Quantum Mechanics I

A Problem Text

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and

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Dedication

To all students of quantum mechanics past, present, and future, but especially to the first students who will learn quantum mechanics not as a mystery which cannot be understood, but as reality which must be experienced, explored, and harnessed.

Preface

The aim of this book is to enable students to solve problems in their first course in quantum mechanics. Student understanding of modern notation, appropriate application of the postulates of quantum mechanics, and appreciation of fundamental quantum mechanical concepts, all as a consequence of solving problems, are also goals. The emphasis on the student solving problems, with theory and rationale embedded in and around this focus on detailed solved problems, has led to this concept of a "problem text."

It is the outgrowth of a project started in 1997 to present material from the perspective of guided problem solving. It is largely the material presented by Larry Sorensen in a one-quarter, 400-level physics course as part of an evening Master of Science program at the University of Washington. The project originally intended only to typeset problems, posed both traditionally and then with guidance that Professor Sorensen dubbed his "garden path" version, and solutions. The stroll along the "garden path" was intended to make the homework sets accessible and an efficient use of the student's time. The population of his quantum mechanics courses was educationally diverse. Occasional doctoral candidates occupied the seats in his auditorium, as did occasional undergraduates. Most students were first time graduate students, many of whom had backgrounds in various fields of engineering. A majority of the clientele held professional positions. Some had limited preparation in physics and mathematics. Everyone appreciated Larry's orientation toward student learning, regardless of any person's starting point, and insistence on efficient use of the student's time and energy, particularly those with day jobs and families. The original concept seemed successful and was subsequently amplified and augmented.

Quantum Mechanics I may be used as a primary text, a supplementary text used with a standard textbook, or a self-study guide. Rudimentary knowledge of differential and integral calculus and differential equations is required. Comprehensive knowledge of these subjects is not required, rather, this volume may assist building competency within these areas. Prior knowledge of linear algebra is unnecessary, and again, use of this book will build competency within this area. Low-dimensional vectors and matrix operators are completely developed and extended to larger dimensions and functions. Indeed, the complete exposure to the appropriate arguments of linear algebra within the context of a first course in quantum mechanics may be responsible for its degree of student accessibility. Solutions immediately follow each prescript. Theory and rationale are addressed both in prescript and postscript narratives, and occasionally within the solutions themselves. The location of solutions immediately following each prescript, complete treatment of theory and rationale, unsolved exercises, and a higher degree of detail than is normally seen in the solutions distinguish Quantum Mechanics I from problem books intended solely as supplementary texts. Advantages of treating the theory within the focus of solved problems are repeated exposure to the notation and the mathematical techniques.

The student should attempt to solve each problem that offers challenge after reading the prescript. Solutions should be reviewed only after a problem has been completed, or in the event of an impasse. The prescripts provide varying amounts of information and explanation depending on the degree of complexity, the specific skills and techniques required, and the material previously encountered. Each prescript is intended to provide enough guidance to allow the student to obtain his/her own result. The solutions should be reviewed only after a result is obtained and for the purposes of verification, and learning new perspectives, skills, techniques, notation, and how the notation is used. Should the student's answer not be in agreement with that in the book, the conveniently located detailed solution presents the opportunity for immediate corrective learning. Of course, reading a portion of a solution to get "unstuck" may be an efficient use of the student's

time and energy. Postscripts offer amplification, additional explanation, and alternate perspectives. All should be examined. Unsolved exercises generally parallel the solved problems and are intended as a second opportunity at a particular skill, technique, or concept; and are provided to be used in conjunction with the student's classwork.

Quantum Mechanics I deliberately emphasizes fundamental skills and techniques for a variety of reasons. Dirac notation, to cite one example among many possibilities, may be best learned in the context of something the student already knows. Fundamental and non-intuitive concepts seem best presented without the complexity that can serve to mask them. The educationally diverse clientele for whom this material was initially prepared often required significant review or were encountering it for the first time. The emphasis on fundamentals means that each student will not be challenged by every problem posed.

The postulates of quantum mechanics are beyond important. One view is that the entirety of quantum mechanics is the postulates. They are presented on the first page of chapter 1 to direct what is initially appropriately addressed. They are repeated on the first page of chapter 2 for emphasis and amplification. They are frequently explicitly revisited throughout the book. The postulates are realistically part of every problem. One mechanism for coping with the discomfiture of some of the counter-intuitive issues often met in the study of quantum mechanics is reconciliation with the postulates. If things are consistent with the postulates, then there is no actual issue. This is the mechanism I use to not be too bothered by quantum mechanics, and to support my standards of understanding and describing truth. I recommend it to you.

Dave DeBruyne

Prologue

The only way to learn physics is to do physics. However, almost all physics textbooks leave a huge gap between the level of the problems that they solve as examples, and the level of the problems that they assign to the students to do as homework and to thereby learn the physics. This book attempts to fill this gap for the first quantum mechanics course which our students find particularly difficult.

The level of our solved problems is the same as that of the solutions that we expect from our students. We try very hard not to leave out any of the "unnecessary" or "obvious" steps until the concepts are well rooted. Clearly no book can show you how to solve every problem. Our goal was to help you learn how to solve a representative subset of all beginning quantum mechanics problems.

We tried to select a minimum number of core concepts that all physicists would agree are essential for beginning quantum mechanics. We hope that you will find it possible to bridge the gap between these problems and the other problems that you want to solve. Most of our students have been able to make the necessary quantum leap.

There is a physics joke about the stages of learning quantum mechanics:

(1) You don't know what it means, you don't know how to calculate anything, and it doesn't bother you.
(2) You don't know what it means, you don't know how to calculate anything, and it bothers you.
(3) You don't know what it means, you know how to calculate things, and it bothers you.
(4) You don't know what it means, you know how to calculate things, and it doesn't bother you.

This book has been designed to help you learn to calculate. Our goal is to get you to stage (4).

We show you how to calculate by example: first we provide a set of paradigmatic problems and their complete solutions. By studying these detailed solutions, and by then using them to solve the additional practice problems we provide, our students have been able to master the fundamentals of quantum calculations. We consider these fundamentals to include the Dirac, Schrodinger, and Heisenberg formulations, which we treat with equal footing throughout the text.

Learning how to calculate is essential because the only language in which we can express, analyze, and discuss quantum mechanics is mathematics. As Willis Lamb put it in 1969:

> "I have taught graduate courses in quantum mechanics at Columbia, Stanford, Oxford, and Yale, and for almost all of them have dealt with measurement in the following manner. On beginning the lectures I told the students, 'You must first learn the rules of calculation in quantum mechanics, and then I will discuss the theory of measurement and discuss the meaning of the subject.' Almost invariably, the time allotted to the course ran out before I had to fulfill my promise."

As Weinberg put it

> "There is a good deal of confusion about this, because quantum mechanics can seem eerie if described in ordinary language."

According to Mermin, most physicists are at stage (3) or (4):

"...contemporary physicists come in two varieties. Type 1 physicists are bothered by EPR and Bell's Theorem. Type (2) (the majority) are not, but one has to distinguish two sub-varieties. Type 2a physicists explain why they are not bothered. Their explanations tend either to miss the point entirely (like Born's to Einstein) or to contain physical assertions that can be shown to be false. Type 2b are not bothered and refuse to explain why."

Of course the goal of physics is to reach stage (5): to know what it means to be able to calculate everything and not to be bothered by the way the universe works. Unfortunately, it has become traditional to teach quantum mechanics as a subject of great mystery that no one understands:

"If quantum mechanics hasn't profoundly shocked you, you cannot have understood it yet." (Bohr)

There is no reality in the absence of observation. (The Copenhagen Interpretation)

"Shut up and calculate." (Mermin's operational version of the Copenhagen Interpretation)

It seems crazy to us to continue to teach generation after generation of our students that they will not be able to understand quantum mechanics. All physicists eventually understand quantum mechanics to some extent. Of course, there are still open questions about the meaning of quantum mechanics; for example, Einstein's reservations about the meaning of quantum mechanics are legendary:

"I recall that during one walk Einstein suddenly stopped, turned to me and asked whether I really believed that the moon exists only when I look at it. The rest of this walk was devoted to a discussion of what a physicist should mean by the term *to exist*." (Pais)

"Quantum mechanics is very impressive. But an inner voice tells me that it is not yet the real thing. The theory yields a lot, but it hardly brings us any closer to the secret of the Old One. In any case I am convinced that He doesn't play dice." (Einstein)

"What nature demands from us is not a quantum theory or a wave theory; rather, nature demands from us a synthesis of these two views which thus far has exceeded the mental powers of physicists. I cannot seriously believe in the quantum theory because the theory is incompatible with the principle that physics is to represent reality in space and time, without spooky actions at a distance." (Einstein)

Even today, the "mysteries" of quantum mechanics continue to echo and to morph:

"No theory of reality compatible with quantum theory can require spatially separate events to be independent." (Bell)

"...experiments have now shown that what bothered Einstein is not a debatable point but the observed behavior of the real world." (Mermin)

"Anybody who's not bothered by Bell's theorem has to have rocks in his head." (Wightman)

"Evidently, God not only plays dice but plays blind-folded, and, at times, throws them where you can't see them." (Hawking)

"And let no one use the Einstein-Podolsky-Rosen experiment to claim that information

> can be transmitted faster than light, or to postulate any 'quantum interconnectedness' between separate consciousnesses. Both are baseless. Both are mysticism. Both are moonshine." (Wheeler)
>
> "Niels Bohr brainwashed a whole generation of theorists into thinking that the job (interpreting quantum mechanics) was done 50 years ago." (Gell-Mann)

The formalism of quantum theory leads to results that agree with experiment with great accuracy and covers an extremely wide range of phenomena. As yet there are no experimental indications of any domain in which it might break down. Nevertheless, there still remain a number of basic questions concerning its fundamental significance which are obscure and confused.

> "Quantum mechanics, that mysterious, confusing discipline, which none of us really understands but which we know how to use." (Bohm and Hiley, quoting Gell-Mann)
>
> "Einstein said that if quantum mechanics is right, the world is crazy... Well, Einstein was right. The world is crazy." (Greenberger)
>
> "Most physicists are very naive; most still believe in real waves or real particles." (Zeilinger)

So, is there a problem, or isn't there? Note Feynman's changing perspective on this question:

> "...I think I can safely say that nobody understands quantum mechanics. So do not take the lecture too seriously, feeling that you have to understand in terms of some model what I am going to describe, but just relax and enjoy it. I am going to tell you what nature behaves like. If you will simply admit that she maybe does behave like this, you will find her a delightful, entrancing thing. Do not keep saying to yourself, if you can possibly avoid it 'But how can it be like that?' because you will get 'down the drain' into a blind alley from which nobody has yet escaped. Nobody knows how it can be like that." (1964)
>
> "We have always had a great deal of difficulty understanding the world view that quantum mechanics represents. At least I do, because I'm an old enough man that I haven't got to the point that this stuff is obvious to me. Okay, I still get nervous about it... You know how it always is, every new idea, it takes a generation or two until it is obvious that there's no real problem. I cannot define the real problem, therefore I suspect there's no real problem, but I'm not sure there's no real problem." (1982)

Quantum mechanics demands the most extraordinary change in our scientific world view of any physical theory. As a boy, Feynman studied Calculus Made Easy by S. P. Thompson that begins "What one fool can do, another can." He dedicated his book QED: The Strange Theory of Light and Matter to his readers with similar words: "What one fool can understand, another can." In a similar spirit, we hope that this book will help you start on your own journey towards understanding quantum mechanics.

As Feynman concludes his Lectures on Physics:

> "The quantum mechanics which was discovered in 1926 has had nearly 40 years of development, and rather suddenly it has begun to be exploited in many practical and real ways. I am sorry to say, gentlemen, that to participate in this adventure it is absolutely imperative that you learn quantum mechanics as soon as possible. I wanted most to give you some appreciation of the wonderful world and the physicist's way of

looking at it, which, I believe, is a major part of the true culture of our times. Perhaps you will not only have some appreciation of this culture; it is even possible that you may want to join in the greatest adventure that the human mind has ever begun."

Perhaps it is only a matter of time:

> "A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die, and a new generation grows up that is familiar with it." (Planck)

But surely, inevitably, the present drive for quantum computation and quantum cryptography will continue to force us towards a more realistic experimental practical understanding of quantum mechanics. You are the new generation–you are in the best of company–welcome to the inquiry!

Larry Sorensen

Table of Contents

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Chapter 1

Discrete Systems I The Postulates and Initial Essentials

One view is that the entirety of quantum mechanics is the postulates. The postulates expose symbology, terminology, and vocabulary for which familiarity is necessary. The discussion following the postulates identifies additional concepts, conditions, and implications. The essential goal of the first five chapters is an initial quantitative interpretation of the postulates.

1–1. What are the postulates of quantum mechanics?

The postulates direct what is initially appropriately addressed.

---

1. The state of a system is represented by a vector $|\psi>$ in Hilbert space.

2. Every observable quantity is represented by a Hermitian operator.

3. A measurement of an observable quantity represented by the operator $\mathcal{A}$ can yield only the eigenvalues of $\mathcal{A}$.

4. If a system is in state $|\psi>$, a measurement of the observable quantity represented by the operator $\mathcal{A}$ that yields the eigenvalue α does so with the probability

$$P(\alpha) \quad \propto \quad \left| <\alpha|\psi> \right|^2,$$

where $|\alpha>$ is the eigenstate corresponding to the eigenvalue α.

5. A measurement of the observable quantity represented by the operator $\mathcal{A}$ with the result α changes the state of the system to the eigenstate $|\alpha>$.

6. The state vector obeys the time dependent Schrodinger equation

$$\mathcal{H}|\psi> \;=\; i\hbar\frac{d}{dt}|\psi>,$$

where $\mathcal{H}$ is the quantum mechanical Hamiltonian operator.

Though there is rationale to the order of presentation, there is no actual rank among the postulates so the numbering is largely cosmetic. The terms state vector, observable, eigenvalue, probability, eigenvector, and Schrodinger postulates are used for reference rather than a numbering system. Where do the postulates initially point?

The **state vector postulate:** The state vector encodes all information that can be known about the system. A state vector is also called a state function or wave function (or wavefunction), though those terms are generally reserved for continuous systems, and the term state vector also applies to continuous systems. Concepts such as eigenvalues, eigenvectors, probability, and expectation value are more straight forward in discrete systems, thus discrete systems are emphasized

initially while building toward continuous systems. Also where practical, continuous systems are treated as generalizations of discrete systems to infinite dimensions. The symbol for the state vector, $|\psi>$, is written in Dirac notation. Familiarity with Dirac notation is a practical necessity for any modern investigation of quantum mechanical phenomena. This postulate indicates the necessity of understanding the concepts of a space in general and Hilbert space in particular. The spaces of interest to quantum mechanics are complex linear vector spaces. The field of complex numbers requires abstraction beyond classical mechanics and beyond the field of real numbers.

The **observables postulate:** An observable quantity is anything that can be measured. Position, momentum, energy, and angular momentum are the primary observable quantities addressed in this text. The outcome of a physical measurement is necessarily a real number. The objects of quantum mechanics possess intrinsically complex components and elements, thus, a challenge is presented in predicting outcomes with real number results. Operators may be expressed as matrix operators for discrete systems and differential operators for continuous systems, though an infinite by infinite matrix operator can contain the same information as a differential operator. Hermitian operators have four extraordinary and advantageous properties. It is beneficial to appreciate that (1) all Hermitian operators can be diagonalized, (2) the eigenvalues of Hermitian operators are real numbers, (3) the eigenvectors of all Hermitian operators are orthogonal, and (4) the eigenvectors of all Hermitian operators form a basis for the space in which they exist.

The **eigenvalue postulate:** An observable quantity is represented by an operator. Each operator has exactly one set of eigenvalues which are characteristics of the operator. Eigenvalues are comparable to normal modes in a mechanical system. For example, plucking an individual guitar string can initially set it vibrating unpredictably, however, it will quickly settle into a linear combination of the fundamental mode, the first overtone, the second overtone, and other overtones. Each possible mode of vibration is an eigenvalue of that guitar string. Obtaining eigenvalues is a dominant activity in quantum mechanics, because they are the only thing that **can** be measured. Eigenvalues of an observable quantity must be real. Imaginary or complex energy, for instance, are senseless concepts; a measured energy must be a real quantity. Eigenvalues, even for continuous systems, are discrete, limiting the possible values of any quantum mechanical measurement.

The **probability postulate:** The probability postulate features more Dirac notation and the interpretation of a state vector containing information about the probability of a measurement. A probability of zero means that an outcome cannot occur. A probability of one means an outcome is certain. Since only eigenvalues are possible results of a measurement, a calculation of the probabilities of all possibilities must sum to one. Notice that the probability is written as a proportionality. Normalization is the mathematical process of ensuring that the probabilities of all possibilities is one in order to obtain equalities instead of proportionalities. Notice also that the interpretation of state vector containing information about the probability of a measurement indicates a form of a product squared. The product is known as an inner product. The square of the norm is necessary because the objects of quantum mechanics possess intrinsically complex components and elements, and a probability is necessarily a real number. The probabilistic interpretation of quantum mechanics can be unsettling because it also limits what can be known and dictates that some things that can be known classically must remain unknown quantum mechanically.

The **eigenvector postulate:** An eigenstate is an eigenvector for a discrete system, and can be called an eigenvector even for a continuous system. The eigenvalues of an operator are properties of that operator. Each eigenvalue will have a corresponding eigenvector in a given basis. Should the basis change, the appearance of the operator changes, the eigenvectors change, but the eigenvalues of the operator remain the same. Ideally, each eigenvalue has a distinct eigenvector.

Some operators, however, have two or more eigenvalues that correspond to the same eigenvector in which case a complete set of commuting observables is required to remove or lift the degeneracy, which is to say uniquely identify the eigenstate. The eigenvector postulate embeds the mystery of the collapse of the wave function. Again, consider a guitar string. Hit an individual guitar string and it will settle into a combination of its normal modes quickly, but in a finite amount of time that could be measured. In non-relativistic quantum mechanics, the system settles into the state corresponding to the eigenvalue measured in the limit of zero time.

The **Schrodinger postulate:** Dirac notation is used to express the Schrodinger postulate in a differential equation. The Hamiltonian is the energy operator of classical mechanics, and the quantum mechanical Hamiltonian operator is the energy operator of quantum mechanics. It is surprising to some that the Schrodinger equation is a postulate. The Schrodinger equation is written in many forms and the form $\mathcal{H}\,|\,E> \;=\; E_n\,|\,E>$ is one of the most useful. Notice that the derivative is a time derivative. Thus, the Schrodinger equation governs the time evolution of a system. Notice also that time as a variable is limited to the Schrodinger postulate alone.

Postscript: The intent of introducing the postulates first is to motivate what follows in this chapter in particular, and in the rest of the text in general. The postulates seem to require knowledge of Dirac notation, a generalized concept of vectors, an appreciation of operators, Hermiticity, eigenvalues, eigenvectors, probability, and many other ingredients. These and other aspects of terminology, vocabulary, and mathematical technique are addressed in the problems that follow. Like problem 1–1, a few problems seek only to guide though most problems will have a prescript discussion with subsequent calculations intended to provide insight into the symbology and how it is used, and expose appropriate mathematical mechanics. Some problems have postscripts, like this one, intended to amplify, or further explain, and/or highlight particular portions of the problem.

Appendix A is the arithmetic of imaginary and complex numbers. Quantum mechanics is addressed in a complex linear vector space. The numbers, components, and elements of the scalars, vectors, and operators of quantum mechanics are intrinsically complex. Competency in quantum mechanical calculation requires mastery of complex arithmetic. Those desiring an introduction or some review should complete Appendix A before proceeding.

Linear independence is necessary to the general field of linear algebra to found the concept of a set of basis vectors. The observables postulate guarantees that anything that could be physically measured will be represented by a Hermitian operator. Hermitian operators have four advantageous properties. (1) All Hermitian operators can be diagonalized, (2) the eigenvalues of Hermitian operators are real numbers, (3) the eigenvectors of all Hermitian operators are orthogonal, and (4) the eigenvectors of all Hermitian operators form a basis for the space in which they exist. Property (4) states that the eigenvectors of a Hermitian operator necessarily form an appropriate basis, and are thus guaranteed to have the property of linear independence. Traditionally presented material on linear independence is included in appendix B for completeness.

Chapter 1 occasionally relies on results that are stated without proof, for instance, the four advantageous properties of Hermitian operators listed in the above paragraph. All claims will be supported as familiarity, technique, and background develop and evolve.

Again, one view is that the entirety of quantum mechanics is the postulates.

1–2. What is a ket?

A **ket** is a column vector written in **Dirac notation**. Dirac's ket is more general that the "magnitude and direction" concept of classical mechanics. A vector is simply a quantity requiring more than one number to describe. A force may be described as 10 Newtons at 30^o to the horizontal, which is two numbers. Another description of the same force is $5\sqrt{3}\,\widehat{x} + 5\,\widehat{y}$ Newtons, again two numbers are required to express a vector quantity in two dimensions. In three dimensions, three numbers are required. In four dimensions, four numbers are required. Four dimensions become difficult to imagine, though there are some routine uses for four dimensions. Five dimensions, however, requires five numbers, six dimensions requires six numbers and infinite dimensions requires infinite numbers. A vector is simply a quantity requiring more than one number to describe.

Dirac notation uses some symbol that uniquely identifies the ket, often the corresponding eigenvalue for an eigenvector, between the symbols "$|$" and "$>$", for instance, $|\,\psi>$, $|\,\alpha>$, $|\,1>$, $|\,\hbar>$, and $|\,i>$ are examples of how kets are written. Specific examples are seen below.

$$|\,b> \rightarrow \begin{pmatrix} 2i \\ 3-i \end{pmatrix}, \quad |-1> \rightarrow \begin{pmatrix} -4 \\ i\cos(\phi) \\ 1+5i \end{pmatrix}, \quad |\,\alpha> \rightarrow \begin{pmatrix} \sqrt{3}\,i \\ \sin(\theta) \\ e^{i\theta} \\ 2-5i \\ -8 \end{pmatrix}, \quad |\,\lambda = 2> \rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}.$$

Postscript: A ket is a column vector in Dirac notation. The symbol $|\,b>$ is a column vector in two dimensions, $|-1>$ is three dimensions, $|\,\alpha>$ is five dimensions, and $|\,\lambda = 2>$ indicates infinite dimensions. A vector is simply a quantity requiring more than one number to describe. The number of numbers required is not limited. The symbols between the "$|$" and "$>$" are not explained at this point, other than they must uniquely identify the ket from others in their system.

Notice that three of the four examples given have components with complex values. The last example is a unit vector. Whether of finite or infinite dimensions, unit vectors play a significant role in quantum mechanics.

There are an infinite number of ways to describe a force depending on the coordinate system chosen and the frame of reference. Similarly, there are an infinite number of ways to describe any vector. The symbol $|\,b>$ is a ket vector, but without reference to any coordinate system or frame of reference. The set of symbols $\begin{pmatrix} 2i \\ 3-i \end{pmatrix}$ is a **representation** of that ket vector for which a specific coordinate system and frame of reference are implied.

Notice that the symbol "$\rightarrow$" is used to specify the initial representation of $|\,b>$. Specifying a vector with a single arrow upon its initial representation denotes that $|\,b>$ is abstract and expressible in an infinite number of forms. The act of representing $|\,b>$ as a column vector with specific components fixes the coordinate system and frame of reference after which "$=$" symbols are appropriate for subsequent calculations. Many texts do not try to make this distinction, and use an equality symbol to denote their representations.

1–3. Form bras corresponding to the kets of problem 1–2.

A **bra** is a row vector that is the complex conjugate analogy of a ket. Make the column vector into a row vector and complex conjugate all of the components. The symbol identifying the ket is retained, but in a bra goes between a "$<$" and a "$|$."

$$<b| \;=\; \big(-2i\,,\;\; 3+i\big) \qquad <-1| \;=\; \big(-4\,,\;\; -i\cos(\phi)\,,\;\; 1-5i\big)$$

$$<\alpha| \;=\; \big(-\sqrt{3}\,i\,,\;\; \sin(\theta)\,,\;\; e^{-i\theta}\,,\;\; 2+5i\,,\;\; -8\big) \qquad <\lambda=2| \;=\; \big(0,\;\; 0,\;\; 1,\;\; 0,\;\; 0,\cdots\big)$$

Postscript: There is no rank between bras an kets. Bras can be formed from kets, or kets can be formed from bras. A state vector, per the state vector postulate, in normally a ket. An eigenvector of an operator will be a ket in our development. Normally kets are encountered initially, then corresponding bras are formed as seen in this problem.

Terminology for making the column vector into a row vector and complex conjugating components is to form a **transpose conjugate** or **adjoint**. A bra is a transpose conjugate, or adjoint, of the corresponding ket, and a ket is a transpose conjugate, or adjoint, of the corresponding bra.

The origin of the terms "bra" and "ket" is Dirac's efficient manner of forming inner products, which look like $<\alpha\,|\,\beta>$, and which is called a bracket, or **braket**, or bra-ket. The separated parts, "bras" and "kets," are identifiable vector entities. Inner products will be addressed directly.

1–4. Add the following ket vectors where possible.

$$|\,\alpha> \rightarrow \begin{pmatrix} 2i \\ 3-4i \\ -6 \\ 2+7i \end{pmatrix} \qquad |\,5> \rightarrow \begin{pmatrix} 1 \\ 3-5i \\ 4 \\ -8i \end{pmatrix} \qquad |\,\hbar> \rightarrow \begin{pmatrix} 6+i \\ -6i \\ 5+4i \\ 3-2i \\ 3 \end{pmatrix} \qquad |\,e> \rightarrow \begin{pmatrix} 4-5i \\ -2+3i \\ 9-4i \\ 0 \\ -7i \end{pmatrix}$$

Kets and bras add just like vectors from introductory physics, simply add like component. Two kets must have the same number of components to be added, thus, $|\,\alpha>$ and $|\,5>$ can be added, $|\,\hbar>$ and $|\,e>$ can be added, but no other additions are possible among the four kets given.

$$|\,\alpha> \;+\; |\,5> \;=\; \begin{pmatrix} 2i \\ 3-4i \\ -6 \\ 2+7i \end{pmatrix} + \begin{pmatrix} 1 \\ 3-5i \\ 4 \\ -8i \end{pmatrix} = \begin{pmatrix} 2i+1 \\ 3-4i+3-5i \\ -6+4 \\ 2+7i-8i \end{pmatrix} = \begin{pmatrix} 1+2i \\ 6-9i \\ -2 \\ 2-i \end{pmatrix}$$

$$|\,\hbar> \;+\; |\,e> \;=\; \begin{pmatrix} 6+i \\ -6i \\ 5+4i \\ 3-2i \\ 3 \end{pmatrix} + \begin{pmatrix} 4-5i \\ -2+3i \\ 9-4i \\ 0 \\ -7i \end{pmatrix} = \begin{pmatrix} 6+i+4-5i \\ -6i-2+3i \\ 5+4i+9-4i \\ 3-2i+0 \\ 3-7i \end{pmatrix} = \begin{pmatrix} 10-4i \\ -2-3i \\ 14 \\ 3-2i \\ 3-7i \end{pmatrix}$$

Postscript: There is no significance to the symbols between the "$|$" and "$>$" at this point other than to uniquely identify the ket. The symbols between the "$|$" and "$>$" will often be eigenvalues.

1–5. Form bras from the kets given in problem 1–4 and add the resulting bras where possible.

Form row vectors from the column vectors given remembering to conjugate the components, then add like components. Again, two bras must have the same number of components to be added, thus, $<\alpha|$ and $<5|$ can be added, $<\hbar|$ and $<e|$ can be added, but no other additions are possible among the four bras formed.

$$\begin{aligned} <\alpha| + <5| &= \big(-2i,\ 3+4i,\ -6,\ 2-7i\big) + \big(1,\ 3+5i,\ 4,\ 8i\big) \\ &= \big(-2i+1,\ 3+4i+3+5i,\ -6+4,\ 2-7i+8i\big) \\ &= \big(1-2i,\ 6+9i,\ -2,\ 2+i\big) \\ <\hbar| + <e| &= \big(6-i,\ 6i,\ 5-4i,\ 3+2i,\ 3\big) + \big(4+5i,\ -2-3i,\ 9+4i,\ 0,\ 7i\big) \\ &= \big(6-i+4+5i,\ 6i-2-3i,\ 5-4i+9+4i,\ 3+2i+0,\ 3+7i\big) \\ &= \big(10+4i,\ -2+3i,\ 14,\ 3+2i,\ 3+7i\big) \end{aligned}$$

Postscript: Notice that $<\alpha| + <5|$ is the bra (transpose conjugate or adjoint) corresponding to the ket $|\alpha> + |5>$, and that $<\hbar| + <e|$ and $|\hbar> + |e>$ also correspond.

1–6. Use the vectors of problems 1–4 and 1–5 to do these subtractions where possible.

(a) $<\alpha| - <5|$

(b) $|\hbar> - |e>$

(c) $|e> - |\hbar>$

(d) $<5| - <e|$

(e) $|e> - |\alpha>$

(f) $|\hbar> - <e|$

Again, like introductory physics, subtract like components. The vectors must have the same number of components to be added or subtracted. Additionally, they must be of the same type; bras cannot be added/subtracted to/from kets, and kets cannot be added/subtracted to/from bras. Only the subtractions in parts (a), (b), and (c) are possible.

$$\begin{aligned} \text{(a)}\quad <\alpha| - <5| &= \big(-2i,\ 3+4i,\ -6,\ 2-7i\big) - \big(1,\ 3+5i,\ 4,\ 8i\big) \\ &= \big(-2i-1,\ 3+4i-3-5i,\ -6-4,\ 2-7i-8i\big) \\ &= \big(-1-2i,\ -i,\ -10,\ 2-15i\big) \end{aligned}$$

$$\text{(b)}\quad |\hbar> - |e> = \begin{pmatrix} 6+i \\ -6i \\ 5+4i \\ 3-2i \\ 3 \end{pmatrix} - \begin{pmatrix} 4-5i \\ -2+3i \\ 9-4i \\ 0 \\ -7i \end{pmatrix} = \begin{pmatrix} 6+i-4+5i \\ -6i+2-3i \\ 5+4i-9+4i \\ 3-2i-0 \\ 3+7i \end{pmatrix} = \begin{pmatrix} 2+6i \\ 2-9i \\ -4+8i \\ 3-2i \\ 3+7i \end{pmatrix}$$

$$\begin{aligned} \text{(c)}\ <e| - <\hbar| &= \big(4+5i,\ -2-3i,\ 9+4i,\ 0,\ 7i\big) - \big(6-i,\ 6i,\ 5-4i,\ 3+2i,\ 3\big) \\ &= \big(4+5i-6+i,\ -2-3i-6i,\ 9+4i-5+4i,\ 0-3-2i,\ 7i-3\big) \\ &= \big(-2+6i,\ -2-9i,\ 4+8i,\ -3-2i,\ -3+7i\big) \end{aligned}$$

(d) Similar types, but dissimilar number of components so not possible.

(e) Similar types, but dissimilar number of components so not possible.

(f) Similar number of components, but dissimilar types so not possible.

Postscript: A more general manner of stating the subtractions in parts (d), (e), and (f) are not possible is that the two objects are not in the same space.

1–7. (a) Multiply $|\chi> \rightarrow \begin{pmatrix} 2-i \\ 3i \end{pmatrix}$, $|W> \rightarrow \begin{pmatrix} 4+3i \\ -5 \\ 6i \end{pmatrix}$ and corresponding bras by $\delta = 3-2i$.

(b) Find $<\chi\,\delta|$ and $<W\,\delta|$.

Scalar multiplication means to multiply each component by the scalar. The designation "scalar" is well conceived because scalar multiplication "scales" the vector, for instance

$$2\,|\chi> \;=\; 2\begin{pmatrix} 2-i \\ 3i \end{pmatrix} \;=\; \begin{pmatrix} 2(2-i) \\ 2(3i) \end{pmatrix} \;=\; \begin{pmatrix} 4-2i \\ 6i \end{pmatrix}$$

thus, the vector is scaled up by a factor of 2. The "scaling" is more difficult to see for complex scalars, though the process is the same.

$$\delta\,|\chi> \;=\; (3-2i)\begin{pmatrix} 2-i \\ 3i \end{pmatrix} \;=\; \begin{pmatrix} (3-2i)(2-i) \\ (3-2i)(3i) \end{pmatrix} \;=\; \begin{pmatrix} 6-3i-4i-2 \\ 9i+6 \end{pmatrix} \;=\; \begin{pmatrix} 4-7i \\ 6+9i \end{pmatrix}$$

$$\begin{aligned} <W\,|\,\delta \;&=\; \big(4-3i\,,\; -5\,,\;\; -6i\big)(3-2i) \;=\; \big((4-3i)(3-2i)\,,\; -5(3-2i)\,,\;\; (-6i)(3-2i)\big) \\ &=\; \big(12-8i-9i-6\,,\; -15+10i\,,\; -18i-12\big) \;=\; \big(6-17i\,,\; -15+10i\,,\;\; -12-18i\big)\,. \end{aligned}$$

The meaning of $<W\,\delta|$ is different than $<W\,|\,\delta$. Given a scalar like δ, if it is outside of the bra, it means multiply by the given δ. However, if it is inside of the bra, $<W\,\delta|$ means $<W\,|\,\delta^*$, or

$$\begin{aligned} <W\,\delta| \;&=\; \big(4-3i\,,\; -5\,,\;\; -6i\big)(3+2i) \;=\; \big((4-3i)(3+2i)\,,\; -5(3+2i)\,,\;\; (-6i)(3+2i)\big) \\ &=\; \big(12+8i-9i+6\,,\; -15-10i\,,\; -18i+12\big) \;=\; \big(18-i\,,\; -15-10i\,,\;\; 12-18i\big)\,. \end{aligned}$$

Just as the components of a ket are conjugated to form the corresponding bra, a scalar between the "$<$" and the "$|$" in a bra is implied to be conjugated.

$$\begin{aligned} <\chi\,|\,\delta \;&=\; \big(2+i\,,\; -3i\big)(3-2i) \;=\; \big((2+i)(3-2i)\,,\;\; (-3i)(3-2i)\big) \\ &=\; \big(6-4i+3i+2\,,\; -9i-6\big) \;=\; \big(8-i\,,\; -6-9i\big). \end{aligned}$$

$$\begin{aligned} <\chi\,\delta| \;&=\; \big(2+i\,,\; -3i\big)(3+2i) \;=\; \big((2+i)(3+2i)\,,\;\; (-3i)(3+2i)\big) \\ &=\; \big(6+4i+3i-2\,,\; -9i+6\big) \;=\; \big(4+7i\,,\; 6-9i\big). \end{aligned}$$

Notice that the components of $<\chi\,\delta|$ are complex conjugates to those of $\delta\,|\,\chi> \;=\; |\,\delta\,\chi>$, but $<\chi\,|\,\delta$ is unrelated to $\delta\,|\,\chi>$.

$$\delta\,|\,W> \;=\; (3-2i)\begin{pmatrix}4+3i\\-5\\6i\end{pmatrix} \;=\; \begin{pmatrix}(3-2i)(4+3i)\\(3-2i)(-5)\\(3-2i)6i\end{pmatrix} \;=\; \begin{pmatrix}12+9i-8i+6\\-15+10i\\18i+12\end{pmatrix} \;=\; \begin{pmatrix}18+i\\-15+10i\\12+18i\end{pmatrix}.$$

Notice that this ket has components that are complex conjugates of the bra $<W\,\delta|$, but is unrelated to $<W\,|\,\delta$.

Postscript: $<W\,\delta|$ means $<W\,|\,\delta^*$, though $|\,\delta\,W>$ and $\delta\,|\,W>$ have the same meaning.

1–8. What is a space, a subspace, a dual space, and what is the Hilbert space?

A **space** is a collection of all possible objects having the same number of components over a known field. The field is complex numbers in quantum mechanics. The number of components determine the dimension of the space. The ket vectors $|\,\alpha>$ and $|\,5>$ each have four components, those components are complex numbers, so they belong to the space $\mathbb{C}^4$. The vectors $|\,\hbar>$ and $|\,e>$ each have five complex components so belong to $\mathbb{C}^5$. The symbology

$$|\,\alpha>,\;\; |\,5> \;\in\; \mathbb{C}^4 \qquad \text{and} \qquad |\,\hbar>,\;\; |\,e> \;\in\; \mathbb{C}^5$$

denotes these facts, where the symbol "$\in$" is read "is an element of." Quantum mechanics is most generally done in $\mathbb{C}^\infty$ which is to indicate infinite dimensions of complex components.

Introductory physics is often addressed in $\mathbb{R}^3$, meaning three dimensions over the field of real numbers. Adding $2\widehat{x}+5\widehat{y}$ to $4\widehat{x}+3\widehat{y}+7\widehat{z}$ to obtain $6\widehat{x}+8\widehat{y}+7\widehat{z}$ is not mixing $\mathbb{R}^2$ and $\mathbb{R}^3$, rather this addition is done in $\mathbb{R}^3$ where the z component of the first vector is zero.

Real numbers are a subset of complex numbers. Every real number can be written $a \;=\; a+0i$. Introductory physics could be done in the larger space $\mathbb{C}^3$ by designating an imaginary component of zero for each real number, which is an unnecessary complication, and thus, introductory physics is generally addressed in the subspace of $\mathbb{C}^3$ denoted $\mathbb{R}^3$. A **subspace** is a subset of a larger space. Much of the remainder of chapter 1 is done in $\mathbb{C}^2$ or $\mathbb{C}^3$ which are subspaces of $\mathbb{C}^\infty$.

The bra vectors $<\alpha|$ and $<5|$ also belong to $\mathbb{C}^4$, but it is a different $\mathbb{C}^4$ than for $|\,\alpha>$ and $|\,5>$. The bra vectors $<\alpha|$ and $<5|$ belong to the $\mathbb{C}^4$ that is the dual space of the $\mathbb{C}^4$ containing the vectors $|\,\alpha>$ and $|\,5>$. A **dual space** is a transpose conjugate space in quantum mechanics. The bras $<\hbar|$ and $<e|$ are in the dual space of $|\,\hbar>$ and $|\,e>$. Similarly, the kets $|\,\hbar>$ and $|\,e>$ are in the dual space of the $\mathbb{C}^5$ containing $<\hbar|$ and $<e|$.

The **Hilbert space** is that space comprised by the sum of all $\mathbb{C}^n$, for all n. The Hilbert space contains all objects in $\mathbb{C}^1$, $\mathbb{C}^2$, $\mathbb{C}^3$,..., to $\mathbb{C}^\infty$ including all dual spaces.

Postscript: The Hilbert space contains not only all possible vectors, kets and bras, but also all possible operators, all possible functions, all possible spaces, or said more generally, all possibilities. A mathematician will address a Hilbert space as defined by a specific set of properties. A physicist includes all possibilities into one and speaks of the Hilbert space.

1–9. Find the norms of $|\beta> \rightarrow \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}$, $|\chi> \rightarrow \begin{pmatrix} 2-i \\ 3i \end{pmatrix}$, $|W> \rightarrow \begin{pmatrix} 4+3i \\ -5 \\ 1-6i \end{pmatrix}$, and $<\hbar|$.

There are many concepts in $\mathbb{R}^3$ which simply do not translate completely to a space of any dimension over a complex field, and/or any dimension larger than 3. In fact, that is one reason to write, for example, $|v> = \begin{pmatrix} 4 \\ 3 \\ 7 \end{pmatrix}$ instead of $\vec{v} = 4\,\widehat{x} + 3\,\widehat{y} + 7\,\widehat{z}$. The difference in notation in $\mathbb{R}^3$ is cosmetic. Should the space be $\mathbb{C}^3$, $|W> = \begin{pmatrix} 4+3i \\ -5 \\ 1-6i \end{pmatrix}$ is clear, but $\vec{W} = (4+3i)\,\widehat{x} - 5\,\widehat{y} + (1-6i)\,\widehat{z}$ may not be so clear. For instance, what is the length of $\vec{W}$?

The length of the real valued $\vec{v} = 4\,\widehat{x} + 3\,\widehat{y} + 7\,\widehat{z}$ is the square root of the dot product,

$$|\vec{v}| = \sqrt{\vec{v}\cdot\vec{v}} = \sqrt{4\times 4 + 3\times 3 + 7\times 7} = \sqrt{16+9+49} = \sqrt{74}$$

in whatever units are given. How can a "length" be obtained when the vector has complex components or is in four or more dimensions; does the term "length" even have meaning?

The concept of a length generalizes to the concept of a **norm** for a vector with complex components and/or more than three components. A norm is the generalization of the square root of a dot product, for instance,

$$\left|\vec{\beta}\right| = \sqrt{\vec{\beta}\cdot\vec{\beta}} = \sqrt{1\times 1 + 2\times 2 + 3\times 3 + 4\times 4} = \sqrt{1+4+9+16} = \sqrt{30}\,,$$

so the norm of $|\beta>$ is $\sqrt{30}$, denoted $\big||\beta>\big| = \sqrt{30}$.

It is helpful to see that $\vec{\beta}$ and $|\beta>$ are just two different ways to express the same thing. Forming the bra of $|\beta>$, we write

$$<\beta|\beta> = \big(1,\ 2,\ 3,\ 4\big)\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}$$

and imagine rotating the column vector counter clockwise over the row vector and multiplying the corresponding components, and adding the products to obtain 30. Then the norm of $|\beta>$ is the square root, or $\big||\beta>\big| = \sqrt{30}$. This is often done in two steps, a typical calculation is

$$\big||\beta>\big|^2 = <\beta|\beta> = \big(1,\ 2,\ 3,\ 4\big)\begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} = 1+4+9+16 = 30 \quad\Rightarrow\quad \big||\beta>\big| = \sqrt{30}\,.$$

Remember that the product of any complex number and its complex conjugate is the sum of the square of the real part and the square of the imaginary part,

$$\big(a+bi\big)\big(a-bi\big) = a^2 - abi + abi + b^2 = a^2 + b^2\,.\ \text{Thus}$$

$$\big|\,|\chi>\big|^2 \;=\; <\chi\,|\,\chi> \;=\; \begin{pmatrix}2+i\,, & -3i\end{pmatrix}\begin{pmatrix}2-i\\ 3i\end{pmatrix} \;=\; 4+1+9 \;=\; 14 \quad\Rightarrow\quad \big|\,|\chi>\big| \;=\; \sqrt{14}$$

The products $<\beta\,|\,\beta>$ and $<\chi\,|\,\chi>$ are known as **inner products**. These are also known as **brakets** when using Dirac notation, but inner product is the more general term. An inner product is a generalization of a dot product to more than three dimensions and/or to a field allowing complex components. A norm is a generalization of length to more than three dimensions and/or to a field allowing complex components.

Notice that the probability postulate contains the inner product $<\alpha\,|\,\psi>$. Calculating inner products should become routine. Notice also that $<\alpha\,|\,\psi>$ is between two " | " symbols with a power of 2 in the probability postulate, meaning a norm squared.

Probability is a real number between 0 and 1. A complex number times its conjugate is a real number. Thus any component of a bra multiplied by its corresponding ket is a real number, and the sum of real numbers is a real number. A vector times its transpose conjugate is a real number.

Probabilities must be real numbers. The outcome of a measurement of an observable quantity such as position, momentum, energy, or angular momentum also must be a real number. The inner product, a vector times its transpose conjugate, illustrates one manner in which a real number is extracted from objects with complex components.

$$<W\,|\,W> \;=\; \begin{pmatrix}4-3i\,, & -5\,, & 1+6i\end{pmatrix}\begin{pmatrix}4+3i\\ -5\\ 1-6i\end{pmatrix} \;=\; 16+9+25+1+36 \;=\; 87 \quad\Rightarrow\quad \big|\,|W>\big| \;=\; \sqrt{87}$$

$$<\hbar\,|\,\hbar> \;=\; \begin{pmatrix}6-i\,, & 6i\,, & 5-4i\,, & 3+2i\,, & 3\end{pmatrix}\begin{pmatrix}6+i\\ -6i\\ 5+4i\\ 3-2i\\ 3\end{pmatrix}$$

$$=\; 36+1+36+25+16+9+4+9 \;=\; 136 \quad\Rightarrow\quad \big|\,|\hbar>\big| \;=\; \sqrt{136}$$

1–10. Normalize $|\beta> \;\rightarrow\; \begin{pmatrix}1\\2\\3\\4\end{pmatrix}$, $|\chi> \;\rightarrow\; \begin{pmatrix}2-i\\3i\end{pmatrix}$, $|W> \;\rightarrow\; \begin{pmatrix}4+3i\\-5\\1-6i\end{pmatrix}$, and $<\hbar|$.

Normalization is the process of adjusting the "length," or length analog, of a vector to 1.

The state vector contains all the information that can be known about a system. The direction, or direction analog, of the state vector is what contains this information. Any vector of any length (length analog) in the same direction (direction analog) contains the same information. The probability postulate uses a proportionality, $P(\alpha) \;\propto\; \big|<\alpha\,|\,\psi>\big|^2$, which may be written as an equality with a proportionality constant. The probability of certainty must be 1, a condition which may be addressed

$$P(\psi) \;=\; 1 \quad\Rightarrow\quad K\Big(\big|<\psi\,|\,\psi>\big|^2\Big) \;=\; 1 \quad\Rightarrow\quad K \;=\; \frac{1}{\big|<\psi\,|\,\psi>\big|^2}$$

thus the proportionality constant is the inverse of the norm squared. The usual procedure is to symmetrize by placing a factor of $\sqrt{K}$ with both the bra and the ket, for example

$$|\,\beta> \;=\; \frac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \quad \Rightarrow \quad <\beta\,| \;=\; \big(1\,,\;\; 2\,,\;\; 3\,,\;\; 4\big)\,\frac{1}{\sqrt{30}}$$

are the normalized vectors $|\,\beta>$ and $<\beta\,|$. Notice that

$$<\beta\,|\,\beta> \;=\; \big(1\,,\;\; 2\,,\;\; 3\,,\;\; 4\big)\,\frac{1}{\sqrt{30}}\,\frac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix} \;=\; \frac{1}{30}\big(1+4+9+16\big) \;=\; \frac{30}{30} \;=\; 1\,.$$

The normalization condition is that $<\psi\,|\,\psi> \;=\; 1\,,$ and simply means that the probability of certainty is 1. Having found the norms of the last three vectors in the previous problem, the conclusion to this problem is simply writing the answers.

$$|\,\chi> \;=\; \frac{1}{\sqrt{14}} \begin{pmatrix} 2-i \\ 3i \end{pmatrix}\,, \qquad |\,W> \;=\; \frac{1}{\sqrt{87}} \begin{pmatrix} 4+3i \\ -5 \\ 1-6i \end{pmatrix}\,,$$

$$<\hbar\,| \;=\; \big(6-i\,,\;\; 6i\,,\;\; 5-4i\,,\;\; 3+2i\,,\;\; 3\big)\,\frac{1}{\sqrt{136}}$$

Postscript: Notice that the ket/bra notation does not change when the vector is normalized because, for instance, $|\,\chi> = \begin{pmatrix} 2-i \\ 3i \end{pmatrix}$ and $|\,\chi> \;=\; \frac{1}{\sqrt{14}} \begin{pmatrix} 2-i \\ 3i \end{pmatrix}$ are the same vector quantum mechanically. Only the direction (direction analog) contains information. The length (length analog), if not 1 initially, must be adjusted to be consistent with the probability postulate.

The factor $\sqrt{K} \;=\; \frac{1}{<\psi\,|\,\psi>}$ is called a **normalization constant**. It is conventionally placed to the left of a ket and to the right of a bra.

The probability postulate is occasionally written as an equality,

$$P\,(\alpha) \;=\; \frac{\big|\,<\alpha\,|\,\psi>\,\big|^2}{<\alpha\,|\,\alpha><\psi\,|\,\psi>}\,,$$

though it is more generally stated as a proportionality. Division of each vector $|\,i>$ by $<i\,|\,i>$ once, whether in the normalization process or the probability calculation, is necessary to obtain consistent probabilities.

It is not mandatory to normalize a state vector, however, doing so as a first step has the advantages of clarity, organizational consistency, and more accessible probability calculations. We will generally normalize a state vector as the first step in all calculations.

The time evolution of a state vector is governed solely by the Schrodinger postulate. Given a normalized state vector, that is a length analog or norm of 1, the only possible evolution over time is analogous to changing direction. The Schrodinger equation changes only the direction (direction analog) of the state vector.

1–11. Given $|\gamma> \rightarrow \begin{pmatrix} 3+2i \\ 4 \\ -i \end{pmatrix}$ and $|\omega> \rightarrow \begin{pmatrix} -5 \\ i \\ -4-3i \end{pmatrix}$,

(a) normalize each vector,

(b) obtain the inner products $<\gamma|\omega>$ and $<\omega|\gamma>$ using your normalized vectors,

(c) and compare $<\gamma|\omega>$ with $<\omega|\gamma>$.

Part (a) is a straightforward application of the normalization process. Of course, $<\gamma|\gamma> = 1$ and $<\omega|\omega> = 1$ following normalization. Part (c) asks does $<\gamma|\omega> = <\omega|\gamma>$?

(a) $$<\gamma|\gamma> = \begin{pmatrix} 3-2i, & 4, & i \end{pmatrix} N^* N \begin{pmatrix} 3+2i \\ 4 \\ -i \end{pmatrix} = |N|^2(9+4+16+1) = |N|^2 30 = 1$$

$$\Rightarrow \quad N = \frac{1}{\sqrt{30}} \quad \Rightarrow \quad |\gamma> = \frac{1}{\sqrt{30}} \begin{pmatrix} 3+2i \\ 4 \\ -i \end{pmatrix} \text{ where } N \text{ is a normalization constant.}$$

$$<\omega|\omega> = \begin{pmatrix} -5, & -i, & -4+3i \end{pmatrix} N^* N \begin{pmatrix} -5 \\ i \\ -4-3i \end{pmatrix} = |N|^2(25+1+16+9)$$

$$= |N|^2 51 = 1 \quad \Rightarrow \quad N = \frac{1}{\sqrt{51}} \quad \Rightarrow \quad |\omega> = \frac{1}{\sqrt{51}} \begin{pmatrix} -5 \\ i \\ -4-3i \end{pmatrix}$$

(b) $$<\gamma|\omega> = \begin{pmatrix} 3-2i, & 4, & i \end{pmatrix} \frac{1}{\sqrt{30}} \frac{1}{\sqrt{51}} \begin{pmatrix} -5 \\ i \\ -4-3i \end{pmatrix}$$

$$= \frac{1}{\sqrt{5\cdot 3\cdot 2\cdot 17\cdot 3}} \Big((3-2i)(-5) + 4(i) + i(-4-3i) \Big)$$

$$= \frac{1}{3\sqrt{5\cdot 2\cdot 17}} \Big(-15+10i+4i-4i+3 \Big) = \frac{1}{3\sqrt{170}} \big(-12+10i \big)$$

$$<\omega|\gamma> = \begin{pmatrix} -5, & -i, & -4+3i \end{pmatrix} \frac{1}{\sqrt{51}} \frac{1}{\sqrt{30}} \begin{pmatrix} 3+2i \\ 4 \\ -i \end{pmatrix}$$

$$= \frac{1}{3\sqrt{170}} \Big((-5)(3+2i) - i(4) + (-4+3i)(-i) \Big)$$

$$= \frac{1}{3\sqrt{170}} \big(-15-10i-4i+4i+3 \big) = \frac{1}{3\sqrt{170}} \big(-12-10i \big)$$

(c) $<\gamma\,|\,\omega> \neq <\omega\,|\,\gamma>$ but $<\gamma\,|\,\omega> = <\omega\,|\,\gamma>^*$; these are complex conjugates.

Postscript: Notice that **an inner product is a scalar**. A scalar is a tensor of zero rank, but a simpler explanation is that a scalar is an individual number that scales. Normalization constants are good examples. Given $|\,\chi> = \begin{pmatrix} 2-i \\ 3i \end{pmatrix}$, the normalized $|\,\chi> = \frac{1}{\sqrt{14}} \begin{pmatrix} 2-i \\ 3i \end{pmatrix}$ is scaled down by $\frac{1}{\sqrt{14}}$. Each component is $\frac{1}{\sqrt{14}}$ smaller than an original component, or each component is scaled to $\frac{1}{\sqrt{14}}$ of its original magnitude.

Recognizing that an inner product is a scalar also means that all properties of scalars, whether real or complex, apply. For instance, scalars commute so inner products commute, scalars can be removed from integrals, so inner products can be removed from integrals, etc.

In general, $<\gamma\,|\,\omega> = <\omega\,|\,\gamma>^*$, where the superscript " * " indicates a complex conjugate. A proof in three dimensions is left as an exercise.

1–12. For $\beta = 2+3i$, $\mathcal{H} \to \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix}$, and $\mathcal{K} \to \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix}$,

find (a) $\beta\,\mathcal{H}$, (b) $\beta\,\mathcal{K}$, (c) $\mathcal{H} + \mathcal{K}$, and (d) $\mathcal{H} - \mathcal{K}$.

This problem introduces matrix operators, demonstrates scalar multiplication of operators, and matrix operator addition and subtraction. The concepts conveyed in the subspaces of $\mathbb{C}^2$ and $\mathbb{C}^3$ can be extended to larger spaces including $\mathbb{C}^\infty$. Many topics, for instance orbital angular momentum and spin, can be addressed in $\mathbb{C}^2$ and $\mathbb{C}^3$.

A **matrix operator** is an array, known simply as a matrix in the language of linear algebra, but known as an operator in quantum mechanics. An operator may be a matrix operator or a differential operator. The postulates are most readily explained using matrix operators in $\mathbb{C}^2$ and $\mathbb{C}^3$ and then extended to $\mathbb{C}^\infty$, where all differential operators exist. Notice that four of the six postulates address operators. Operators represent physically measurable quantities, for instance energy, position, momentum, or angular momentum. All of the information of the system is contained in the state vector $|\,\psi>$. All of the information about the measurable quantity is contained in the operator representing that measurable quantity.

Scalar multiplication of operators is comparable to scalar multiplication of vectors, multiply each of the elements by the scalar, for instance

$$2\,\mathcal{H} = 2\begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} = \begin{pmatrix} 2\cdot 2 & 2\cdot 3i & 2(-4i) \\ 2(-3i) & 2\cdot 0 & 2\cdot 5 \\ 2\cdot 4i & 2\cdot 5 & 2\cdot 6 \end{pmatrix} = \begin{pmatrix} 4 & 6i & -8i \\ -6i & 0 & 10 \\ 8i & 10 & 12 \end{pmatrix}$$

thus, each of the elements is scaled larger by a factor of 2. Scaling by a factor of $\beta = 2+3i$ is more difficult to imagine, though the process is the same.

Addition and subtraction is accomplished by adding/subtracting like elements, for instance

$$\begin{pmatrix} 3 & 4+3i \\ 4-3i & 5 \end{pmatrix} + \begin{pmatrix} 2i & -7 \\ -7 & -2i \end{pmatrix} = \begin{pmatrix} 3+2i & 4+3i-7 \\ 4-3i-7 & 5-2i \end{pmatrix} = \begin{pmatrix} 3+2i & -3+3i \\ -3-3i & 5-2i \end{pmatrix},$$

$$\begin{pmatrix} 3 & 4+3i \\ 4-3i & 5 \end{pmatrix} - \begin{pmatrix} 2i & -7 \\ -7 & -2i \end{pmatrix} = \begin{pmatrix} 3-2i & 4+3i+7 \\ 4-3i+7 & 5+2i \end{pmatrix} = \begin{pmatrix} 3-2i & 11+3i \\ 11-3i & 5+2i \end{pmatrix}.$$

(a) $$(2+3i)\begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} = \begin{pmatrix} (2+3i)2 & (2+3i)3i & (2+3i)(-4i) \\ (2+3i)(-3i) & (2+3i)0 & (2+3i)5 \\ (2+3i)4i & (2+3i)5 & (2+3i)6 \end{pmatrix}$$

$$= \begin{pmatrix} 4+6i & -9+6i & 12-8i \\ 9-6i & 0 & 10+15i \\ -12+8i & 10+15i & 12+18i \end{pmatrix}$$

(b) $$(2+3i)\begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix} = \begin{pmatrix} (2+3i)2i & (2+3i)5 & (2+3i)(1+i) \\ (2+3i)0 & (2+3i)3i & (2+3i)(-8) \\ (2+3i)1 & (2+3i)(-8) & (2+3i)(-5i) \end{pmatrix}$$

$$= \begin{pmatrix} -6+4i & 10+15i & 2+2i+3i-3 \\ 0 & -9+6i & -16-24i \\ 2+3i & -16-24i & 15-10i \end{pmatrix} = \begin{pmatrix} -6+4i & 10+15i & -1+5i \\ 0 & -9+6i & -16-24i \\ 2+3i & -16-24i & 15-10i \end{pmatrix}$$

(c) $$\begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} + \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix} = \begin{pmatrix} 2+2i & 3i+5 & -4i+1+i \\ -3i+0 & 0+3i & 5-8 \\ 4i+1 & 5-8 & 6-5i \end{pmatrix}$$

$$= \begin{pmatrix} 2+2i & 5+3i & 1-3i \\ -3i & 3i & -3 \\ 1+4i & -3 & 6-5i \end{pmatrix}$$

(d) $$\begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} - \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix} = \begin{pmatrix} 2-2i & 3i-5 & -4i-1-i \\ -3i-0 & 0-3i & 5+8 \\ 4i-1 & 5+8 & 6+5i \end{pmatrix}$$

$$= \begin{pmatrix} 2-2i & -5+3i & -1-5i \\ -3i & -3i & 13 \\ -1+4i & 13 & 6+5i \end{pmatrix}$$

Postscript: Linear algebra addresses matrices of unequal dimensions, for instance, 2 X 3 or 5 X 4. Square matrix operators, for instance, 2 X 2, 3 X 3, 4 X 4,... dominate quantum mechanics. Hermitian operators in matrix form are necessarily square.

Operators must be of the same dimension to be added/subtracted, for instance a 2 X 2 matrix cannot be added/subtracted to/from a 3 X 3 matrix. Said another way, operators must be of the same space/subspace to be added/subtracted.

1–13. For $|v> \rightarrow \begin{pmatrix} 4 \\ 3i \\ 1-5i \end{pmatrix}$, $\mathcal{H} \rightarrow \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix}$, and $\mathcal{K} \rightarrow \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix}$,

find each operator/vector or vector/operator product possible.

First, notice the product $\mathcal{H}\,|\psi>$ in the Schrodinger postulate. This is an operator/vector product.

Operator/vector products or vector/operator products are possible only when the two objects are of the same space/subspace. A two dimensional vector cannot be multiplied by a three dimensional operator, nor can a two dimensional operator be multiplied by a three dimensional vector. A vector and an operator must have the same number of dimensions to be multiplied in any sense.

Operator/vector or vector/operator products are extensions of an inner product. A 2 X 2 example of an operator/vector product is

$$\begin{pmatrix} 3 & 4i \\ -4i & 5 \end{pmatrix} \begin{pmatrix} 6i \\ 2 \end{pmatrix}.$$

Again, imagine rotating the column vector counter clockwise over the matrix operator and forming an inner product with each row. That would look like

$$\begin{pmatrix} 3 & 4i \\ -4i & 5 \end{pmatrix} \begin{pmatrix} 6i \\ 2 \end{pmatrix} = \begin{pmatrix} 3 \cdot 6i + 4i \cdot 2 \\ -4i \cdot 6i + 5 \cdot 2 \end{pmatrix} = \begin{pmatrix} 18i + 8i \\ 24 + 10 \end{pmatrix} = \begin{pmatrix} 26i \\ 34 \end{pmatrix}.$$

An inner product is a scalar, but there is one scalar for each row, thus, an operator/vector product is a vector. Should this represent a Hamiltonian acting on a state vector per the product $\mathcal{H}\,|\psi>$ in the Schrodinger postulate, a changed state vector is the result.

The expressions

$$\begin{pmatrix} 6i \\ 2 \end{pmatrix} \begin{pmatrix} 3 & 4i \\ -4i & 5 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 3 & 4i \\ -4i & 5 \end{pmatrix} \begin{pmatrix} -6i\,, & 2 \end{pmatrix}$$

do not make sense under an extension of an inner product, however,

$$\begin{pmatrix} -6i\,, & 2 \end{pmatrix} \begin{pmatrix} 3 & 4i \\ -4i & 5 \end{pmatrix}$$

does make sense within the inner product analogy, thus

$$\begin{pmatrix} -6i\,, & 2 \end{pmatrix} \begin{pmatrix} 3 & 4i \\ -4i & 5 \end{pmatrix} = \begin{pmatrix} -18i - 8i\,, & 24 + 10 \end{pmatrix} = \begin{pmatrix} -26i\,, & 34 \end{pmatrix}$$

is an example of a vector/operator product.

There are four possible products between the vector and the two operators given. They are $\mathcal{H}\,|v>$, $\mathcal{K}\,|v>$, $<v|\,\mathcal{H}$, and $<v|\,\mathcal{K}$.

$$\mathcal{H}\,|\,v> \;=\; \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} \begin{pmatrix} 4 \\ 3i \\ 1-5i \end{pmatrix} \;=\; \begin{pmatrix} 2(4) & + & 3i(3i) & + & -4i(1-5i) \\ -3i(4) & + & 0(3i) & + & 5(1-5i) \\ 4i(4) & + & 5(3i) & + & 6(1-5i) \end{pmatrix}$$

$$= \begin{pmatrix} 8-9-4i-20 \\ -12i+0+5-25i \\ 16i+15i+6-30i \end{pmatrix} \;=\; \begin{pmatrix} -21-4i \\ 5-37i \\ 6+i \end{pmatrix}$$

$$\mathcal{K}\,|\,v> \;=\; \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix} \begin{pmatrix} 4 \\ 3i \\ 1-5i \end{pmatrix} \;=\; \begin{pmatrix} 2i(4) & + & 5(3i) & + & (1+i)(1-5i) \\ 0(4) & + & 3i(3i) & + & (-8)(1-5i) \\ 1(4) & + & -8(3i) & + & -5i(1-5i) \end{pmatrix}$$

$$= \begin{pmatrix} 8i+15i+1-5i+i+5 \\ 0-9-8+40i \\ 4-24i-5i-25 \end{pmatrix} \;=\; \begin{pmatrix} 6+19i \\ -17+40i \\ -21-29i \end{pmatrix}$$

$$<v\,|\,\mathcal{H} \;=\; \Big(4\,,\;\; -3i\,,\;\; 1+5i\Big) \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix}$$

$$= \Big(4(2) \;+\; -3i(-3i) \;+\; (1+5i)(4i)\,,$$
$$4(3i) \;+\; -3i(0) \;+\; (1+5i)(5)\,,$$
$$4(-4i) \;+\; -3i(5) \;+\; (1+5i)(6)\Big)$$

$$= \Big(8-9+4i-20\,,\quad 12i+0+5+25i\,,\quad -16i-15i+6+30i\Big)$$

$$= \Big(-21+4i\,,\quad 5+37i\,,\quad 6-i\Big)$$

$$<v\,|\,\mathcal{K} \;=\; \Big(4\,,\;\; -3i\,,\;\; 1+5i\Big) \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix}$$

$$= \Big(4(2i) \;+\; -3i(0) \;+\; (1+5i)(1)\,,$$
$$4(5) \;+\; -3i(3i) \;+\; (1+5i)(-8)\,,$$
$$4(1+i) \;+\; -3i(-8) \;+\; (1+5i)(-5i)\Big)$$

$$= \Big(8i-0+1+5i\,,\quad 20+9-8-40i\,,\quad 4+4i+24i-5i+25\Big)$$

$$= \Big(1+13i\,,\quad 21-40i\,,\quad 29+23i\Big)$$

Postscript: Notice that $\mathcal{H}\,|\,v>$ and $<v\,|\,\mathcal{H}$ are corresponding ket and bra, but that $\mathcal{K}\,|\,v>$ and $<v\,|\,\mathcal{K}$ appear unrelated.

The terms operator/vector and vector/operator product are rarely encountered. Conventional terminology is that an operator operates to the right on a ket and to the left on a bra.

1–14. Find all possible operator/operator products for $\mathcal{C} \rightarrow \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}$ and $\mathcal{D} \rightarrow \begin{pmatrix} 4 & -5i \\ 5i & 4 \end{pmatrix}$, and for the $\mathcal{H}$ and $\mathcal{K}$ given in the previous problem, ignoring powers.

Operators must have the same dimensions to be multiplied. $\mathcal{C}$ and $\mathcal{D}$ can be multiplied, $\mathcal{H}$ and $\mathcal{K}$ can be multiplied, but the 2 X 2 matrices cannot be multiplied the 3 X 3 matrices or vice versa.

Matrix multiplication, or an operator/operator product, is our final generalization of an inner product. A 2 X 2 example of an operator/operator product is

$$\mathcal{C}\,\mathcal{D} \;=\; \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} \begin{pmatrix} 4 & -5i \\ 5i & 4 \end{pmatrix}.$$

First, imagine each column of the right operator as an individual ket. Then imagine rotating each individual column vector counter clockwise over the first operator and forming an inner product with each row for all columns. That is

$$\mathcal{C}\,\mathcal{D} \;=\; \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} \begin{pmatrix} 4 & -5i \\ 5i & 4 \end{pmatrix} \;=\; \begin{pmatrix} 3(4) & + & 4i(5i) & \quad & 3(-5i) & + & 4i(4) \\ -4i(4) & + & 3(5i) & & -4i(-5i) & + & 3(4) \end{pmatrix}$$

$$= \begin{pmatrix} 12-20 & -15i+16i \\ -16i+15i & -20+12 \end{pmatrix} \;=\; \begin{pmatrix} -8 & i \\ -i & -8 \end{pmatrix}$$

which is the operator/operator product. An inner product is a scalar, an operator/vector product is a vector, and an operator/operator product is an operator.

There are two operator/operator products possible for any two operators in the same space. The order in which the two operators are multiplied matters. In the other order, the product is

$$\mathcal{D}\,\mathcal{C} \;=\; \begin{pmatrix} 4 & -5i \\ 5i & 4 \end{pmatrix} \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} \;=\; \begin{pmatrix} 4(3) & + & -5i(-4i) & \quad & 4(4i) & + & -5i(3) \\ 5i(3) & + & 4(-4i) & & 5i(4i) & + & 4(3) \end{pmatrix}$$

$$= \begin{pmatrix} 12-20 & 16i-15i \\ 15i-16i & -20+12 \end{pmatrix} \;=\; \begin{pmatrix} -8 & i \\ -i & -8 \end{pmatrix}.$$

This operator/operator product is the same in both orders in this case, which is unusual.

$$\mathcal{H}\mathcal{K} \;=\; \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix}$$

$$= \begin{pmatrix} 2(2i)+3i(0)-4i(1) & 2(5)+3i(3i)-4i(-8) & 2(1+i)+3i(-8)-4i(-5i) \\ -3i(2i)+0(0)+5(1) & -3i(5)+0(3i)+5(-8) & -3i(1+i)+0(-8)+5(-5i) \\ 4i(2i)+5(0)+6(1) & 4i(5)+5(3i)+6(-8) & 4i(1+i)+5(-8)+6(-5i) \end{pmatrix}$$

$$= \begin{pmatrix} 4i+0-4i & 10-9+32i & 2+2i-24i-20 \\ 6+0+5 & -15i+0-40 & -3i+3+0-25i \\ -8+0+6 & 20i+15i-48 & 4i-4-40-30i \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 1+32i & -18-22i \\ 11 & -40-15i & 3-28i \\ -2 & -48+35i & -44-26i \end{pmatrix}$$

$$\mathcal{K}\mathcal{H} = \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix} \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix}$$

$$= \begin{pmatrix} 2i(2)+5(-3i)+(1+i)(4i) & 2i(3i)+5(0)+(1+i)(5) & 2i(-4i)+5(5)+(1+i)(6) \\ 0(2)+3i(-3i)-8(4i) & 0(3i)+3i(0)-8(5) & 0(-4i)+3i(5)-8(6) \\ 1(2)-8(-3i)-5i(4i) & 1(3i)-8(0)-5i(5) & 1(-4i)-8(5)-5i(6) \end{pmatrix}$$

$$= \begin{pmatrix} 4i-15i+4i-4 & -6+0+5+5i & 8+25+6+6i \\ 0+9-32i & 0+0-40 & 0+15i-48 \\ 2+24i+20 & 3i-0-25i & -4i-40-30i \end{pmatrix}$$

$$= \begin{pmatrix} -4-7i & -1+5i & 39+6i \\ 9-32i & -40 & -48+15i \\ 22+24i & -22i & -40-34i \end{pmatrix}$$

Notice that none of the elements of the two product matrices are the same, and thus $\mathcal{H}\mathcal{K} \neq \mathcal{K}\mathcal{H}$.

Postscript: If the product of two objects is the same regardless of the order of the multiplication, the two objects are said to **commute**. All scalars, including complex scalars, commute with all other scalars. Problem 1–11 demonstrates that vectors do not commute with other vectors in general. Though $\mathcal{C}\mathcal{D} = \mathcal{D}\mathcal{C}$, the fact that $\mathcal{H}\mathcal{K} \neq \mathcal{K}\mathcal{H}$, demonstrates that operators do not commute with other operators in general.

1–15. Show by explicit multiplication in $\mathbb{C}^3$ that an identity operator multiplying

(a) a ket,

(b) a bra,

(c) a matrix operator from the left, and

(d) a matrix operator from the right results in the original ket, bra, or matrix operator.

The **identity operator** is the analogy of "1" in the real number system. One times a number is the original number. This problem introduces the identity operator but also intends to persuade that any legitimate multiplication by the identity operator results in the original object.

$$\mathcal{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ in } \mathbb{C}^2 \qquad \text{and} \qquad \mathcal{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ in } \mathbb{C}^3.$$

An identity operator is a matrix with 1's on the principal diagonal and zeros elsewhere. Assume

$$|v> \rightarrow \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} \qquad \text{and} \qquad \mathcal{A} \rightarrow \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}.$$

Of course $\mathcal{I}|v> = |v>$, $<v|\mathcal{I} = <v|$, $\mathcal{I}\mathcal{A} = \mathcal{A}$, and $\mathcal{A}\mathcal{I} = \mathcal{A}$.

(a) $\mathcal{I}\,|\,v> = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} b_1+0+0 \\ 0+b_2+0 \\ 0+0+b_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = |\,v> \,.$

(b) $<v\,|\,\mathcal{I} = \begin{pmatrix} b_1,\, b_2,\, b_3 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} b_1{+}0{+}0,\, 0{+}b_2{+}0,\, 0{+}0{+}b_3 \end{pmatrix} = \begin{pmatrix} b_1,\, b_2,\, b_3 \end{pmatrix} = <v\,|\,.$

(c) $\mathcal{I}\mathcal{A} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$

$= \begin{pmatrix} a_{11}+0+0 & a_{12}+0+0 & a_{13}+0+0 \\ 0+a_{21}+0 & 0+a_{22}+0 & 0+a_{23}+0 \\ 0+0+a_{31} & 0+0+a_{32} & 0+0+a_{33} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \mathcal{A}\,.$

(d) $\mathcal{A}\mathcal{I} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$= \begin{pmatrix} a_{11}+0+0 & 0+a_{12}+0 & 0+0+a_{13} \\ a_{21}+0+0 & 0+a_{22}+0 & 0+0+a_{23} \\ a_{31}+0+0 & 0+a_{32}+0 & 0+0+a_{33} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \mathcal{A}\,.$

Postscript: A scalar times an operator, from either side, is another operator. The meaning of

$$\alpha\mathcal{I} \quad \text{is} \quad \alpha \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix} \quad \text{in} \quad \mathbb{C}^3\,,$$

which is an operator with the scalar on the principal diagonal and zeros elsewhere. Operating on a vector or operator with this yields the same result as multiplication of the vector or operator by the scalar. The scalar times the identity operator is what is intended when an author sets a scalar equal to an operator. For instance,

$$\mathcal{A}\mathcal{B} = \alpha \quad \text{means} \quad \mathcal{A}\mathcal{B} = \alpha\mathcal{I}\,.$$

The concept of a diagonal operator is also introduced. The identity operator is diagonal. A **diagonal operator** is an operator with any non-zero elements on the principal diagonal and all off-diagonal elements of zero, like $\begin{pmatrix} -5 & 0 \\ 0 & 3 \end{pmatrix}$ in $\mathbb{C}^2$, and $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix}$ in $\mathbb{C}^3$.

1–16. Given $\mathcal{L}^2 = \mathcal{L}_x^2 + \mathcal{L}_y^2 + \mathcal{L}_z^2$ and

$$\mathcal{L}_x \to \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\,, \qquad \mathcal{L}_y \to \frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar\,, \qquad \mathcal{L}_z \to \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar\,,$$

show that $\mathcal{L}^2 = 2\hbar^2\mathcal{I}$.

Powers are the operator multiplied by itself, for instance $\mathcal{H}^2 = \mathcal{H}\mathcal{H}$ or $\mathcal{C}^3 = \mathcal{C}\mathcal{C}\mathcal{C}$, or

$$\mathcal{L}_x^2 = \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar = \frac{\hbar^2}{2}\begin{pmatrix}1&0&1\\0&1+1&0\\1&0&1\end{pmatrix} = \frac{\hbar^2}{2}\begin{pmatrix}1&0&1\\0&2&0\\1&0&1\end{pmatrix}$$

where elements that are all 1's or 0's make the matrix arithmetic particularly straightforward. The given matrices, $\mathcal{L}_x$, $\mathcal{L}_y$, and $\mathcal{L}_z$ are the component orbital angular momentum operators. They offer a convenient platform to consolidate operator arithmetic having realism, introduce operator powers, and employ an identity operator $\mathcal{I}$.

$$\mathcal{L}^2 = \mathcal{L}_x^2 + \mathcal{L}_y^2 + \mathcal{L}_z^2$$

$$\to \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar + \frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar\frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar + \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar$$

$$= \frac{1}{2}\begin{pmatrix}1&0&1\\0&1+1&0\\1&0&1\end{pmatrix}\hbar^2 + \frac{1}{2}\begin{pmatrix}1&0&-1\\0&1+1&0\\-1&0&1\end{pmatrix}\hbar^2 + \begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\hbar^2$$

$$= \begin{pmatrix}1/2&0&1/2\\0&1&0\\1/2&0&1/2\end{pmatrix}\hbar^2 + \begin{pmatrix}1/2&0&-1/2\\0&1&0\\-1/2&0&1/2\end{pmatrix}\hbar^2 + \begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\hbar^2$$

$$= \begin{pmatrix}1&0&0\\0&2&0\\0&0&1\end{pmatrix}\hbar^2 + \begin{pmatrix}1&0&0\\0&0&0\\0&0&1\end{pmatrix}\hbar^2 = \begin{pmatrix}2&0&0\\0&2&0\\0&0&2\end{pmatrix}\hbar^2 = 2\hbar^2\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix} = 2\hbar^2\mathcal{I}\,.$$

1–17. Use $\mathcal{C}$, $\mathcal{D}$, $\mathcal{H}$, and $\mathcal{K}$ from problems 1–13 and 1–14 to find $\big[\mathcal{C},\mathcal{D}\big]$ and $\big[\mathcal{H},\mathcal{K}\big]$.

The objects $\big[\mathcal{C},\mathcal{D}\big]$ and $\big[\mathcal{H},\mathcal{K}\big]$ are called commutators. In general, a **commutator** is defined

$$\big[\mathcal{A},\mathcal{B}\big] \;=\; \mathcal{A}\mathcal{B} \;-\; \mathcal{B}\mathcal{A}$$

thus, if $\big[\mathcal{A},\mathcal{B}\big] \;=\; 0$, the operators $\mathcal{A}$ and $\mathcal{B}$ commute. The required product operators were calculated in problem 1–14.

$$\big[\mathcal{C},\mathcal{D}\big] \;=\; \mathcal{C}\mathcal{D} \;-\; \mathcal{D}\mathcal{C} \;=\; \begin{pmatrix} -8 & i \\ -i & -8 \end{pmatrix} \;-\; \begin{pmatrix} -8 & i \\ -i & -8 \end{pmatrix} \;=\; \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \;=\; 0 \quad \text{in } \mathbb{C}^2 .$$

$$\big[\mathcal{H},\mathcal{K}\big] \;=\; \mathcal{H}\mathcal{K}-\mathcal{K}\mathcal{H} \;=\; \begin{pmatrix} 0 & 1+32i & -18-22i \\ 11 & -40-15i & 3-28i \\ -2 & -48+35i & -44-26i \end{pmatrix} \;-\; \begin{pmatrix} -4-7i & -1+5i & 39+6i \\ 9-32i & -40 & -48+15i \\ 22+24i & -22i & -40-34i \end{pmatrix}$$

$$=\; \begin{pmatrix} 4+7i & 2+27i & -57-28i \\ 2+32i & -15i & 51-43i \\ -24-24i & -48+57i & -4+8i \end{pmatrix} .$$

Postscript: The meaning of zero in the equation $\big[\mathcal{A},\mathcal{B}\big] \;=\; 0$ is a zero matrix, a matrix with all elements 0, such as $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ in $\mathbb{C}^2$. One purpose of the commutator is to show that two operators commute. The calculation for $\big[\mathcal{H},\mathcal{K}\big]$ is unlikely because it can be seen by inspection that the product matrices do not commute.

A commutator is an operator. The product of two operators is an operator, and the difference of two operators is an operator. It is important to understand that a commutator is an operator.

The operators for the observable quantities position and momentum are denoted $\mathcal{X}$ and $\mathcal{P}$ respectively. A significant statement of the relation between these two observable quantities is

$$\big[\mathcal{X},\mathcal{P}\big] \;=\; i\hbar$$

where $i\hbar$ means $i\hbar\mathcal{I}$ for the appropriate space. This is known as the **fundamental canonical commutator** when expressed for position and momentum. It is known as a **canonical commutator** when expressed for other observable quantities. The Heisenberg uncertainty relation applies to all observable quantities having a canonical commutation relation.

The identity operator $\mathcal{I}$ commutes with all other operators in the same space. Thus, a scalar multiple of an identity operator, like $\mathcal{L}^2$, commutes with all other operators in the same space.

1–18. Which of the following operators are Hermitian?

$$\mathcal{C} \to \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}, \quad \mathcal{D} \to \begin{pmatrix} 4 & -5i \\ 5i & 4 \end{pmatrix}, \quad \mathcal{H} \to \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix}, \quad \mathcal{K} \to \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix}.$$

Every observable quantity is represented by a **Hermitian operator**. The property of Hermiticity is defined $\mathcal{A} = \mathcal{A}^\dagger$ where the superscript dagger indicates an **adjoint** which means a transpose conjugate. Transpose means make all the rows columns, or make all the columns rows. Then complex conjugate each element to obtain the adjoint operator. For instance

$$\mathcal{C} \to \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} \quad \Rightarrow \quad \mathcal{C}^T = \begin{pmatrix} 3 & -4i \\ 4i & 3 \end{pmatrix} \quad \Rightarrow \quad \mathcal{C}^{T*} = \mathcal{C}^\dagger = \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} = \mathcal{C}$$

and since $\mathcal{C}^\dagger = \mathcal{C} \iff \mathcal{C} = \mathcal{C}^\dagger$, $\mathcal{C}$ is Hermitian. Another example is

$$\mathcal{Q} \to \begin{pmatrix} 1 & 2+i \\ 2-i & 3i \end{pmatrix} \quad \Rightarrow \quad \mathcal{Q}^T \to \begin{pmatrix} 1 & 2-i \\ 2+i & 3i \end{pmatrix} \quad \Rightarrow \quad \mathcal{Q}^{T*} \to \begin{pmatrix} 1 & 2+i \\ 2-i & -3i \end{pmatrix} \neq \mathcal{Q}$$

because though the other three elements are identical, the element in the second row and second column is not the same, therefore $\mathcal{Q}$ is not Hermitian.

$$\mathcal{D} \to \begin{pmatrix} 4 & -5i \\ 5i & 4 \end{pmatrix} \quad \Rightarrow \quad \mathcal{D}^T = \begin{pmatrix} 4 & 5i \\ -5i & 4 \end{pmatrix} \quad \Rightarrow \quad \mathcal{D}^{T*} = \mathcal{D}^\dagger = \begin{pmatrix} 4 & -5i \\ 5i & 4 \end{pmatrix} = \mathcal{D}$$

so $\mathcal{D}$ is Hermitian.

$$\mathcal{H} \to \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} \Rightarrow \mathcal{H}^T = \begin{pmatrix} 2 & -3i & 4i \\ 3i & 0 & 5 \\ -4i & 5 & 6 \end{pmatrix} \Rightarrow \mathcal{H}^{T*} = \mathcal{H}^\dagger = \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix} = \mathcal{H}$$

thus $\mathcal{H}$ is Hermitian.

$$\mathcal{K} \to \begin{pmatrix} 2i & 5 & 1+i \\ 0 & 3i & -8 \\ 1 & -8 & -5i \end{pmatrix} \Rightarrow \mathcal{K}^T = \begin{pmatrix} 2i & 0 & 1 \\ 5 & 3i & -8 \\ 1+i & -8 & -5i \end{pmatrix} \Rightarrow \mathcal{K}^{T*} = \begin{pmatrix} -2i & 0 & 1 \\ 5 & -3i & -8 \\ 1-i & -8 & 5i \end{pmatrix} \neq \mathcal{K}$$

because seven of the nine elements differ, so $\mathcal{K}$ is not Hermitian.

Postscript: Observable quantities must be real numbers. The methods of calculating results that are real numbers from a space with intrinsically complex numbers, components, and elements are built into the postulates. A measurement of an observable quantity represented by an operator must be one of the eigenvalues of that operator. One of the advantageous properties of Hermitian operators is that their eigenvalues are real numbers!

A number times its complex conjugate is a real number. An inner product of a bra times its corresponding ket is a real number. Forming a bra from its corresponding ket is a multicomponent

generalization of conjugating a complex number, and is in fact, transpose conjugation. Calling a bra the adjoint of its corresponding ket is entirely correct. The process of transpose conjugating an operator, forming an adjoint operator, is simply a further generalization.

Examine the main diagonal of all five examples. The process of transposing elements, making all rows columns or all columns rows, does not affect elements on the main diagonal. An operator with an imaginary or complex number on the main diagonal cannot be Hermitian because that element will remain in the same position during the process of transposition and then be changed by the process of conjugation. Hermitian operators must have real numbers on the principal diagonal.

Some of the most favorable Hermitian operators are diagonal operators, like $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$ or $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix}$, with real numbers on the main diagonal and zeros elsewhere.

Remember that real numbers are a subset of complex numbers that do not have an imaginary part, or have an imaginary part that is zero. One way to demonstrate that a number is real is to show that it is the same as its complex conjugate. That $\alpha = \alpha^*$ means α is a real number.

Hermitian operators are also known as **self adjoint** operators.

1–19. Calculate the determinants of

$$\mathcal{Q} \to \begin{pmatrix} 1 & 2+i \\ 2-i & 3i \end{pmatrix}, \qquad \mathcal{C} \to \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}, \qquad \text{and} \qquad \mathcal{H} \to \begin{pmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{pmatrix}.$$

A measurement can only yield an eigenvalue and the measurement of any eigenvalue collapses the system to the eigenvector corresponding to that eigenvalue. Evaluating determinants is a skill that is central to the manual method of solving the eigenvalue/eigenvector problem.

An integral with limits is a scalar, (though it may take considerable effort to evaluate). Similarly, a **determinant** is a scalar. $\det \mathcal{A}$ is a scalar associated with a square matrix operator.

A determinant is a function of a square matrix that is the alternating sum of the products of the elements of any row or column and the respective cofactors.

Symbolically, $\mathcal{A} \to \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \Rightarrow \det \mathcal{A} = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{21}a_{12}$, and

$$\mathcal{A} \to \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \Rightarrow \det \mathcal{A} = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

$$= a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{21} \begin{vmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{vmatrix} + a_{31} \begin{vmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{vmatrix}$$

$$= a_{11}\big(a_{22}a_{33} - a_{32}a_{23}\big) - a_{21}\big(a_{12}a_{33} - a_{32}a_{13}\big) + a_{31}\big(a_{12}a_{23} - a_{22}a_{13}\big)$$

$$= a_{11}a_{22}a_{33} - a_{11}a_{32}a_{23} + a_{21}a_{32}a_{13} - a_{21}a_{12}a_{33} + a_{31}a_{12}a_{23} - a_{31}a_{22}a_{13}.$$

This can be extended to arbitrary or infinite dimension. For evaluation of determinants beyond dimension 3, refer to Arfken[1], Boas[2], or a favorite linear algebra text.

$$\det \mathcal{Q} = \begin{vmatrix} 1 & 2+i \\ 2-i & 3i \end{vmatrix} = (1)(3i) - (2-i)(2+i) = 3i - 4 - 1 = -5 + 3i\,.$$

$$\det \mathcal{C} = \begin{vmatrix} 3 & 4i \\ -4i & 3 \end{vmatrix} = (3)(3) - (-4i)(4i) = 9 - 16 = -7\,.$$

$$\det \mathcal{H} = \begin{vmatrix} 2 & 3i & -4i \\ -3i & 0 & 5 \\ 4i & 5 & 6 \end{vmatrix}$$

$$= (2)(0)(6) - (2)(5)(5) + (-3i)(5)(-4i) - (-3i)(3i)(6) + (4i)(3i)(5) - (4i)(0)(-4i)$$

$$= 0 - 50 - 60 - 54 - 60 - 0 = -224\,.$$

Postscript: Notice that the determinant of the non-Hermitian operator is a complex number, but that the determinants of the two Hermitian operators are real numbers. The determinant of a Hermitian operator must be a real number.

If $\det \mathcal{A} = 0$, $\mathcal{A}$ is **singular**. The inverse of a singular operator does not exist.

1–20. Given the matrix operator $\begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}$,

(a) show that $|2> = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is an eigenvector with eigenvalue 2,

(b) and that $|3> = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ is an eigenvector with eigenvalue 3.

(c) Interpret these facts geometrically.

This problem is a numerical introduction to the eigenvalue/eigenvector equation. Both eigenvalues and eigenvectors are central to interpreting the postulates.

The product of an operator and a vector is another vector, $\mathcal{A}\,|v> = |w>$. For some matrices and all Hermitian operators, there are products of the operator and special vectors such that the new vector is a product of a scalar and the original vector, *i.e.*,

$$\mathcal{A}\,|v_i> = \alpha_i\,|v_i>\,.$$

[1] Arfken *Mathematical Methods for Physicists,* Academic Press, 1970, chap 4.

[2] Boas *Mathematical Methods in the Physical Sciences,* John Wiley & Sons, 1983, pp. 87–94.

This **eigenvalue/eigenvector equation** actually describes a family of equations, thus subscripts are sometimes used, though $\mathcal{A}\,|\,v> \;=\; \alpha\,|\,v>$ has the same meaning as the above equation. There are as many matching scalars and vectors as the dimension of the space for operators having an eigenvalue/eigenvector relation. The scalars are known as **eigenvalues** and the vectors are known as **eigenvectors**. It is popular to place the eigenvalue between the | and > that indicate the ket to identify the corresponding eigenvector. Thus, demonstrate that

$$\begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \;=\; 2 \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

for part (a), for instance. This is simply a numerical statement of the eigenvalue/eigenvector equation. Consider "length" and "direction" of the vectors for part (c).

(a) $\begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1+1 \\ -2+4 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \end{pmatrix} = 2 \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, so for the operator $\mathcal{A} = \begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}$,

2 is an eigenvalue, and $|\,2> \;=\; \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ is the corresponding eigenvector.

(b) $\begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 1+2 \\ -2+8 \end{pmatrix} = \begin{pmatrix} 3 \\ 6 \end{pmatrix} = 3 \begin{pmatrix} 1 \\ 2 \end{pmatrix}$, so for the operator $\mathcal{A} = \begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}$,

3 is an eigenvalue, and $|\,3> \;=\; \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ is the corresponding eigenvector.

In a 2 dimensional space, we expect exactly two eigenvalues and two eigenvectors.

(c) In part (a), the effect of the operator on its eigenvector is a vector twice as long and in exactly the same direction as the original vector. In part (b), the effect of the operator on its eigenvector is a vector three times as long as the original vector and in exactly the same direction. An operator acting on an eigenvector results in changing the "length" of the vector without rotating it. The length of the eigenvector is changed by a factor equal to its eigenvalue.

Postscript: The eigenvalue/eigenvector equation is some form of $\mathcal{A}\,|\,v> \;=\; \alpha\,|\,v>$. An operator acting on an eigenvector returns the same vector scaled.

The eigenvectors in this problem were deliberately not normalized to allow integer arithmetic. $|\,2> \;=\; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $|\,3> \;=\; \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ when normalized.

Physicists use various methods to denote eigenvectors other than by placing the eigenvalue between the | and > that indicate the eigenvector or **eigenket**. For instance, $|\,v_1>$ or $|\,1>$ might identify the first eigenvector and $|\,v_2>$ or $|\,2>$ might denote the second eigenvector. Indices known as quantum numbers are often placed between the | and > that indicate the eigenket.

Again, the eigenvalue/eigenvector equation always denotes a family of equations. Subscripts are not always used. $\mathcal{A}\,|\,v> \;=\; \alpha\,|\,v>$ has the same meaning as $\mathcal{A}\,|\,v_i> \;=\; \alpha_i\,|\,v_i>$. There are as many eigenvalues and eigenvectors as the dimension of the operator under consideration.

The prefix "eigen" on the words "value" and "vector" is from German and translates roughly to the word "characteristic" in English. Thus, an eigenvalue is a characteristic value of the operator, and an eigenvector is a characteristic vector of the operator.

1–21. Find the eigenvalues and normalized eigenvectors of

$$\mathcal{F} \rightarrow \begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}, \qquad \mathcal{C} \rightarrow \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}, \qquad \text{and} \qquad \mathcal{H} \rightarrow \begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix}.$$

Here is a roadmap to solve an eigenvalue/eigenvector problem manually.

(1) Set $\det\left(\mathcal{A} - \alpha\mathcal{I}\right) = 0$. This is known as the **characteristic equation**.

(2) Solve the characteristic equation. The solutions are the eigenvalues.

(3) Use the eigenvalue/eigenvector equation to solve for the eigenvectors.

(4) Normalize the eigenvectors.

There are some conventions associated with the eigenvalue/eigenvector problem. We will work from the eigenvalue of least magnitude to the eigenvalue of greatest magnitude. If the simultaneous equations that result from the eigenvalue/eigenvector equation are indeterminate, choose values that allow integer arithmetic, usually meaning choose the first non-zero element of the eigenket to be positive and real, most often 1. This is a convention that is popular but not universal[3]. The operator $\mathcal{H}$ in this problem can be addressed with integers if the last non-zero element of the eigenvector is chosen to be 1.

$$\det\left(\mathcal{F}-\alpha\mathcal{I}\right) = \det\left[\begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix} - \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix}\right] = \det\begin{pmatrix} 1-\alpha & 1 \\ -2 & 4-\alpha \end{pmatrix} = (1-\alpha)(4-\alpha)-(1)(-2)$$

$= 4 - 5\alpha + \alpha^2 + 2 = \alpha^2 - 5\alpha + 6$. The characteristic equation is $\alpha^2 - 5\alpha + 6 = 0$

$\Rightarrow \quad (\alpha - 2)(\alpha - 3) = 0 \quad \Rightarrow \quad \alpha = 2\,,\ \alpha = 3\,,$ are the eigenvalues. $\mathcal{A}\,|\,v> = \alpha\,|\,v>$ for

$$\alpha = 2 \text{ is } \begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 2\begin{pmatrix} a \\ b \end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} a & + & b & = & 2a \\ -2a & + & 4b & = & 2b \end{array} \quad \Rightarrow \quad \begin{array}{rcl} b & = & a \\ -2a & = & -2b \end{array}$$

so let $a = 1 \quad \Rightarrow \quad b = 1 \quad \Rightarrow \quad |\,2> = N\begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and normalizing

$$\begin{pmatrix} 1\,, & 1 \end{pmatrix} N^* N \begin{pmatrix} 1 \\ 1 \end{pmatrix} = |\,N\,|^2(1+1) = |\,N\,|^2(2) = 1 \quad \Rightarrow \quad N = \frac{1}{\sqrt{2}}$$

$$\Rightarrow \quad |\,2> = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ is the normalized eigenvector. } \mathcal{A}\,|\,v> = \alpha\,|\,v> \text{ for } \alpha = 3 \text{ is}$$

$$\begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 3\begin{pmatrix} a \\ b \end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} a & + & b & = & 3a \\ -2a & + & 4b & = & 3b \end{array} \quad \Rightarrow \quad \begin{array}{rcl} b & = & 2a \\ -2a & = & -b \end{array}$$

[3] Shankar, *Principles of Quantum Mechanics* (Plenum Press, New York, 1994), 2nd ed., p. 34.

then $a = 1 \quad \Rightarrow \quad b = 2 \quad \Rightarrow \quad |3> = N\begin{pmatrix}1\\2\end{pmatrix}$, and normalizing

$$(1,\ 2)N^*N\begin{pmatrix}1\\2\end{pmatrix} = |N|^2(1+4) = |N|^2(5) = 1 \quad \Rightarrow \quad N = \frac{1}{\sqrt{5}}$$

$$\Rightarrow \quad |3> = \frac{1}{\sqrt{5}}\begin{pmatrix}1\\2\end{pmatrix} \text{ is the normalized eigenvector.}$$

$$\det\left(\mathcal{C}-\alpha\mathcal{I}\right) = \det\left[\begin{pmatrix}3 & 4i\\ -4i & 3\end{pmatrix} - \begin{pmatrix}\alpha & 0\\ 0 & \alpha\end{pmatrix}\right] = \det\begin{pmatrix}3-\alpha & 4i\\ -4i & 3-\alpha\end{pmatrix} = (3-\alpha)(3-\alpha)-(4i)(-4i)$$

$= 9-6\alpha+\alpha^2-16 = \alpha^2-6\alpha-7$. The characteristic equation is $\alpha^2-6\alpha-7 = 0$
$\Rightarrow \ (\alpha+1)(\alpha-7)=0 \ \Rightarrow \ \alpha=-1,\ \alpha=7,$ are the eigenvalues. $\mathcal{C}\,|v> = \alpha\,|v>$ for $\alpha=-1,$

$$\begin{pmatrix}3 & 4i\\ -4i & 3\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} = -1\begin{pmatrix}a\\b\end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} 3a & + & 4ib & = & -a \\ -4ia & + & 3b & = & -b \end{array} \quad \Rightarrow \quad \begin{array}{rcl} ib & = & -a \\ -ia & = & -b \end{array}$$

thus $a = 1 \quad \Rightarrow \quad b = i \quad \Rightarrow \quad |-1> = N\begin{pmatrix}1\\i\end{pmatrix}$, and normalizing

$$(1,\ -i)N^*N\begin{pmatrix}1\\i\end{pmatrix} = |N|^2(1+1) = |N|^2(2) = 1 \quad \Rightarrow \quad N = \frac{1}{\sqrt{2}}$$

$$\Rightarrow \quad |-1> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \text{ is the normalized eigenvector. } \mathcal{C}\,|v> = \alpha\,|v> \text{ for } \alpha = 7 \text{ is}$$

$$\begin{pmatrix}3 & 4i\\ -4i & 3\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} = 7\begin{pmatrix}a\\b\end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} 3a & + & 4ib & = & 7a \\ -4ia & + & 3b & = & 7b \end{array} \quad \Rightarrow \quad \begin{array}{rcl} ib & = & a \\ -ia & = & b \end{array}$$

so $a = 1 \quad \Rightarrow \quad b = -i \quad \Rightarrow \quad |7> = N\begin{pmatrix}1\\-i\end{pmatrix}$, and normalizing

$$(1,\ i)N^*N\begin{pmatrix}1\\-i\end{pmatrix} = |N|^2(1+1) = |N|^2(2) = 1 \quad \Rightarrow \quad N = \frac{1}{\sqrt{2}}$$

$$\Rightarrow \quad |7> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \text{ is the second normalized eigenvector. Then for } \mathcal{H},$$

$$\det\begin{pmatrix}1-\alpha & 0 & -2i\\ 0 & 1-\alpha & 0\\ 2i & 0 & 4-\alpha\end{pmatrix} = (1-\alpha)^2(4-\alpha)-(2i)(1-\alpha)(-2i) = (1-2\alpha+\alpha^2)(4-\alpha)-4(1-\alpha)$$

$= 4-9\alpha+6\alpha^2-\alpha^3-4+4\alpha = -\alpha^3+6\alpha^2-5\alpha \quad \Rightarrow \quad \alpha^3-6\alpha^2+5\alpha = 0$ is the characteristic equation and can be factored $\alpha(\alpha-1)(\alpha-5) = 0 \quad \Rightarrow \quad \alpha = 0,\ 1,$ and 5 are the eigenvalues.

$$\mathcal{H}\,|v> = 0\,|v> \ \Rightarrow \ \begin{pmatrix}1 & 0 & -2i\\ 0 & 1 & 0\\ 2i & 0 & 4\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = 0\begin{pmatrix}a\\b\\c\end{pmatrix} \ \Rightarrow \ \begin{array}{rcrcrcl} a & + & -2ic & = & 0 & & a = 2ic \\ & & b & = & 0 & \Rightarrow & b = 0 \\ 2ia & + & 4c & = & 0 & & ia = -2c \end{array}$$

so $b=0$ and pick $c=1$ so that integers may be used $\Rightarrow$ $a=2i$ $\Rightarrow$ $|0> = N\begin{pmatrix}2i\\0\\1\end{pmatrix}$.

$$\big(-2i\,,\,0\,,\,1\big)N^*N\begin{pmatrix}2i\\0\\1\end{pmatrix} = |N|^2(4+0+1) = |N|^2(5) = 1 \Rightarrow N = \frac{1}{\sqrt{5}} \Rightarrow |0> = \frac{1}{\sqrt{5}}\begin{pmatrix}2i\\0\\1\end{pmatrix}.$$

$$\mathcal{H}|v> = 1|v> \Rightarrow \begin{pmatrix}1&0&-2i\\0&1&0\\2i&0&4\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = 1\begin{pmatrix}a\\b\\c\end{pmatrix} \Rightarrow \begin{array}{rcrcrcl} a&+&-2ic&=&a&& c=0\\ &&b&=&b&\Rightarrow& b=b\\ 2ia&+&4c&=&c&& 2ia=-3c\end{array}$$

so $c=0$ $\Rightarrow$ $a=0$ and let $b=1$ $\Rightarrow$ $|1> = N\begin{pmatrix}0\\1\\0\end{pmatrix}$.

$$\big(0\,,\;1\,,\;0\big)N^*N\begin{pmatrix}0\\1\\0\end{pmatrix} = |N|^2(0+1+0) = |N|^2(1) = 1 \Rightarrow N=1 \Rightarrow |1> = \begin{pmatrix}0\\1\\0\end{pmatrix}.$$

$$\mathcal{H}|v> = 5|v> \Rightarrow \begin{pmatrix}1&0&-2i\\0&1&0\\2i&0&4\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix} = 5\begin{pmatrix}a\\b\\c\end{pmatrix} \Rightarrow \begin{array}{rcrcrcl} a&+&-2ic&=&5a&& -ic=2a\\ &&b&=&5b&\Rightarrow& b=0\\ 2ia&+&4c&=&5c&& 2ia=c\end{array}$$

so $b=0$ then let $a=1$ $\Rightarrow$ $c=2i$ $\Rightarrow$ $|5> = N\begin{pmatrix}1\\0\\2i\end{pmatrix}$.

$$\big(1\,,\,0\,,\,-2i\big)N^*N\begin{pmatrix}1\\0\\2i\end{pmatrix} = |N|^2(1+0+4) = |N|^2(5) = 1 \Rightarrow N = \frac{1}{\sqrt{5}} \Rightarrow |5> = \frac{1}{\sqrt{5}}\begin{pmatrix}1\\0\\2i\end{pmatrix}.$$

Postscript: The characteristic equation arises from the eigenvalue/eigenvector equation,

$$\mathcal{A}|a> = \alpha|a> \quad\Rightarrow\quad \mathcal{A}|a> - \alpha|a> = 0 \quad\Rightarrow\quad \big(\mathcal{A}-\alpha\mathcal{I}\big)|a> = 0$$

and $|a> \neq 0$ for a real system, so the only non-trivial solution is when $\det\big(\mathcal{A}-\alpha\mathcal{I}\big) = 0$.

The primary difficulty using this "manual" method is that the characteristic equation can be difficult to solve. The matrix operators in this text either represent physical systems or are designed to communicate concepts for which convenient eigenvalues are generally designed into the problems and exercises presented. Numerous computer applications are available to find eigenvalues and eigenvectors. A computer application may be a practical necessity to obtain eigenvalues and eigenvectors for an arbitrary matrix operator.

The method of obtaining eigenvalues and eigenvectors known as diagonalization will be developed using the manual method introduced in this problem. The method of diagonalization extends to $\mathbb{C}^\infty$ in which the manual method does not apply. The intent is to first expose diagonalization in $\mathbb{C}^2$ and $\mathbb{C}^3$. The genuine power of the method of obtaining eigenvalues and eigenvectors using diagonalization is its existence.

1–22. What are the eigenvalues and eigenvectors for $\mathcal{L}_y \rightarrow \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$?

Obtaining eigenvalues and eigenvectors in a realistic application such as a component orbital angular momentum operator (less scalar factors) seems appropriate before addressing diagonalization.

$$\det\left(\mathcal{L}_y - \alpha\mathcal{I}\right) = \det\begin{pmatrix} -\alpha & -i & 0 \\ i & -\alpha & -i \\ 0 & i & -\alpha \end{pmatrix} = (-\alpha)^3 - (-\alpha)(i)(-i) - (-i)(i)(-\alpha) = -\alpha^3 + \alpha + \alpha = 0$$

$\Rightarrow \quad \alpha^3 - 2\alpha = 0 \quad \Rightarrow \quad \alpha(\alpha^2 - 2) = \alpha(\alpha - \sqrt{2}\,)(\alpha + \sqrt{2}\,) = 0 \quad \Rightarrow \quad \alpha = -\sqrt{2},\ 0,\ \sqrt{2}$ are the eigenvalues. Starting with the smallest eigenvalue to obtain eigenvectors,

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \left(-\sqrt{2}\right)\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} & -bi & & = & -\sqrt{2}\,a \\ ai & - & ci & = & -\sqrt{2}\,b \\ & bi & & = & -\sqrt{2}\,c \end{array}$$

Adding the top and bottom equations, $-\sqrt{2}\,a - \sqrt{2}\,c = 0 \quad \Rightarrow \quad a = -c$. Using this in the middle equation, we get $ai + ai = -\sqrt{2}\,b \quad \Rightarrow \quad -\dfrac{2ai}{\sqrt{2}} = b \quad \Rightarrow \quad b = -\sqrt{2}\,ai$. If we choose $a = 1$, then $b = -\sqrt{2}\,i$, and $c = -1$, so the eigenket is

$$|-\sqrt{2}> \;=\; A\begin{pmatrix} 1 \\ -\sqrt{2}i \\ -1 \end{pmatrix} \quad \Rightarrow \quad <-\sqrt{2}\,|-\sqrt{2}> \;=\; \left(1,\ \sqrt{2}\,i,\ -1\right)A^*A\begin{pmatrix} 1 \\ -\sqrt{2}\,i \\ -1 \end{pmatrix}$$

$= |\,A\,|^2(1+2+1) \quad \Rightarrow \quad 4\,|\,A\,|^2 = 1 \quad \Rightarrow \quad |-\sqrt{2}> = \dfrac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2}\,i \\ -1 \end{pmatrix}$ for the eigenvalue $-\sqrt{2}$.

To find the eigenvector corresponding to the next smallest eigenvalue 0,

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} & -bi & & = & 0 \\ ai & - & ci & = & 0 \\ & bi & & = & 0 \end{array}$$

The top and bottom equations say $b = 0$, and the middle equation says $a = c$, so by convention, $a = 1 \quad \Rightarrow \quad c = 1$, and the eigenket is

$$|\,0> \;=\; A\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad \Rightarrow \quad <0\,|\,0> \;=\; \left(1,\ 0,\ 1\right)A^*A\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \;=\; |\,A\,|^2(1+0+1) = 2\,|\,A\,|^2 \;=\; 1$$

$$\Rightarrow \qquad |\,0> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad \text{for the eigenvalue } 0\,.$$

For the eigenvector corresponding to the largest eigenvalue,

$$\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \sqrt{2} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcl} -bi & = & \sqrt{2}\,a \\ ai - ci & = & \sqrt{2}\,b \\ bi & = & \sqrt{2}\,c \end{array}$$

Adding the top and bottom equations, we get $\sqrt{2}\,a + \sqrt{2}\,c = 0 \quad \Rightarrow \quad a = -c$. Using this in the middle equation, we get

$$ai + ai = \sqrt{2}\,b \quad \Rightarrow \quad \frac{2ai}{\sqrt{2}} = b \quad \Rightarrow \quad b = \sqrt{2}\,ai\,.$$

If we choose $a = 1$, then $b = \sqrt{2}\,i$, and $c = -1$, the eigenket is

$$|\sqrt{2}> = A \begin{pmatrix} 1 \\ \sqrt{2}\,i \\ -1 \end{pmatrix} \quad \Rightarrow \quad <\sqrt{2}\,|\sqrt{2}> = \left(1,\ -\sqrt{2}\,i,\ -1\right) A^* A \begin{pmatrix} 1 \\ \sqrt{2}\,i \\ -1 \end{pmatrix}$$

$$= |A|^2(1+2+1) \quad \Rightarrow \quad 4|A|^2 = 1 \quad \Rightarrow \quad |\sqrt{2}> = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2}i \\ -1 \end{pmatrix} \text{ for the eigenvalue } \sqrt{2}\,.$$

1–23. Find the normal modes of oscillation for a frictionless system of two identical masses connected to each other and outside walls by ideal springs with the same spring constant.

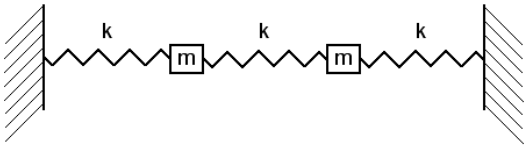

Figure 1–1. Two identical masses, three identical springs.

A brief excursion to classical mechanics is appropriate to explain the general meaning of an eigenvalue, and also to generally expose how the eigenvalue/eigenvector problem arises naturally from physical systems, including quantum mechanical systems.

Normal modes of oscillation are also known as natural frequencies, characteristic modes, and characteristic frequencies. Imagine displacing one or both masses. The masses may oscillate unpredictably at first, but given some time for the energy to be distributed throughout the system, this system will oscillate in one of two modes at one of two frequencies. These are the normal modes of oscillation, or just normal modes. Calculating eigenvalues in a quantum mechanical system is comparable to finding the normal modes in a classical mechanical system.

The ideal springs provide restoring forces $F = -kx$. Let the displacement of the mass on the left be x_1 and the mass on the right be x_2. The restoring force on the masses are

$$F_1 = -kx_1 + k\,(x_2 - x_1) \quad \Rightarrow \quad ma_1 = -2kx_1 + kx_2 \quad \Rightarrow \quad ma_1 + 2kx_1 - kx_2 = 0$$

$$F_2 = -kx_2 - k\,(x_2 - x_1) \quad \Rightarrow \quad ma_2 = kx_1 - 2kx_2 \quad \Rightarrow \quad ma_2 - kx_1 + 2kx_2 = 0$$

where the two equations on the right can be expressed as the matrix equation

$$\begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} + \begin{pmatrix} 2k & -k \\ -k & 2k \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$$

which when multiplied by $\begin{pmatrix} \frac{1}{m} & 0 \\ 0 & \frac{1}{m} \end{pmatrix}$ is

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} + \begin{pmatrix} \frac{2k}{m} & -\frac{k}{m} \\ -\frac{k}{m} & \frac{2k}{m} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$$

and since $a_i = -\omega^2 x_i$, this is

$$\begin{pmatrix} -\omega^2 & 0 \\ 0 & -\omega^2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \begin{pmatrix} \frac{2k}{m} & -\frac{k}{m} \\ -\frac{k}{m} & \frac{2k}{m} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0 \quad \Rightarrow \quad \begin{pmatrix} \frac{2k}{m} - \omega^2 & -\frac{k}{m} \\ -\frac{k}{m} & \frac{2k}{m} - \omega^2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0$$

which will have a non-trivial solution when the determinant of the matrix is zero, so

$$\det \begin{pmatrix} \frac{2k}{m} - \omega^2 & -\frac{k}{m} \\ -\frac{k}{m} & \frac{2k}{m} - \omega^2 \end{pmatrix} = 0 \quad \Rightarrow \quad \left(\frac{2k}{m} - \omega^2\right)^2 - \frac{k^2}{m^2} = 0$$

$$\Rightarrow \quad \frac{4k^2}{m^2} - \frac{4k}{m}\omega^2 + \omega^4 - \frac{k^2}{m^2} = 0 \quad \Rightarrow \quad \omega^4 - \frac{4k}{m}\omega^2 + \frac{3k^2}{m^2} = 0$$

$$\left(\omega^2 - \frac{3k}{m}\right)\left(\omega^2 - \frac{k}{m}\right) = 0 \quad \Rightarrow \quad \omega = \sqrt{\frac{3k}{m}}, \quad \omega = \sqrt{\frac{k}{m}}$$

are the normal modes of oscillation.

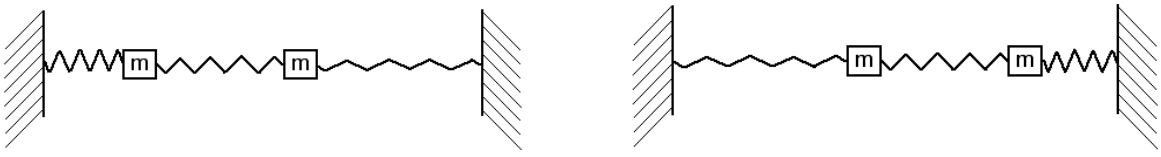

Figure 1–2. Normal mode for $\omega = \sqrt{\frac{k}{m}}$.

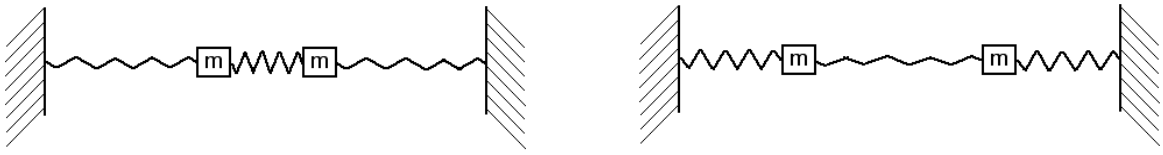

Figure 1–3. Normal mode for $\omega = \sqrt{\frac{3k}{m}}$.

Postscript: Notice that $\det(\mathcal{A} - \omega\mathcal{I}) = 0$ simply emerges. Its solutions are called normal modes, characteristics of the system, that are readily interpreted as eigenvalues. An analogy is that a quantum mechanical system exists only in a linear combination of states comparable to normal modes/eigenvalues, thus, only one of the "normal modes/eigenvalues" can be measured.

This system with only two normal modes lends itself directly to exposing how an eigenvalue/eigenvector problem naturally describes a physical system. The problem is more complicated

for an individual guitar string. Plucking a guitar string can initially set it vibrating unpredictably, however, it will quickly settle into a linear combination of the fundamental mode, the first overtone, the second overtone, and other overtones. Each possible mode of vibration is a normal mode/eigenvalue of that guitar string. There are an infinite number of modes of vibration for an "ideal" guitar string. The eigenvalues of this two mass system exist in $\mathbb{R}^2$. The eigenvalues of an ideal guitar string exist in $\mathbb{R}^\infty$. The eigenvalues of a quantum mechanical system also exist in $\mathbb{R}^\infty$, though a subspace may be used for some systems. The components and elements of the vectors and operators from which the quantum mechanical eigenvalues are extracted exist in $\mathbb{C}^\infty$, though the eigenvalues exist in $\mathbb{R}^\infty$. The normal modes of a guitar string are likely a better overall analogy to the eigenvalues of a realistic quantum mechanical system than the two mass/three spring system because of the infinity of eigenvalues intrinsic.

Calculating eigenvalues in a quantum mechanical system is comparable to finding the normal modes in a classical mechanical system.

1–24. What are the eigenvalues and eigenvectors for $\mathcal{D} \rightarrow \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}$?

The given $\mathcal{D}$ is a **diagonal operator**. This means that all non-zero elements are on the main diagonal, and all elements not on the main diagonal are zero. Notice that the non-zero elements are arbitrary. This problem provides a convenient and useful result.

$\det \begin{pmatrix} \alpha-\lambda & 0 & 0 \\ 0 & \beta-\lambda & 0 \\ 0 & 0 & \gamma-\lambda \end{pmatrix} = (\alpha-\lambda)(\beta-\lambda)(\gamma-\lambda)$ where the only non-zero contribution to the determinant is from the main diagonal, so the characteristic equation can be written

$$(\alpha-\lambda)(\beta-\lambda)(\gamma-\lambda) = 0 \quad \Rightarrow \quad \lambda = \alpha, \ \lambda = \beta, \text{ and } \lambda = \gamma.$$

This is a significant finding. The eigenvalues in a diagonal matrix are the elements on the main diagonal. The eigenvalues in a diagonal matrix are found by inspection. Eigenvectors are found

$$\begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \alpha \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} \alpha a &= \alpha a \\ \beta b &= \alpha b \\ \gamma c &= \alpha c \end{aligned}$$

where the top equation says $a = a$, so let $a = 1$. The second and third equations say that $b = c = 0$ in general. The middle equation can be written $(\beta-\alpha)\,b = 0$, and in general $\beta \neq \alpha$, thus $b = 0$. The same argument applies to the bottom equation which can be written $(\gamma-\alpha)\,c = 0$, and in general $\gamma \neq \alpha$, thus $c = 0$ and the eigenvector is $|\alpha> = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, which is already normalized. For the eigenvalue β,

$$\begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \beta \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} \alpha a &= \beta a \\ \beta b &= \beta b \\ \gamma c &= \beta c \end{aligned}$$

where the middle equation says $b = b$, so let $b = 1$. Since $\alpha \neq \beta$ and $\gamma \neq \beta$ in general, $a = c = 0$ and $|\beta> = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, which again is already normalized. For γ,

$$\begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \gamma \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} \alpha a &= \gamma a \\ \beta b &= \gamma b \\ \gamma c &= \gamma c \end{aligned}$$

$\Rightarrow \quad c = c$, so let $c = 1$ and $a = b = 0$ because $\alpha \neq \gamma$ and $\beta \neq \gamma$ in general, so $|\gamma> = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$, which is also conveniently already normalized.

Postscript: The vectors $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, and $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ are the **unit vectors** in $\mathbb{C}^3$. The vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ are the **unit vectors** in $\mathbb{C}^2$. The vectors $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$, and $\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$ are the **unit vectors** in $\mathbb{C}^4$, and $\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$, $\begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$, and $\begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}$ are the **unit vectors** in $\mathbb{C}^\infty$.

The eigenvalues of a diagonal operator are the elements on the principal diagonal, and the eigenvectors are the unit vectors with the 1 in the position corresponding to the position of the eigenvalue in the operator. So, what are the eigenvalues and eigenvectors of $\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix}$?

$|2> = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|3> = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, and $|4> = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ by inspection. For $\begin{pmatrix} \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 59 \end{pmatrix}$,

$|\sqrt{3}> = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|0> = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, and $|59> = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ by inspection. For $\begin{pmatrix} -\frac{\hbar}{2} & 0 \\ 0 & \frac{\hbar}{2} \end{pmatrix}$,

$|-\frac{\hbar}{2}> = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|\frac{\hbar}{2}> = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, by inspection. Read the eigenvalue off of the main diagonal and its eigenvector is the corresponding unit vector. The last is a spin $\frac{1}{2}$ operator, by the way.

This problem is in $\mathbb{C}^3$, but could have been done in $\mathbb{C}^4$, with a few more steps, or even $\mathbb{C}^\infty$

with a bit more writing. The Hamiltonian for a quantum mechanical simple harmonic oscillator is

$$\mathcal{H} \;=\; \begin{pmatrix} \frac{1}{2}\,\hbar\omega & 0 & 0 & 0 & \dots \\ 0 & \frac{3}{2}\,\hbar\omega & 0 & 0 & \dots \\ 0 & 0 & \frac{5}{2}\,\hbar\omega & 0 & \dots \\ 0 & 0 & 0 & \frac{7}{2}\,\hbar\omega & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\Rightarrow \qquad |\,\frac{1}{2}\,\hbar\omega> \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |\,\frac{3}{2}\,\hbar\omega> \;=\; \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad |\,\frac{5}{2}\,\hbar\omega> \;=\; \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}, \quad |\,\frac{7}{2}\,\hbar\omega> \;=\; \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix}, \quad \dots$$

are the eigenvalues and corresponding eigenvectors.

Working with diagonal operators is particularly convenient. The intent is to develop a method of diagonalizing as many operators as possible. The method of diagonalizing operators is broad and quite useful, but it cannot be applied universally. Not all matrices can be diagonalized, however, all Hermitian operators can be diagonalized!

1–25. Diagonalize $\qquad \mathcal{C} \;\rightarrow\; \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} \qquad$ and $\qquad \mathcal{H} \;\rightarrow\; \begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix}.$

Some matrices, and all Hermitian operators, can be diagonalized by a **unitary transformation**. A **unitary operator** is an operator whose product with its adjoint is the identity,

$$\mathcal{U}\,\mathcal{U}^{\dagger} \;=\; \mathcal{U}^{\dagger}\mathcal{U} \;=\; \mathcal{I}\,.$$

Multiplication of a vector by a unitary operator preserves the norm of a vector. A unitary operation is analogous to an identity operation with a rotation.

All Hermitian matrices can be diagonalized[4] using a **unitary transformation**

$$\mathcal{U}^{\dagger}\mathcal{A}\,\mathcal{U} \;=\; \mathcal{A}'$$

where the operator $\mathcal{A}'$ is diagonal. The appropriate unitary operator to diagonalize $\mathcal{A}$ is constructed from its eigenvectors. Our convention is to form $\mathcal{U}$ keeping the eigenvectors in columns, place them in a matrix from left to right in the order of the eigenvector corresponding to the lowest eigenvalue to the eigenvector corresponding to the highest eigenvalue. In problem 1–21, the eigenvectors of $\mathcal{C}$ were found

$$|-1> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |7> = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix} \;\Rightarrow\; \mathcal{U} \;=\; \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} \;\Rightarrow\; \mathcal{U}^{\dagger} \;=\; \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix}$$

[4] Byron and Fuller, *Mathematics of Classical and Quantum Physics* (Dover Publications, Inc., New York, 1969), p. 165–168.

$$\Rightarrow \quad \mathcal{U}^\dagger \mathcal{C}\, \mathcal{U} = \mathcal{U}^\dagger \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix} = \mathcal{U}^\dagger \begin{pmatrix} \frac{3}{\sqrt{2}} - \frac{4}{\sqrt{2}} & \frac{3}{\sqrt{2}} + \frac{4}{\sqrt{2}} \\ -\frac{4i}{\sqrt{2}} + \frac{3i}{\sqrt{2}} & -\frac{4i}{\sqrt{2}} - \frac{3i}{\sqrt{2}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{7}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & -\frac{7i}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} -1/2 - 1/2 & 7/2 - 7/2 \\ -1/2 + 1/2 & 7/2 + 7/2 \end{pmatrix} = \begin{pmatrix} -1 & 0 \\ 0 & 7 \end{pmatrix}$$

from which $|-1> = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|7> = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ by inspection.

From problem 1–21,

$$|0> = \frac{1}{\sqrt{5}} \begin{pmatrix} 2i \\ 0 \\ 1 \end{pmatrix}, \quad |1> = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |5> = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 0 \\ 2i \end{pmatrix} \quad \Rightarrow \quad \mathcal{U} = \begin{pmatrix} \frac{2i}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{5}} & 0 & \frac{2i}{\sqrt{5}} \end{pmatrix}$$

$$\Rightarrow \quad \mathcal{U}^\dagger = \begin{pmatrix} -\frac{2i}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{5}} & 0 & -\frac{2i}{\sqrt{5}} \end{pmatrix} \quad \Rightarrow \quad \mathcal{U}^\dagger \mathcal{H}\, \mathcal{U} = \mathcal{U}^\dagger \begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix} \begin{pmatrix} \frac{2i}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{5}} & 0 & \frac{2i}{\sqrt{5}} \end{pmatrix}$$

$$= \mathcal{U}^\dagger \begin{pmatrix} \frac{2i}{\sqrt{5}} - \frac{2i}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} + \frac{4}{\sqrt{5}} \\ 0 & 1 & 0 \\ -\frac{4}{\sqrt{5}} + \frac{4}{\sqrt{5}} & 0 & \frac{2i}{\sqrt{5}} + \frac{8i}{\sqrt{5}} \end{pmatrix} = \begin{pmatrix} -\frac{2i}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{5}} & 0 & -\frac{2i}{\sqrt{5}} \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{5}{\sqrt{5}} \\ 0 & 1 & 0 \\ 0 & 0 & \frac{10i}{\sqrt{5}} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & -\frac{10i}{5} + \frac{10i}{5} \\ 0 & 1 & 0 \\ 0 & 0 & \frac{5}{5} + \frac{20}{5} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 5 \end{pmatrix} \quad \Rightarrow \quad |0> = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1> = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |5> = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

by inspection.

Postscript: A primary advantage of the method of diagonalization is that it exists. Obtaining eigenvalues from which to get eigenvectors by the manual method, and then using those eigenvectors to build unitary operators to diagonalize the original operator to get eigenvalues which are already known is circular, at best. Other than to understand a process and expose the symbology, the intent is to exploit the fact that diagonalization applies to any Hermitian operator rather than participate in circular mathematical mechanics. Diagonalizing an operator to obtain eigenvectors which are unit vectors is a non-circular mathematical advantage of the process, nevertheless.

The operator and eigenvectors were transformed, but the eigenvalues were not. The eigenvalues of an operator are invariant under a unitary transformation. A unitary transformation built from the eigenvectors of a Hermitian operator "rotates," or re-orients, the eigenvectors of that operator to align with the unit vectors in the appropriate space without affecting the eigenvalues. Proof of the invariance of eigenvalues under a unitary transformation is problem 3–13.

All Hermitian operators can be diagonalized. Not all non-Hermitian operators can be diagonalized. Doubters should attempt to diagonalize $\mathcal{F} \rightarrow \begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}$ for which $|2> = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $|3> = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$ were found to be the normalized eigenvectors.

1–26. Show that $\left(\mathcal{BC}\right)^{\dagger} = \mathcal{C}^{\dagger}\mathcal{B}^{\dagger}$.

The adjoint of a product of two operators is the product of the adjoints in reverse order.

This problem develops a useful fact and also exposes the convention of Dirac notation that anything between the "$<$" and a"$|$" in a bra are considered conjugated in the case of scalars or transpose conjugated in the case of vectors and operators. It also demonstrates the concepts that if removed from a bra, the object removed must be explicitly denoted as a conjugate/adjoint, and that the object removed is located at the far right.

$<v\mathcal{BC}| = <v|\left(\mathcal{BC}\right)^{\dagger}$, but removing $\mathcal{C}$ and $\mathcal{B}$ individually, $<v\mathcal{BC}| = <v\mathcal{B}|\mathcal{C}^{\dagger} = <v|\mathcal{C}^{\dagger}\mathcal{B}^{\dagger}$

where $\mathcal{B}^{\dagger}$ is located to the far right, thus $<v|\left(\mathcal{BC}\right)^{\dagger} = <v|\mathcal{C}^{\dagger}\mathcal{B}^{\dagger} \quad \Rightarrow \quad \left(\mathcal{BC}\right)^{\dagger} = \mathcal{C}^{\dagger}\mathcal{B}^{\dagger}$.

Postscript: That an operator removed from a bra must be located at the far right is the property of commutivity. Two more proofs that $\left(\mathcal{BC}\right)^{\dagger} = \mathcal{C}^{\dagger}\mathcal{B}^{\dagger}$ are provided in chapter 3.

1–27. Use a unitary transformation to show that the eigenvalues of a Hermitian operator are real.

The previous problem developed a useful fact that is used in this problem demonstrating the utility of the method of diagonalization. The symbolic use of an appropriate unitary transformation, known to exist for every Hermitian operator per the previously cited work of Byron and Fuller, is illustrated in this problem. This problem shows some of the power of method of diagonalization.

This is a two part proof. First, the elements on the main diagonal of a Hermitian operator are demonstrated to be real. That a scalar is equal to its conjugate means that it is a real number. The second part of the proof relies on the fact that all Hermitian operators can be diagonalized.

Hermitian means $\mathcal{A} = \mathcal{A}^{\dagger}$ so $\mathcal{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \mathcal{A}^{\dagger} = \begin{pmatrix} a_{11}^{*} & a_{21}^{*} & a_{31}^{*} & \cdots \\ a_{12}^{*} & a_{22}^{*} & a_{32}^{*} & \cdots \\ a_{13}^{*} & a_{23}^{*} & a_{33}^{*} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$

for Hermitian $\mathcal{A}$, from which we can conclude $a_{ii} = a_{ii}^{*}$, so that the elements on the main diagonal are necessarily real.

Consider the unitary transformation $\mathcal{U}^{\dagger}\mathcal{A}\mathcal{U}$ diagonalizing $\mathcal{A}$, where $\mathcal{U}$ is constructed from the eigenvectors of $\mathcal{A}$. The adjoint of a product is the product of the adjoints in reverse order,

$$\left(\mathcal{U}^{\dagger}\mathcal{A}\mathcal{U}\right)^{\dagger} = \left(\mathcal{U}\right)^{\dagger}\left(\mathcal{A}\right)^{\dagger}\left(\mathcal{U}^{\dagger}\right)^{\dagger} = \mathcal{U}^{\dagger}\mathcal{A}^{\dagger}\mathcal{U} = \mathcal{U}^{\dagger}\mathcal{A}\mathcal{U}$$

thus, the diagonal operator $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ is Hermitian. The eigenvalues of the diagonal operator $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ are on the principal diagonal, and the elements on the principal diagonal of any Hermitian operator where just shown to be real, therefore the eigenvalues of $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ are real. Because the unitary transformation does not affect the eigenvalues, the eigenvalues of $\mathcal{A}$ are identical to those of $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$, so the eigenvalues of any Hermitian operator $\mathcal{A}$ must be real.

Postscript: Notice that it is not necessary to identify the eigenvectors/basis vectors of $\mathcal{A}$.

Again, problem 3–13 shows that unitary transformation does not affect eigenvalues. Eigenvalues are properties of the operator, regardless of its form. $\mathcal{A}$ and $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ are actually the same operator represented in different bases. Eigenvectors differ, but eigenvalues do not.

1–28. What is a basis?

A **basis** is a set of vectors such that every vector in the space can be uniquely expressed as a linear combination of the basis vectors. A basis is a generalization of a choice of coordinate system and frame of reference to $\mathbb{C}^n$, where $1 < n \leq \infty$.

All vectors in $\mathbb{R}^2$ can be expressed as a linear combination of the unit vectors $\widehat{x}$, $\widehat{y}$ in Cartesian coordinates, so these unit vectors form a basis in $\mathbb{R}^2$. The unit vectors in polar coordinates, $\widehat{r}$ and $\widehat{\theta}$, is also a basis in $\mathbb{R}^2$. Any vector quantity in $\mathbb{R}^2$ can be uniquely expressed as the sum of multiples of $\widehat{x}$ and $\widehat{y}$, or different multiples of $\widehat{r}$ and $\widehat{\theta}$. The Cartesian unit vectors $\widehat{x}$, $\widehat{y}$, and $\widehat{z}$ form a basis in $\mathbb{R}^3$, as do the spherical polar unit vectors $\widehat{r}$, $\widehat{\theta}$, and $\widehat{\phi}$.

The same vector will have different components in different bases. For instance, a force of 10 N at 45° to the horizontal can be described $\begin{pmatrix} 5\sqrt{2} \\ 5\sqrt{2} \end{pmatrix}$ in Cartesian coordinates, but the same vector is described $\begin{pmatrix} 10 \\ \pi/4 \end{pmatrix}$ when the basis is changed to polar coordinates. The components of a fixed vector are different in different bases.

The definition of a basis is the same for spaces over a complex field. For instance, in $\mathbb{C}^2$, any two vectors from which every other vector in the space can be constructed constitute a basis in $\mathbb{C}^2$. $\mathbb{C}^3$ requires a minimum of three vectors to construct every other vector in the space. $\mathbb{C}^n$ requires a minimum of n vectors to form a basis.

The eigenvalues of a Hermitian operator are real numbers. All Hermitian operators can be diagonalized. A third advantage of Hermitian operators is their eigenvectors constitute a basis in the appropriate $\mathbb{C}^n$. The eigenvectors of a Hermitian operator constitute a basis for the space in which they exist!

That any vector in $\mathbb{C}^2$ can be constructed from $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ should be straightforward. For instance

$$|\,k> \;=\; \begin{pmatrix} 2+3i \\ 5-4i \end{pmatrix} \;=\; (2+3i)\begin{pmatrix} 1 \\ 0 \end{pmatrix} \;+\; (5-4i)\begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

These unit vectors were obtained in the last problem by diagonalizing $\mathcal{C} \rightarrow \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}$ whose

eigenvectors were found to be $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}$ and $\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}$, or just $\begin{pmatrix}1\\ i\end{pmatrix}$ and $\begin{pmatrix}1\\ -i\end{pmatrix}$ in unnormalized form. That any vector in $\mathbb{C}^2$ can be constructed from $\begin{pmatrix}1\\ i\end{pmatrix}$ and $\begin{pmatrix}1\\ -i\end{pmatrix}$ is more difficult to picture, nevertheless, these eigenvectors of a Hermitian operator are guaranteed to form a basis. Just like the vector force 10 N at 45° to the horizontal has different components in different bases, the elements of the operator $\mathcal{C}$ are $\begin{pmatrix}-1 & 0\\ 0 & 7\end{pmatrix}$ using the basis vectors $\begin{pmatrix}1\\ 0\end{pmatrix}$ and $\begin{pmatrix}0\\ 1\end{pmatrix}$, though it is represented $\begin{pmatrix}3 & 4i\\ -4i & 3\end{pmatrix}$ using the basis vectors $\begin{pmatrix}1\\ i\end{pmatrix}$ and $\begin{pmatrix}1\\ -i\end{pmatrix}$; different basis vectors require different elements to convey the same information.

All the information that can be known about a system is encoded in its state vector, $|\psi>$. Just as a force of 10 N at 45° to the horizontal can be described $\begin{pmatrix}5\sqrt{2}\\ 5\sqrt{2}\end{pmatrix}$ in the Cartesian basis or $\begin{pmatrix}10\\ \pi/4\end{pmatrix}$ in the polar basis, the state vector $|\psi>$ has different components in different bases, which means only that the appearance of the information it contains will vary depending on the basis used, the actual information it contains is invariant.

The preferred strategy is to diagonalize a Hermitian operator, which frequently can be done symbolically, and use the unit vectors appropriate to the space as the basis.

Postscript: A set of vectors such that every vector in the space can be uniquely expressed as a linear combination is said to **span** the space, or is **complete**. That a set of vectors span a space or is complete are equivalent to stating that the set of vectors constitute a basis.

Another description of the unitary transformations $\mathcal{U}^\dagger \mathcal{A}\, \mathcal{U}$ where $\mathcal{U}$ is unitary, is a **change of basis**. A unitary transformation changes the vectors used to span the space.

The vectors in a complex vector space are abstract objects. Accept them as the abstractions that they are. At least a portion of the difficulty with the concept of a basis in a complex vector space seems to be "picturing" the vectors as is common in $\mathbb{R}^2$ or $\mathbb{R}^3$. An Argand diagram is a two dimensional diagram using the x axis to plot the real part of a complex number and the y axis to plot the imaginary part. Argand diagrams for $2+5i$ and $3+4i$ are seen in figure 1–4. Notice that it takes two dimensions to picture a complex scalar. Now try to picture $|c> = \begin{pmatrix}2+5i\\ 3+4i\end{pmatrix}$.

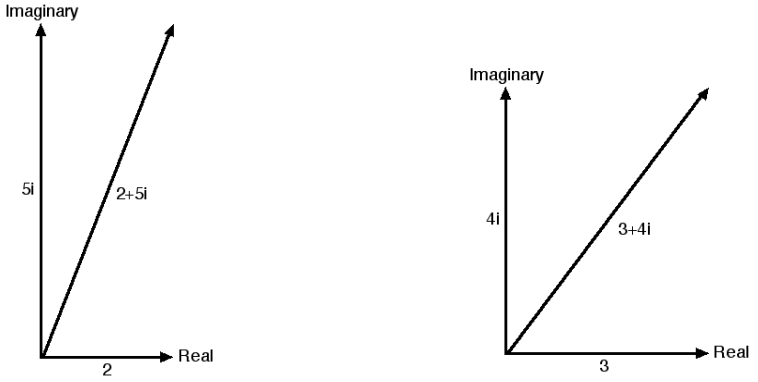

Figure 1–4. Argand diagrams for $2+5i$ and $3+4i$.

Imagine rotating one or both of the Argand diagrams in space so that the two origins coincide and all four axes are mutually exclusive, that is, at right angles or equivalent. Four mutually perpendicular (or equivalent) axes seem possible only as an abstraction. A vector in $\mathbb{C}^n$ requires n real dimensions and n imaginary dimensions for a total of $2n$ dimensions. Pictures in $\mathbb{R}^n$ for $n > 3$ are problematic. Pictures in $\mathbb{C}^n$ for $n > 1$ are also problematic and complicated by the fact each component effectively requires two dimensions.

The concept of a basis spanning a space is essential, however, it is rare that basis vectors are identified, other than the unit vectors, just as it was unnecessary to identify eigenvectors/basis vectors of the original $\mathcal{A}$ in the previous problem. The unit vectors are particularly convenient bases for their spaces. An example for $\mathbb{C}^2$ was given above.

$$|\,v> \;=\; \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \;=\; \alpha \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \;+\; \beta \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \;+\; \gamma \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad \text{in } \mathbb{C}^3\,, \text{ and in } \mathbb{C}^4\,,$$

$$|\,v> \;=\; \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} \;=\; \alpha \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \;+\; \beta \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \;+\; \gamma \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \;+\; \delta \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}\,,$$

which is a process that can be imagined in $\mathbb{C}^n$ or even $\mathbb{C}^\infty$. The unit vectors are the basis vectors of a diagonal matrix. That any Hermitian operator can be diagonalized is assurance that the unit vectors appropriate to the space is one possible basis.

The Hilbert space is basis independent. The Hilbert space contains all bases. The three most frequent references to bases will be to the **position basis**, the **momentum basis**, and the **energy basis**. That sets of vectors exist that span position, momentum, and energy spaces is a key concept. The state vector describing the system and the operators describing the observables will have different components and elements in different bases.

1–29. What are the properties of orthogonality and orthonormality?

Orthogonality is a generalization of mutual right angles to more than three dimensions and to $\mathbb{C}^n$.

The unit vectors $\widehat{x}$, $\widehat{y}$ in Cartesian coordinates in $\mathbb{R}^2$ are at right angles. Calculate the dot product $\left(4\widehat{x} + 5\widehat{y}\right) \cdot \left(2\widehat{x} - 3\widehat{y}\right)$. That is the x component times the x component added to the y component times the y component or $8 - 15 = -7$ is the dot product of these two vectors. A picture is the right angle projection of one vector onto the other. What is $\left(2\widehat{x} + 5\widehat{y}\right) \cdot \left(5\widehat{x} - 2\widehat{y}\right)$? Well, it's $10 - 10 = 0$, and this means the right angle projection of one vector onto another is zero, or in $\mathbb{R}^2$, these two vectors are perpendicular. The property of perpendicularity is more difficult to picture in three dimensions, but the dot product $\left(4\,\widehat{x} + 5\,\widehat{y} + 1\,\widehat{z}\right) \cdot \left(2\,\widehat{x} - 3\,\widehat{y} + 7\,\widehat{z}\right) = 0$ so these two vectors are perpendicular in $\mathbb{R}^3$.

An inner product is a generalization of dot product to more than three dimensions and to $\mathbb{C}^n$. What is the inner product of $|-1> \;=\; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$ and $|\,7> \;=\; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$, the eigenvectors of $\mathcal{C}$ from problem 1–21?

$$<-1\,|\,7> \;=\; \left(1\,,\;\; -i\right) \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \;=\; \frac{1}{2}(1 - 1) \;=\; 0$$

which is the analogy of perpendicular, or at "right angles" in $\mathbb{C}^2$. The terminology is that these two eigenvectors are **orthogonal**. It does not lend itself to a picture, as with many concepts in a complex vector space. What are the inner products of $|0> = \frac{1}{\sqrt{5}}\begin{pmatrix}2i\\0\\1\end{pmatrix}$, $|1> = \begin{pmatrix}0\\1\\0\end{pmatrix}$ and $|5> = \frac{1}{\sqrt{5}}\begin{pmatrix}1\\0\\2i\end{pmatrix}$, the eigenvectors of $\mathcal{H}$ from problem 1–21?

$$<0|1> = \big(-2i,\ 0,\ 1\big)\frac{1}{\sqrt{5}}\begin{pmatrix}0\\1\\0\end{pmatrix} = \frac{1}{\sqrt{5}}\big(0+0+0\big) = 0\,,$$

$$<0|5> = \big(-2i,\ 0,\ 1\big)\frac{1}{\sqrt{5}}\frac{1}{\sqrt{5}}\begin{pmatrix}1\\0\\2i\end{pmatrix} = \frac{1}{5}\big(-2i+0+2i\big) = 0\,,$$

$$<1|5> = \big(0,\ 1,\ 0\big)\frac{1}{\sqrt{5}}\begin{pmatrix}1\\0\\2i\end{pmatrix} = \frac{1}{\sqrt{5}}\big(0+0+0\big) = 0\,.$$

Each eigenvector is orthogonal to the others. These examples in $\mathbb{C}^2$ and $\mathbb{C}^3$ cannot be translated to an $\mathbb{R}^3$ equivalent where pictures are formed. However, the extension of a dot product in $\mathbb{R}^2$ or $\mathbb{R}^3$ to $\mathbb{C}^n$ seems straightforward given that the inherent abstractions are accepted. Orthogonality of vectors allows for infinite mutually exclusive direction analogs in a complex vector space.

If $<i|j> = 0$, the vectors $|i>$ and $|j>$ are said to be orthogonal.

Orthonormal means orthogonal and normalized. If $<i|j> = 0$, the vectors $|i>$ and $|j>$ are orthogonal, but if also $<i|i> = 1$ for all i, the vectors are orthonormal. Any orthogonal set can be made orthonormal by the process of normalization. In fact, because these two sets of vectors in $\mathbb{C}^2$ and $\mathbb{C}^3$ were normalized in problem 1–21, they are already orthonormal.

$$<-1|-1> = \big(1,\ -i\big)\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} = \frac{1}{2}\big(1+1\big) = 1\,,$$

$$<7|7> = \big(1,\ i\big)\frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = \frac{1}{2}\big(1+1\big) = 1\,.$$

$$<0|0> = \big(-2i,\ 0,\ 1\big)\frac{1}{\sqrt{5}}\frac{1}{\sqrt{5}}\begin{pmatrix}2i\\0\\1\end{pmatrix} = \frac{1}{5}\big(4+0+1\big) = 1\,,$$

$$<1|1> = \big(0,\ 1,\ 0\big)\begin{pmatrix}0\\1\\0\end{pmatrix} = 0+1+0 = 1\,,$$

$$<5|5> = \big(1,\ 0,\ -2i\big)\frac{1}{\sqrt{5}}\frac{1}{\sqrt{5}}\begin{pmatrix}1\\0\\2i\end{pmatrix} = \frac{1}{5}\big(1+0+4\big) = 1\,.$$

Postscript: $<i\,|\,j> = \delta_{ij}$ is a concise statement of orthonormality. The Kronecker delta is

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j\,, \\ 0 & \text{if } i \neq j\,. \end{cases}$$

Thus, the statement $<i\,|\,j> = \delta_{ij}$ says that if the inner product of like vectors is one, and the inner product of unlike vectors is zero, the vectors are orthonormal.

Notice that $\mathcal{C}$ and $\mathcal{H}$ from problem 1–21 are Hermitian. A fourth advantage of Hermiticity is that the eigenvectors of a Hermitian operator are orthogonal! That Hermitian operators have eigenvectors that are intrinsically orthogonal and can be made orthonormal by the process of normalization is a significant factor in quantum mechanical calculation.

Orthogonality presents an intrinsically abstract concept. There are a variety of coordinate systems in $\mathbb{R}^3$ with mutually exclusive basis vectors. Cartesian coordinates, spherical polar coordinates, and circular cylindrical coordinates are three commonly encountered examples. Right angles, however, in $\mathbb{R}^4$ or $\mathbb{R}^n$ for $n > 3$ are difficult, or impossible, to picture. That right angle analogies exist for $\mathbb{C}^n$ for $1 < n \leq \infty$ is acceptable only as the abstract concept that it is.

Notice that though analogies may be made to various features and properties in $\mathbb{R}^2$ and $\mathbb{R}^3$, the vocabulary appropriate to a complex vector space is more general. The concept of length generalizes to that of a **norm**, the dot or scalar product generalizes to an **inner product**, a coordinate system generalizes to a **basis**, and mutual perpendicularity generalizes to **orthogonality**. The terminology of $\mathbb{R}^3$ is inadequate for $\mathbb{C}^n$, suggesting that abstraction is required.

1–30. Show that the eigenvectors of a Hermitian operator with distinct eigenvalues are orthogonal.

This problem uses the eigenvalue/eigenvector equation, the fact $<v\,|\,w> = <w\,|\,v>^*$ in general, the fact eigenvalues of a Hermitian operator are real, and the fact that $<b\,|\,a> = 0$ means the two vectors are orthogonal.

Let $\mathcal{A}\,|\,a> = \alpha\,|\,a>$ and $\mathcal{A}\,|\,b> = \beta\,|\,b>$ represent two eigenvalue/eigenvector equations for the Hermitian operator $\mathcal{A}$. Forming an inner product with opposing eigenvectors,

$$<b\,|\,\mathcal{A}\,|\,a> = <b\,|\,\alpha\,|\,a> \quad \text{and} \quad <a\,|\,\mathcal{A}\,|\,b> = <a\,|\,\beta\,|\,b>$$

and since $<v\,|\,w> = <w\,|\,v>^*$ in general,

$$<b\,|\,\mathcal{A}\,|\,a> = <a\,|\,\mathcal{A}\,|\,b>^* \quad \Rightarrow \quad <b\,|\,\alpha\,|\,a> = <a\,|\,\beta\,|\,b>^*$$

$$\Rightarrow \quad \alpha <b\,|\,a> = \beta^* <a\,|\,b>^* = \beta^* <b\,|\,a> = \beta <b\,|\,a>$$

because the eigenvalues of a Hermitian operator are real, so

$$\alpha <b\,|\,a> - \beta <b\,|\,a> = 0 \quad \Rightarrow \quad \big(\alpha - \beta\big) <b\,|\,a> \quad \Rightarrow \quad <b\,|\,a> = 0$$

meaning the eigenvectors are orthogonal given that $\alpha \neq \beta$, meaning distinct eigenvalues, for all $|\,a>$ and $|\,b>$ that are eigenvectors of a Hermitian $\mathcal{A}$.

Postscript: Notice that $\alpha \neq \beta$, distinct eigenvalues, is a necessary condition for this reduction. Chapter 3 discusses the eigenvectors of a Hermitian operator with non-distinct eigenvalues.

1–31. (a) Show that $\mathcal{W} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 \\ i & -i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}$ is unitary.

(b) Perform the unitary transformation $\mathcal{W}^\dagger \mathcal{H} \mathcal{W}$ where $\mathcal{H} = \begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix}$.

(c) Find the eigenvalues and eigenvectors of $\mathcal{W}^\dagger \mathcal{H} \mathcal{W}$.

(d) Compare the results of part (c) with the results of previous problems for the given $\mathcal{H}$.

This problem attempts to further clarify the meaning of a basis and additionally illustrate the utility of diagonalization. The given $\mathcal{W}$ is unitary meaning $\mathcal{W}^\dagger \mathcal{W} = \mathcal{I}$, the unitary transformation $\mathcal{W}^\dagger \mathcal{H} \mathcal{W}$ provides an apparently unrelated matrix operator (though it actually contains the same information as the given $\mathcal{H}$), and this apparently unrelated matrix will have the same eigenvalues but different eigenvectors than the given $\mathcal{H}$. After completing part (c), there are three versions of $\mathcal{H}$ available. Each of the three apparently different matrices factually has the same eigenvalues but different eigenvectors; these are the same operator expressed in different bases.

A unitary transformation rotates (re-orients) the eigenvectors while preserving all lengths (length analogs). A unitary transformation constructed from the eigenvectors of the operator being transformed rotates (re-orients) the eigenvectors to align with unit vectors. The given $\mathcal{W}$ is constructed from the eigenvectors of an operator other than the given $\mathcal{H}$, thus the unitary transformation $\mathcal{W}^\dagger \mathcal{H} \mathcal{W}$ rotates (re-orients) $\mathcal{H}$ to an arbitrary orientation.

(a) $\mathcal{W} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 \\ i & -i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \quad \Rightarrow \quad \mathcal{W}^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i & 0 \\ 1 & i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}$

$$\Rightarrow \mathcal{W}^\dagger\mathcal{W} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i & 0 \\ 1 & i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 \\ i & -i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+1 & 1-1 & 0 \\ 1-1 & 1+1 & 0 \\ 0 & 0 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(b) $\mathcal{W}^\dagger \mathcal{H} \mathcal{W}$

$$= \mathcal{W}^\dagger \begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 \\ i & -i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i & 0 \\ 1 & i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & -2\sqrt{2}\,i \\ i & -i & 0 \\ 2i & 2i & 4\sqrt{2} \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1+1 & 1-1 & -2\sqrt{2}\,i \\ 1-1 & 1+1 & -2\sqrt{2}\,i \\ 2\sqrt{2}\,i & 2\sqrt{2}\,i & 8 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 & 0 & -2\sqrt{2}\,i \\ 0 & 2 & -2\sqrt{2}\,i \\ 2\sqrt{2}\,i & 2\sqrt{2}\,i & 8 \end{pmatrix} = \begin{pmatrix} 1 & 0 & -\sqrt{2}\,i \\ 0 & 1 & -\sqrt{2}\,i \\ \sqrt{2}\,i & \sqrt{2}\,i & 4 \end{pmatrix}.$$

(c) $\det \begin{pmatrix} 1-\alpha & 0 & -\sqrt{2}\,i \\ 0 & 1-\alpha & -\sqrt{2}\,i \\ \sqrt{2}\,i & \sqrt{2}\,i & 4-\alpha \end{pmatrix} = (1-\alpha)^2(4-\alpha)-(1-\alpha)2-(1-\alpha)2 = 4-9\alpha+6\alpha^2-\alpha^3-4+4\alpha$

$\Rightarrow \quad \alpha^3 - 6\alpha^2 + 5\alpha \;=\; 0 \quad \Rightarrow \quad \alpha(\alpha-1)(\alpha-5) \;=\; 0 \quad \Rightarrow \quad 0\,,\ 1\,,\ 5$ are the eigenvalues. Notice that these are the same as the eigenvalues of $\mathcal{H}$. The eigenvectors, however, will differ.

$$\begin{pmatrix} 1 & 0 & -\sqrt{2}\,i \\ 0 & 1 & -\sqrt{2}\,i \\ \sqrt{2}\,i & \sqrt{2}\,i & 4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \;=\; 0 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{array}{r} a - \sqrt{2}\,ic \;=\; 0 \\ b - \sqrt{2}\,ic \;=\; 0 \\ \sqrt{2}\,ia + \sqrt{2}\,ib + 4c \;=\; 0 \end{array}$$

$$\Rightarrow \quad c = 1 \quad \Rightarrow \quad a = b = \sqrt{2}\,i \quad \Rightarrow \quad |\,0> \;=\; \frac{1}{\sqrt{5}} \begin{pmatrix} \sqrt{2}\,i \\ \sqrt{2}\,i \\ 1 \end{pmatrix}.$$

$$\begin{pmatrix} 1 & 0 & -\sqrt{2}\,i \\ 0 & 1 & -\sqrt{2}\,i \\ \sqrt{2}\,i & \sqrt{2}\,i & 4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \;=\; 1 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{array}{r} a - \sqrt{2}\,ic \;=\; a \\ b - \sqrt{2}\,ic \;=\; b \\ \sqrt{2}\,ia + \sqrt{2}\,ib + 4c \;=\; c \end{array}$$

$\Rightarrow \quad c \;=\; 0$ and $a \;=\; 1 \quad \Rightarrow \quad b \;=\; -1$ where the bottom equation reduces to $a + b \;=\; 0$

requiring $b \;=\; -1$ for $a \;=\; 1 \quad \Rightarrow \quad |\,1> \;=\; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$

$$\begin{pmatrix} 1 & 0 & -\sqrt{2}\,i \\ 0 & 1 & -\sqrt{2}\,i \\ \sqrt{2}\,i & \sqrt{2}\,i & 4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} \;=\; 5 \begin{pmatrix} a \\ b \\ c \end{pmatrix} \Rightarrow \begin{array}{r} a - \sqrt{2}\,ic \;=\; 5a \\ b - \sqrt{2}\,ic \;=\; 5b \\ \sqrt{2}\,ia + \sqrt{2}\,ib + 4c \;=\; 5c \end{array} \Rightarrow \begin{array}{r} -\sqrt{2}\,ic \;=\; 4a \\ -\sqrt{2}\,ic \;=\; 4b \\ \sqrt{2}\,ia + \sqrt{2}\,ib \;=\; c \end{array}$$

let $a \;=\; 1 \quad \Rightarrow \quad c \;=\; 2\sqrt{2}\,i \quad \Rightarrow \quad b \;=\; 1 \quad \Rightarrow \quad |\,5> \;=\; \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 1 \\ 2\sqrt{2}\,i \end{pmatrix}.$

(d) Three versions of $\mathcal{H}$ are now available,

$$\begin{pmatrix} 1 & 0 & -\sqrt{2}\,i \\ 0 & 1 & -\sqrt{2}\,i \\ \sqrt{2}\,i & \sqrt{2}\,i & 4 \end{pmatrix} \Rightarrow |\,0> = \frac{1}{\sqrt{5}} \begin{pmatrix} \sqrt{2}\,i \\ \sqrt{2}\,i \\ 1 \end{pmatrix},\ |\,1> = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix},\ |\,5> = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 1 \\ 2\sqrt{2}\,i \end{pmatrix},$$

$$\begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix} \quad \Rightarrow \quad |\,0> \;=\; \frac{1}{\sqrt{5}} \begin{pmatrix} 2i \\ 0 \\ 1 \end{pmatrix}, \quad |\,1> \;=\; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\,5> \;=\; \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 0 \\ 2i \end{pmatrix},$$

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 5 \end{pmatrix} \quad \Rightarrow \quad |\,0> \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\,1> \;=\; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\,5> \;=\; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

Each operator contains the same information. The operator originally presented is the second. The first and third operators have been rotated (re-oriented) to two different orientations. The diagonal form has been re-oriented so that its eigenvectors align with the unit vectors. Each has the same eigenvalues. Each operator has eigenvectors guaranteed to span $\mathbb{C}^3$ (notice that all three versions are Hermitian) so each set of eigenvectors constitute a basis. The diagonal form, where

eigenvalues and eigenvectors are available by inspection and the unit vectors are comparable to the $\widehat{x}$, $\widehat{y}$, $\widehat{z}$ of introductory physics for the appropriate space, offers distinct advantages.

Each set of eigenvectors for all three versions of $\mathcal{H}$ form a basis in $\mathbb{C}^3$ in the same sense the Cartesian unit vectors $\widehat{x}$, $\widehat{y}$, and $\widehat{z}$ or the spherical polar unit vectors $\widehat{r}$, $\widehat{\theta}$, and $\widehat{\phi}$ span the space of $\mathbb{R}^3$. That every vector in $\mathbb{C}^3$ can be uniquely expressed using the unit vectors should be straight forward. It is more difficult to imagine constructing every possible vector of $\mathbb{C}^3$ from

$$|0> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix}\sqrt{2}\,i\\ \sqrt{2}\,i\\ 1\end{pmatrix}, \quad |1> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\\ 0\end{pmatrix}, \quad |5> \;=\; \frac{1}{\sqrt{10}}\begin{pmatrix}1\\ 1\\ 2\sqrt{2}\,i\end{pmatrix}, \text{ or}$$

$$|0> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix}2i\\ 0\\ 1\end{pmatrix}, \quad |1> \;=\; \begin{pmatrix}0\\ 1\\ 0\end{pmatrix}, \quad |5> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix}1\\ 0\\ 2i\end{pmatrix}.$$

Further, it is completely unnecessary to resolve such constructions. These eigenvectors originate from Hermitian operators, and the property of Hermiticity ensures that these two sets of eigenvectors form a basis from which any vector in $\mathbb{C}^3$ can be uniquely expressed using an appropriate linear combination. Doing so with either of the above set of vectors seems quite inefficient when it can be done with the unit vectors guaranteed to be available using a unitary transformation built from the eigenvectors of their Hermitian operator.

Postscript: The unitary operators and transformations introduced here are used in chapter 2 and discussed in depth in chapter 3. That a unitary transformation is appropriately used to rotate/reorient vectors as well as operators is addressed in both chapters 2 and 3.

Exercises

1–32. Find (a) $|v> + |w>$ and (b) $|v> - |w>$ given that

$$|v> \rightarrow \begin{pmatrix} 5-2i \\ -3-7i \\ -4+3i \end{pmatrix} \quad \text{and} \quad |w> \rightarrow \begin{pmatrix} -3+i \\ 6-5i \\ -2+5i \end{pmatrix}.$$

Exercising vector addition. Add/subtract like components to obtain the sum/difference ket vectors. See problem 1–4.

1–33. What are (a) $<v|$,

(b) $<w|$,

(c) $<v| + <w|$, and

(d) $<v| - <w|$, using the ket vectors of the previous exercise.

(e) Compare parts (c) and (d) with parts (a) and (b) of the previous exercise.

Exercising both forming a bra given a ket, and vector addition of bras. A bra is the complex conjugate analogy to a ket, and a ket is the complex conjugate analogy to a bra in the complex vector space appropriate to quantum mechanics. Part (e) intends you to see that the sums and differences are corresponding bras and kets. See problems 1–3, 1–5, and 1–6.

1–34. (a) Find $<i|i>$ for each $|i>$ from the previous two exercises.

(b) Identify the smallest space of which each inner product is a member.

The expression $<i|i>$ means to calculate the inner product of all corresponding bras and kets, or explicitly, the four products $<v|v>$, $<w|w>$, $<v+w|v+w>$, and $<v-w|v-w>$ for the previous two exercises. Of course, all of the inner products exist in $\mathbb{C}^\infty$, but that is certainly not the smallest space because an inner product is a scalar. So, the likeliest candidate may be $\mathbb{C}^1$. However, you should see that each possible inner product is a real number, thus $<i|i> \in \mathbb{R}^1$.

Probabilities must be real numbers. A member of $\mathbb{C}^1$ times its complex conjugate is a real number. That the inner product of corresponding bras and kets is the sum of complex conjugate products so must be a real number, or stated symbolically $<i|i> \in \mathbb{R}^1$, is not a coincidence.

1–35. Find each ket sum and bra sum possible given

$$|\,c> \;\rightarrow\; \begin{pmatrix} 3i \\ 2-4i \end{pmatrix} \qquad |\,\beta> \;\rightarrow\; \begin{pmatrix} i \\ 0 \\ -2+i \end{pmatrix} \qquad |\,k> \;\rightarrow\; \begin{pmatrix} 5 \\ 2-3i \end{pmatrix} \qquad |\,2> \;\rightarrow\; \begin{pmatrix} 4i \\ -6 \\ 9 \end{pmatrix}.$$

Two vectors must be in the same space to be added. Two of these kets are in $\mathbb{C}^2$, and two are in $\mathbb{C}^3$. There are two ket sums and two bra sums possible. Notice that the sums are corresponding bras and kets in their respective spaces.

1–36. (a) Multiply the above $|\,c>$, $|\,\beta>$, $|\,k>$, and $|\,2>$ and corresponding bras by $\gamma = 1+2i$.

(b) Find $<c\,\gamma|$, $<\beta\,\gamma|$, $<k\,\gamma|$, and $<2\,\gamma|$.

(c) Identify the results from parts (a) and (b) with conjugate components.

See problem 1–7. Exercising different forms of scalar multiplication.

$$\gamma\,|\,c> \;=\; (1+2i)\begin{pmatrix} 3i \\ 2-4i \end{pmatrix} \;=\; \begin{pmatrix} (1+2i)(3i) \\ (1+2i)(2-4i) \end{pmatrix} \;=\; \begin{pmatrix} 3i-6 \\ 2-4i+4i+8 \end{pmatrix} \;=\; \begin{pmatrix} -6+3i \\ 10 \end{pmatrix}$$

$$\begin{aligned} <\beta\,|\,\gamma \;&=\; \big(-i\,,\;\; 0\,,\;\; -2-i\big)(1+2i) \;=\; \big(-i(1+2i)\,,\;\; 0(1+2i)\,,\;\; (-2-i)(1+2i)\big) \\ &=\; \big(-i+2\,,\;\; 0\,,\;\; -2-4i-i+2\big) \;=\; \big(2-i\,,\;\; 0\,,\;\; -5i\big). \end{aligned}$$

There are six more scalar products possible for part (a).

Any scalar within the delimiters of a bra is conjugated, for instance, $<c\,\gamma| \;=\; <c\,|\,\gamma^*$, or

$<c\,\gamma| \;=\; \big(-3i\,,\;\; 2+4i\big)(1-2i) \;=\; \big(-3i-6\,,\;\; 2+4i-4i+8\big) \;=\; \big(-6-3i\,,\;\; 10\big)$.

You should see $<j\,\gamma|$ and $\gamma\,|\,j>$ are corresponding bras and kets for part (c).

1–37. Normalize each of the vectors given in exercise 1–35.

See problems 1–9 and 1–10. The normalized vector is the scalar product of the normalization constant times the original vector, for example

$$\begin{aligned} <c\,|\,N^*N\,|\,c> \;=\; 1 \;\;&\Rightarrow\;\; \big|\,N\,\big|^2\big(-3i\,,\;\; 2+4i\big)\begin{pmatrix} 3i \\ 2-4i \end{pmatrix} \;=\; 1 \;\;\Rightarrow\;\; \big|\,N\,\big|^2(9+4+16) \;=\; 1 \\ &\Rightarrow\;\; \big|\,N\,\big|^2(29) \;=\; 1 \;\;\Rightarrow\;\; N \;=\; \frac{1}{\sqrt{29}} \;\;\Rightarrow\;\; |\,c> \;=\; \frac{1}{\sqrt{29}}\begin{pmatrix} 3i \\ 2-4i \end{pmatrix}. \end{aligned}$$

The length analog of a state vector is determined by the probability postulate. The probability of all possibilities must be 1. The direction analog contains all the information that can differentiate one state vector from another. The Schrodinger postulate, governing time evolution, simply changes the direction analog of the state vector. Thus, $|\,c> \rightarrow \begin{pmatrix} 3i \\ 2-4i \end{pmatrix}$ and $|\,c> \;=\; \frac{1}{\sqrt{29}}\begin{pmatrix} 3i \\ 2-4i \end{pmatrix}$ contain the same information quantum mechanically so renaming the vector is unnecessary.

1–38. Form all possible dissimilar inner products from the vectors given in exercise 1–35.

There are four dissimilar inner products possible, namely $<c\,|\,k>$, $<k\,|\,c>$, $<\beta\,|\,2>$, and $<2\,|\,\beta>$. The inner product $<c\,|\,2>$, for instance, is not possible because $|\,c> \in \mathbb{C}^2$ and $|\,2> \in \mathbb{C}^3$. An inner product is a scalar. An inner product of unrelated bras and kets will generally be a complex scalar. You should notice that reversing the order of the inner products results in the complex conjugate, or symbolically, $<v\,|\,w> = <w\,|\,v>^*$.

1–39. Show that $<v\,|\,w> = <w\,|\,v>^*$ in $\mathbb{C}^3$.

This problem is a limited proof that complex conjugate of an inner product is the same as the inner product in inverse order. If true in $\mathbb{C}^3$, it should be straight forward to see that the process can be extended to larger dimension. Form two general vectors in $\mathbb{C}^3$, such as

$$|\,v> = \begin{pmatrix} a_1 + b_1 i \\ a_2 + b_2 i \\ a_3 + b_3 i \end{pmatrix} \qquad \text{and} \qquad |\,w> = \begin{pmatrix} c_1 + d_1 i \\ c_2 + d_2 i \\ c_3 + d_3 i \end{pmatrix}.$$

Form the inner products $<v\,|\,w>$ and $<w\,|\,v>^*$. Compare them. They will be identical.

1–40. For $\gamma = 1 + 2i$, $\mathcal{A} \to \begin{pmatrix} 1 & 2i \\ -2i & 4 \end{pmatrix}$, $\mathcal{B} \to \begin{pmatrix} 1+3i & -i \\ i & 1-3i \end{pmatrix}$, find

(a) $\gamma\,\mathcal{A}$, (b) $\gamma\,\mathcal{B}$, (c) $\gamma\,\mathcal{A} + \gamma\,\mathcal{B}$, (d) $\mathcal{A} + \mathcal{B}$, and (e) $\gamma\,(\mathcal{A} + \mathcal{B})$.

Operator arithmetic parallels vector arithmetic. Scalar multiplication of operators is a generalization of scalar multiplication of vectors; multiply each element of the operator by the scalar. Operator addition/subtraction is a generalization of vector addition/subtraction, add/subtract similarly located elements. Compare the results of parts (c) and (e) which provide a numerical example that scalars distribute over operators. See problem 1–12.

1–41. For $|\,\lambda> \to \begin{pmatrix} 1+2i \\ 5 \end{pmatrix}$, $\mathcal{C} \to \begin{pmatrix} 2i & -3i \\ 3i & 5 \end{pmatrix}$, $\mathcal{D} \to \begin{pmatrix} 6 & 1-3i \\ 1+3i & 3 \end{pmatrix}$,

(a) find each operator/vector or vector/operator product possible,

(b) and find each operator/operator product possible.

(c) Do these operators commute?

There are four operator/vector or vector/operator products possible, and two operator/operator products possible. In general, vectors do not commute with vectors and operators do not commute with operators. Operator/vector and vector/operator products exist in dual spaces so cannot commute. See problems 1–13, 1–14, and 1–17.

1–42. For $\quad |\,v> \;\rightarrow \begin{pmatrix} 2+i \\ 3i \\ 5 \end{pmatrix}, \quad \mathcal{E} \;\rightarrow \begin{pmatrix} 3 & 1 & -2i \\ -1 & 0 & 0 \\ 2i & 0 & 4 \end{pmatrix}, \quad \mathcal{F} \;\rightarrow \begin{pmatrix} 5 & 2i & 1 \\ -2i & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix},$

(a) find each operator/vector or vector/operator product possible,

(b) and find each operator/operator product possible.

(c) Do these operators commute?

Similar to the previous exercise except in $\mathbb{C}^3$.

1–43. Which of the six operators $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, $\mathcal{D}$, $\mathcal{E}$, and $\mathcal{F}$ given in the last three exercises could potentially represent an observable quantity?

An observable quantity is represented by a Hermitian operator. Which of the six operators is Hermitian? Said another way, which of the six operators is equal to its transpose conjugate? If an operator is not Hermitian, it cannot represent an observable quantity. Three are Hermitian, and three are not Hermitian. See problem 1–18.

1–44. Find the eigenvalues and normalized eigenvectors of

$$\mathcal{A} \;\rightarrow \begin{pmatrix} 1 & 2i \\ -2i & 4 \end{pmatrix} \qquad \text{and} \qquad \mathcal{F} \;\rightarrow \begin{pmatrix} 5 & 2i & 1 \\ -2i & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}.$$

See problems 1–21 and 1–22. The only possible result of a measurement is an eigenvalue. Given that an eigenvalue is measured, the state vector collapses to the corresponding eigenvector. There are realistic physical problems solved in the subspaces of $\mathbb{C}^2$ and $\mathbb{C}^3$, for instance those relating to orbital angular momentum and spin. The broader intent is to convey the concepts and calculations in $\mathbb{C}^2$ and $\mathbb{C}^3$ where they seem accessible, then to generalize to larger spaces including $\mathbb{C}^\infty$. The eigenvalue/eigenvector equation, $\mathcal{H}\,|\,\alpha> \;=\; \alpha\,|\,\alpha>$, is frequently revisited.

Both $\mathcal{A}$ and $\mathcal{F}$ are Hermitian, therefore, have eigenvalues that are real numbers. The primary difficulty with solving the eigenvalue/eigenvector problem manually is solving the characteristic equation, though these two operators have been created explicitly to enable solutions accessible through polynomial factoring.

1–45. Show that your eigenvectors for $\mathcal{A}$ and $\mathcal{F}$ from the previous exercise are orthonormal.

See problem 1–29. Orthonormality means $<i\,|\,j> \;=\; \delta_{ij}$, stating the inner product of different vectors is zero and the inner product of like vectors is one. This also is revisited frequently.

Since both $\mathcal{A}$ and $\mathcal{F}$ are Hermitian, their eigenvectors are guaranteed to be orthogonal. Any vectors that are orthogonal can be made orthonormal through the process of normalization. Should your eigenvectors be properly normalized from exercise 1–44, there are three inner products to show the eigenvectors of $\mathcal{A}$ are orthonormal and six inner products to the same end for $\mathcal{F}$.

The property of Hermiticity guarantees the eigenvectors of an operator are orthogonal. The property of Hermiticity also guarantees the eigenvectors span the space, or said another way, form a basis for the space. Every vector in the complex vector space $\mathbb{C}^2$ can be uniquely expressed using the eigenvectors of $\mathcal{A}$. Every vector in the complex vector space $\mathbb{C}^3$ can be uniquely expressed using the eigenvectors of $\mathcal{F}$. This may be difficult to imagine because it does not lend itself to any sort of a picture. Pictures are formed in $\mathbb{R}^2$ and $\mathbb{R}^3$, but even $\mathbb{C}^2$ requires the equivalent of $\mathbb{R}^4$ which is an abstraction. Abstraction is inherent to a complex vector space.

The mathematical concept of a basis in a complex linear vector space is coupled to linear independence (appendix B) from which orthogonality follows. The probability postulate dictates the concept of a basis is coupled to orthonormality as a practical matter for quantum mechanics.

1–46. Use your eigenvectors for $\mathcal{A}$ and $\mathcal{F}$ to diagonalize these operators.

See problems 1–25. All Hermitian matrices can be diagonalized using a unitary transformation

$$\mathcal{U}^\dagger \mathcal{B}\, \mathcal{U} \;=\; \mathcal{B}'$$

where the operator $\mathcal{B}'$ is diagonal. The appropriate unitary operator to diagonalize $\mathcal{B}$ is constructed from its eigenvectors. Form $\mathcal{U}$ keeping the eigenvectors in columns, place them in a matrix from left to right in the order of the vector corresponding to the lowest eigenvalue to the vector corresponding to the highest eigenvalue. There other mathematical options to form a proper unitary matrix for a unitary transformation. A convention is necessary and dictates how bras and kets transform consistently with the same change of basis (addressed in chapter 3).

The unitary transformation constructed from the eigenvectors of an operator "rotates," or re-orients, the eigenvectors to align with the unit vectors. There are numerous advantages to this concept. The transformed operator is diagonal with eigenvalues on the diagonal, and the basis vectors are unit vectors. The eigenvalues, the only possibilities of any measurement, are obtained by inspection. The eigenvectors of any diagonal matrix are the unit vectors also by inspection. It is straight forward to imagine unit vectors forming a basis that spans the appropriate space.

The eigenvectors of a Hermitian operator form a basis that spans the space. An argument is provided in chapter 3. Some evidence for the moment is imagine a diagonal operator that is now known to have unit vectors as a basis. Then imagine a unitary transformation to an arbitrary basis, per problem 1–31, in other words, instead of using a unitary transformation to diagonalize the operator, use a unitary transformation to un-diagonalize the operator. If the eigenvectors of the diagonal operator which are unit vectors span the space, must the eigenvectors transformed to a non-diagonal basis also span the space? That a unitary transformation does not affect the information that is contained by an operator or a vector will be demonstrated in chapter 3. The eigenvectors of a Hermitian operator form a basis that spans the space.

1–47. Show that the eigenvectors of $\begin{pmatrix} 1 & 0 & -\sqrt{2}\,i \\ 0 & 1 & -\sqrt{2}\,i \\ \sqrt{2}\,i & \sqrt{2}\,i & 4 \end{pmatrix}$,

$$|0> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix} \sqrt{2}\,i \\ \sqrt{2}\,i \\ 1 \end{pmatrix}, \qquad |1> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \qquad |5> \;=\; \frac{1}{\sqrt{10}}\begin{pmatrix} 1 \\ 1 \\ 2\sqrt{2}\,i \end{pmatrix},$$

are orthonormal.

The arbitrary unitary transformation completed in problem 1–31 is a Hermitian operator. The unitary transformation of a Hermitian operator must also be Hermitian. A Hermitian operator has orthogonal eigenvectors, which once normalized, form an orthonormal basis. Starting with

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 5 \end{pmatrix} \quad \Rightarrow \quad |0> \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |1> \;=\; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |5> \;=\; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},$$

it should seem straight forward to imagine recovering either of the other $\mathcal{H}'$ operators expressed in problem 1–31 by using an appropriate unitary transformation.

Reasons to manually diagonalize an operator constructed from its eigenvectors are rare, though the concept is essential. The concept is the foundation for a **complete set of commuting observables** necessary to address **degenerate** systems, which are central topics of chapter 3. The preferred method to obtain a complete set of commuting observables is **simultaneous diagonalization**, meaning diagonalizing two or more operators with the same unitary transformation. Diagonalization of one operator seems a logical step before diagonalizing two or more operators.

1–48. Find the eigenvalues and normalized eigenvectors of $\mathcal{T} \;\rightarrow\; \begin{pmatrix} \kappa & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & \nu \end{pmatrix}$.

Do this by inspection! This should be among the shortest solutions to any quantum mechanics problem ever posed! This exercise is intended to cement the facts that the eigenvalues of a diagonal operator are the elements on the main diagonal, and that eigenvectors of a diagonal operator are the unit vectors where the 1 is in the position corresponding to the vertical location of that eigenvalue. Diagonal operators have many advantageous properties.

Chapter 2

Probability, Statistics, and Stationary States

The two central questions that can be asked of any quantum mechanical measurement are what are the possibilities and what is the probability of each possibility? The possibilities are the eigenvalues. This chapter features the probability calculations, the associated statistical measures of central tendency; expectation value and uncertainty, as well as stationary states. The solutions to the spatial portion of the time-independent Schrodinger equation are known as stationary states. The state vector is a linear combination of the eigenvectors, each with its own probability amplitude. Each eigenvector evolves individually as governed by the time-dependent Schrodinger equation, and the state vector is a linear combination of the time evolving eigenstates.

2–1. Compare and contrast each of the postulates to analogous statements from classical mechanics where a comparison is possible.

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1. The state of a system is represented by a vector $|\psi>$ in Hilbert space.

2. Every observable quantity is represented by a Hermitian operator.

3. A measurement of an observable quantity represented by the operator $\mathcal{A}$ can yield only the eigenvalues of $\mathcal{A}$.

4. If a system is in state $|\psi>$, a measurement of the observable quantity represented by the operator $\mathcal{A}$ that yields the eigenvalue α does so with the probability

$$P(\alpha) \propto \left| <\alpha|\psi> \right|^2,$$

where $|\alpha>$ is the eigenstate corresponding to the eigenvalue α.

5. A measurement of the observable quantity represented by the operator $\mathcal{A}$ with the result α changes the state of the system to the eigenstate $|\alpha>$.

6. The state vector obeys the time dependent Schrodinger equation

$$\mathcal{H}|\psi> = i\hbar\frac{d}{dt}|\psi>,$$

where $\mathcal{H}$ is the quantum mechanical Hamiltonian operator.

The **state vector postulate**. The state vector $|\psi>$ replaces the positions and momentums (or velocities) of classical mechanics.

The **observables postulate**. That observable quantities are described by operators is fundamentally different than the classical description that every dynamical variable is described by a function of position and momentum, for instance.

The **eigenvalue postulate**. Any real value is a possible result of a classical measurement. The only possible result of a quantum mechanical measurement is an eigenvalue of the operator representing the quantity being measured.

The **probability postulate**. There is no classical analogy. The interpretation of the square of an inner product as a probability is unique to quantum mechanics.

The **eigenvector postulate**. There is also no classical analogy for the eigenvector postulate. Classically, measurement of a system does not affect the system.

The **Schrodinger postulate**. The time rate of change of the state variables of a classical system are governed by Hamilton's equations

$$\frac{dx}{dt} = \frac{\partial H}{\partial p} \qquad \text{and} \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial x}\,.$$

The time evolution of a quantum mechanical system is governed by Schrodinger's equation.

Postscript: The state vector postulate includes the principle of superposition. Given $|\,\psi_1>$ and $|\,\psi_2>$ are possible states, then the linear combination, $|\,\psi> \;=\; c_1\,|\,\psi_1> \,+\, c_2\,|\,\psi_2>$, is also a possible state of the system. The $|\,\psi_i>$ are the eigenvectors/eigenstates of the system. The general state vector is the superposition or linear combination of all eigenstates, *i.e.*,

$$|\,\psi> \;=\; c_1\,|\,\psi_1> \,+\, c_2\,|\,\psi_2> \,+\, c_3\,|\,\psi_3> \,+\, \cdots \,=\, \sum_{i=1}^{\infty} c_i\,|\,\psi_i>$$

in the case of an infinity of eigenstates. Each of the coefficients c_i are scalars that indicate the relative "amount" of eigenstate $|\,\psi_i>$ in the superposition that and are often called **probability amplitudes** because the probability of measuring the corresponding eigenvalue is often $|\,c_i\,|^{\,2}$. A coefficient can be zero meaning that the corresponding eigenstate is absent from that state vector.

Observable quantities are those that can be physically measured. That all Hermitian operators can be diagonalized was employed in the first chapter to show that the eigenvalues of Hermitian operators are real numbers. Numbers used to describe physical quantities are necessarily real numbers. This fact is essential to the observables postulate. Also, the eigenvectors of Hermitian operators are orthogonal, therefore, the eigenvectors can be made orthonormal. Further, the eigenvectors of Hermitian operators form a basis appropriate to the space. These four properties of Hermitian operators will be further supported in chapter 3 following additional development of unitary transformations. The observable quantities of position, momentum, energy, and angular momentum are focal.

Though entwined within many of the postulates, quantum mechanics requires the field of complex numbers. The observables postulate specifically denotes Hermitian operators. Hermitian means $\mathcal{A} = \mathcal{A}^{\dagger}$. The dagger means adjoint or transpose conjugate, thus the elements are implied to be from the field of complex numbers.

The eigenvalue postulate is definitely non-classical. The *only* possible result of a measurement is an *eigenvalue* of the operator representing the physical quantity being measured. The familiar continuous ranges of positions, momenta, energies, and angular momenta are not possible quantum mechanically. A system, for instance a hydrogen atom, may have an infinite number of eigenenergies, but they are *quantized* energy eigenvalues instead of being a continuous range.

A proportionality is used in probability postulate. The proportionality is replaced by an equality by dividing by the inner product of unnormalized vectors,

$$P(\alpha) \;\propto\; |<\alpha\,|\,\psi>|^2 \qquad \Rightarrow \qquad P(\alpha) \;=\; \frac{|<\alpha\,|\,\psi>|^2}{<\alpha\,|\,\alpha><\psi\,|\,\psi>}\,,$$

or equivalently, by normalizing vectors before calculating the inner product. The probability postulate is the reason for the process of normalization, and it is also the reason that two state vectors that are proportional represent the same physical state. A probability of 1 means certainty. Thus, the sum of the probabilities of a measurement of all possibilities must be 1 .

The probabilistic interpretation of quantum mechanics defies classical explanation and has perplexed some of the greatest minds of the 20th century who have sought alternatives.

The eigenvector postulate describes what is often called the "collapse of the wave function." It is the statement that the observer interacts with the system; that the observer is part of the system. Regardless of how carefully a measurement is made, the process of measurement changes the system being measured. Further, the measurement changes the system in a specific way, the measurement forces the system into one of its eigenstates. Finally, once in that eigenstate, it remains in that eigenstate until it undergoes its next interaction which is its next "measurement."

The Schrodinger equation is not derived from the postulates of quantum mechanics, rather, *the Schrodinger equation is one of the postulates of quantum mechanics.*

The Schrodinger postulate requires the quantum mechanical Hamiltonian operator, $\mathcal{H}$. The classical Hamiltonian operator is the total energy operator, $H = T + V$, where T is kinetic energy and V is potential energy. Each of the dynamical variables of classical mechanics is replaced by an operator for the transition to the quantum mechanical formulation, $x \rightarrow \mathcal{X}$ and $p \rightarrow \mathcal{P}$ in Hilbert space. The classical Hamiltonian then goes to the quantum mechanical Hamiltonian, $H \rightarrow \mathcal{H}$ for energy, and for angular momentum $L \rightarrow \mathcal{L}$ in Hilbert space.

The meaning of the word "postulate" is that the stated tenet is not derived. The postulates include numerous mysteries and provide some unexpected results. The postulates also indicate that there are things that cannot be known. Return to the postulates as the foundation that they are as necessary. One view is that the entirety of quantum mechanics is the postulates.

2–2. The "$\mathcal{A}$–ness" of a particle or system in the state

$$|\,\psi> \;=\; \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \qquad \text{where} \qquad \mathcal{A} \;=\; \begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix} \qquad \text{is measured.}$$

(a) Normalize $|\,\psi>$.

(b) What are the possible outcomes of a measurement of the "$\mathcal{A}$–ness" of $|\,\psi>$?

(c) Calculate the probability of each possibility.

(d) Show that the sum of the probabilities is 1.

(e) A measurement of the "$\mathcal{A}$–ness" of $|\,\psi>$ yields the value 4. A second measurement of the "$\mathcal{A}$–ness" of $|\,\psi>$ is then made. What are the possibilities and probabilities of the outcomes of this second measurement?

Doing the normalization of part (a) prior to any calculations avoids numerous potential difficulties. The only possible results of a measurement are the eigenvalues of $\mathcal{A}$ per the eigenvalue postulate. There are three possibilities. The eigenvalues and eigenvectors of a diagonal operator are obtained by inspection. The eigenvectors are needed to calculate probabilities. The three probabilities must sum to 1. The eigenvector postulate indicates how to approach part (e).

(a) The normalized state vector is found

$$1 \;=\; \big(1,\,2,\,3\big)\,A^{*}\,A\begin{pmatrix}1\\2\\3\end{pmatrix} \;=\; |\,A\,|^{2}(1{+}4{+}9) \;=\; 1 \quad\Rightarrow\quad A \;=\; \frac{1}{\sqrt{14}} \quad\Rightarrow\quad |\,\psi> \;=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}.$$

(b) The possible results of a measurement are the eigenvalues 3, 4, and 5. The elements on the principal diagonal of a diagonal matrix operator are the eigenvalues.

(c) The eigenvectors are $|\,3> \;=\; \begin{pmatrix}1\\0\\0\end{pmatrix}$, $|\,4> \;=\; \begin{pmatrix}0\\1\\0\end{pmatrix}$, $|\,5> \;=\; \begin{pmatrix}0\\0\\1\end{pmatrix}$ by inspection.

All $|\,\alpha>$ and the $|\,\psi>$ are normalized so $P\,(\alpha) \;=\; \Big|<\alpha\,|\,\psi>\Big|^{2}$, which means

$$P\,(ev=3) \;=\; \left|\big(1,\,0,\,0\big)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^{2} \;=\; \left|\frac{1}{\sqrt{14}}\big(1+0+0\big)\right|^{2} \;=\; \left|\frac{1}{\sqrt{14}}\right|^{2} \;=\; \frac{1}{14}\,,$$

$$P\,(ev=4) \;=\; \left|\big(0,\,1,\,0\big)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^{2} \;=\; \left|\frac{1}{\sqrt{14}}\big(0+2+0\big)\right|^{2} \;=\; \left|\frac{2}{\sqrt{14}}\right|^{2} \;=\; \frac{4}{14}\,,$$

$$P\,(ev=5) \;=\; \left|\big(0,\,0,\,1\big)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^{2} \;=\; \left|\frac{1}{\sqrt{14}}\big(0+0+3\big)\right|^{2} \;=\; \left|\frac{3}{\sqrt{14}}\right|^{2} \;=\; \frac{9}{14}\,.$$

(d) $\displaystyle\sum_{1}^{3} P_i \;=\; \frac{1}{14}+\frac{4}{14}+\frac{9}{14} \;=\; \frac{14}{14} \;=\; 1\,.$

(e) The eigenvector postulate says that the state vector of the system is the eigenstate of $ev=4$ following the first measurement, so the state vector is $|\,\psi'> \;=\; \begin{pmatrix}0\\1\\0\end{pmatrix}$. The probability of obtaining $ev=4$ as a result of the second measurement is 1.

The probability of measuring either of the other two eigenvalues is zero. The probability of measuring $ev=3$ or $ev=5$ is

$$\left|\big(1,\,0,\,0\big)\begin{pmatrix}0\\1\\0\end{pmatrix}\right|^{2} \;=\; \left|\big(0,\,0,\,1\big)\begin{pmatrix}0\\1\\0\end{pmatrix}\right|^{2} \;=\; \big|\,\big(0+0+0\big)\,\big|^{2} \;=\; |\,0\,|^{2} \;=\; 0\,.$$

Postscript: Notice that $\mathcal{A}$ is a Hermitian operator that satisfies the observables postulate.

Notice also that the state vector is not pertinent to the possible results of a measurement. Possibilities are determined solely by the operator. The state vector is pertinent only to the probabilities of the possible results of a measurement.

2–3. What are the possible results and the probability of obtaining each possible result of a measurement of the "$\mathcal{B}$–ness" of a system where

$$\mathcal{B} \;=\; \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix} \qquad \text{and the state is} \qquad |\,\psi> \;=\; \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}.$$

The question asks only for possibilities and probabilities. The possibilities are the eigenvalues, and the probabilities follow from the inner product of the eigenvector and the state vector. Solve the eigenvalue/eigenvector problem for $\mathcal{B}$ to find

$$|\,2> \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad |\,3> \;=\; \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \qquad |\,1> \;=\; \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}.$$

This state vector is normalized in the previous problem. Probabilities must sum to 1.

Using the normalized state vector, the probabilities of each possibility are

$$P\,(ev=2) \;=\; \left| \left(1,\ 0,\ 0\right) \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \right|^2 \;=\; \left| \frac{1}{\sqrt{14}} \left(1+0+0\right) \right|^2 \;=\; \left| \frac{1}{\sqrt{14}} \right|^2 \;=\; \frac{1}{14}\,,$$

$$P\,(ev=3) \;=\; \left| \frac{1}{\sqrt{2}} \left(0,\ 1,\ 1\right) \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \right|^2 \;=\; \left| \frac{1}{\sqrt{28}} \left(0+2+3\right) \right|^2 \;=\; \left| \frac{5}{\sqrt{28}} \right|^2 \;=\; \frac{25}{28}\,,$$

$$P\,(ev=1) \;=\; \left| \frac{1}{\sqrt{2}} \left(0,\ 1,\ -1\right) \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \right|^2 \;=\; \left| \frac{1}{\sqrt{28}} \left(0+2-3\right) \right|^2 \;=\; \left| \frac{-1}{\sqrt{28}} \right|^2 \;=\; \frac{1}{28}\,,$$

$$\text{and} \qquad \frac{2}{28} + \frac{25}{28} + \frac{1}{28} \;=\; \frac{28}{28} \;=\; 1\,, \qquad \text{as it must.}$$

2–4. Use operator $\mathcal{A}$ and operator $\mathcal{B}$ from the previous two problems. The state vector of the system is $|\psi> = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$ also used in the previous two problems for the following questions.

(a) If we measure a value of 3 for $\mathcal{A}$, what are the possible values of successive measurements of $\mathcal{B}$, $\mathcal{A}$, $\mathcal{B}$, etc., and their respective probabilities?

(b) If we measure $\mathcal{A}$ and get 4, what are the possible values of a subsequent measurement of $\mathcal{B}$ and the probabilities of each possibility?

(c) Having measured a value of 4 for $\mathcal{A}$, and then measured a value of 3 for $\mathcal{B}$, what are the possible values of another measurement of $\mathcal{A}$ and their respective probabilities?

(d) Having measured a value of 4 for $\mathcal{A}$, and then measured a value of 1 for $\mathcal{B}$, what are the possible values of a measurement of $\mathcal{A}$ and their respective probabilities?

(e) If we measure 5 for $\mathcal{A}$, what are the possible values of subsequent measurements of $\mathcal{B}$ and their respective probabilities?

The eigenvector postulate indicates that the state vector following a measurement is the eigenstate corresponding to the eigenvalue measured. Use the subsequent state vector determined by the measurement in probability calculations to answer all five questions.

(a) If we measure $\mathcal{A}$ and get $ev = 3$, the state vector of the system is now in the eigenstate of $\mathcal{A}$ corresponding to this eigenvalue, *i.e.*, $|\psi'> = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$. This is identical to the eigenstate of $\mathcal{B}$ corresponding to $ev = 2$. The eigenvectors of $\mathcal{B}$ corresponding to $ev = 3$ or $ev = 1$ both have zero as their first component, so $<ev_{\mathcal{B}} = 3\,|\psi'> = <ev_{\mathcal{B}} = 1\,|\psi'> = 0$. We will measure $ev = 2$ for $\mathcal{B}$ with probability of $|<ev_{\mathcal{B}} = 2\,|\psi'>|^2 = 1$. Subsequent measurements of $\mathcal{A}$, $\mathcal{B}$, $\mathcal{A}$, etc., yield $ev_{\mathcal{A}} = 3$, $ev_{\mathcal{B}} = 2$, $ev_{\mathcal{A}} = 3$, etc. The probability of each measurement is 1.

(b) From the given measurement of $\mathcal{A}$, the state vector of the system is $|\psi'> = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$. The eigenvector corresponding to the eigenvalue measured is now the state vector of the system. Both of the eigenvectors $|ev_{\mathcal{B}} = 3>$ and $|ev_{\mathcal{B}} = 1>$ of operator $\mathcal{B}$ are non-zero in the same component that $|\psi'>$ is non-zero so will have non-zero probabilities. The corresponding component of $|ev_{\mathcal{B}} = 2>$ is zero from which we can conclude that $P(ev_{\mathcal{B}} = 2) = 0$ without calculation. Nevertheless, the probabilities of all possibilities are

$$P(ev_{\mathcal{B}} = 2) = \left| \begin{pmatrix} 1, & 0, & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right|^2 = \left| \begin{pmatrix} 0 + 0 + 0 \end{pmatrix} \right|^2 = |0|^2 = 0,$$

$$P(ev_{\mathcal{B}} = 3) = \left| \frac{1}{\sqrt{2}} \begin{pmatrix} 0, & 1, & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{2}} \begin{pmatrix} 0 + 1 + 0 \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2},$$

$$P(ev_{\mathcal{B}}=1) \;=\; \left|\frac{1}{\sqrt{2}}\,(0,\;1,\;-1)\begin{pmatrix}0\\1\\0\end{pmatrix}\right|^2 \;=\; \left|\frac{1}{\sqrt{2}}\,(0+1+0)\right|^2 \;=\; \left|\frac{1}{\sqrt{2}}\right|^2 \;=\; \frac{1}{2}\,.$$

(c) If 3 was found for the measurement of $\mathcal{B}$, the new state vector is $|\,\psi'> \;=\; \dfrac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\end{pmatrix}$. Then the probabilities for a subsequent measurement of $\mathcal{A}$ follow from the probability postulate,

$$P(ev_{\mathcal{A}}=3) \;=\; \left|(1,\;0,\;0)\,\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\end{pmatrix}\right|^2 \;=\; \left|\frac{1}{\sqrt{2}}\,(0+0+0)\right|^2 \;=\; |\,0\,|^2 \;=\; 0\,,$$

$$P(ev_{\mathcal{A}}=4) \;=\; \left|(0,\;1,\;0)\,\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\end{pmatrix}\right|^2 \;=\; \left|\frac{1}{\sqrt{2}}\,(0+1+0)\right|^2 \;=\; \left|\frac{1}{\sqrt{2}}\right|^2 \;=\; \frac{1}{2}\,,$$

$$P(ev_{\mathcal{A}}=5) \;=\; \left|(0,\;0,\;1)\,\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\end{pmatrix}\right|^2 \;=\; \left|\frac{1}{\sqrt{2}}\,(0+0+1)\right|^2 \;=\; \left|\frac{1}{\sqrt{2}}\right|^2 \;=\; \frac{1}{2}\,.$$

(d) If we found 1 for the measurement of $\mathcal{B}$, the state vector is $|\,\psi'> \;=\; \dfrac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\end{pmatrix}$. In a calculation that is similar to part (c), we find for a measurement of $\mathcal{A}$, $P(ev_{\mathcal{A}}=3) \;=\; 0$, $P(ev_{\mathcal{A}}=4) \;=\; 1/2$, and $P(ev_{\mathcal{A}}=5) \;=\; 1/2$.

(e) The state vector of the system is $\begin{pmatrix}0\\0\\1\end{pmatrix}$ after the given measurement. Again, both $|\,ev_{\mathcal{B}}=3>$ and $|\,ev_{\mathcal{B}}=1>$ of the operator $\mathcal{B}$ have corresponding components that are non-zero but $|\,ev=2>$ does not. The probabilities are $P(ev=2) \;=\; 0$, $P(ev_{\mathcal{B}}=3) \;=\; 1/2$, and $P(ev_{\mathcal{B}}=1) \;=\; 1/2$ for a subsequent measurement of $\mathcal{B}$.

2–5. Find the possibilities and probabilities of a measurement of $\mathcal{L}_y$ for a system in the state

$$|\,\psi> \;=\; \begin{pmatrix}1\\2\\3\end{pmatrix} \qquad \text{where} \qquad \mathcal{L}_y \;=\; \begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}.$$

The probability calculations for this problem require the use of complex numbers. The eigenvalues and normalized eigenvectors from problem 1–22 of chapter 1 are

$$|-\sqrt{2}> \;=\; \frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\,i\\-1\end{pmatrix}, \qquad |\,0> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}, \qquad \text{and} \qquad |\sqrt{2}> \;=\; \frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\,i\\-1\end{pmatrix}.$$

The possibilities are the eigenvalues. Using the normalized state vector from previous problems,

$$P\,(ev = -\sqrt{2}\,) \;=\; \left|\, \big(1,\ \sqrt{2}\,i,\ -1\big)\,\frac{1}{2}\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \right|^2 \;=\; \left|\, \frac{1}{2\sqrt{14}}\,\big(1+2\sqrt{2}\,i-3\big) \right|^2$$
$$=\; \frac{1}{4\cdot 14}\big|\,-2+2\sqrt{2}\,i\,\big|^2 \;=\; \frac{1}{56}\,\big(-2-2\sqrt{2}\,i\big)\,\big(-2+2\sqrt{2}\,i\big)$$
$$=\; \frac{1}{56}\,\big(4+8\big) \;=\; \frac{12}{56} \;=\; \frac{3}{14}\,,$$

$$P\,(ev = 0) \;=\; \left|\, \big(1,\ 0,\ 1\big)\,\frac{1}{\sqrt{2}}\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \right|^2 \;=\; \left|\, \frac{1}{\sqrt{28}}\,\big(1+0+3\big) \right|^2 \;=\; \left|\, \frac{4}{\sqrt{28}} \right|^2 \;=\; \frac{16}{28} \;=\; \frac{8}{14}\,,$$

$$P\,(ev = \sqrt{2}\,) \;=\; \left|\, \big(1,\ -\sqrt{2}\,i,\ -1\big)\,\frac{1}{2}\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \right|^2 \;=\; \left|\, \frac{1}{2\sqrt{14}}\,\big(1-2\sqrt{2}\,i-3\big) \right|^2$$
$$=\; \frac{1}{4\cdot 14}\,\big|\,-2-2\sqrt{2}\,i\,\big|^2 \;=\; \frac{1}{56}\,\big(-2+2\sqrt{2}\,i\big)\,\big(-2-2\sqrt{2}\,i\big)$$
$$=\; \frac{1}{56}\,\big(4+8\big) \;=\; \frac{12}{56} \;=\; \frac{6}{28} \;=\; \frac{3}{14}\,,$$

and the sum of the probabilities is $\;\frac{3}{14}+\frac{8}{14}+\frac{3}{14} \;=\; \frac{14}{14} \;=\; 1\,,\;$ as is necessary.

Postscript: Remember that for any scalar $\alpha\,,\ \ |\,\alpha\,|^{\,2} = \alpha^*\,\alpha\,,$ the product of conjugate quantities, so $|\,\alpha\,|^{\,2}$ is the sum of the squares of the real and imaginary parts of a complex scalar.

2–6. For $\quad |\,\psi> \;=\; \begin{pmatrix}1\\2\\3\end{pmatrix}\,,\qquad \mathcal{C} \;\to\; \begin{pmatrix}3 & 4i\\ -4i & 3\end{pmatrix}\,,\qquad$ and $\qquad \mathcal{H} \;\to\; \begin{pmatrix}1 & 0 & -2i\\ 0 & 1 & 0\\ 2i & 0 & 4\end{pmatrix}\,,\quad$ what measurements can be made, and what are the probabilities of each possible result?

The given $|\,\psi>$ and $\mathcal{C}$ are not in the same space, thus a measurement of "$\mathcal{C}$–ness" is not possible. $|\,\psi>$ and $\mathcal{H}$ are in the same space, so measuring "$\mathcal{H}$–ness" is possible.

The normalized eigenvectors and eigenvalues of $\mathcal{H}$ from problem 1–21 of chapter 1 are

$$|\,0> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix}2i\\0\\1\end{pmatrix}\,,\qquad |\,1> \;=\; \begin{pmatrix}0\\1\\0\end{pmatrix}\,,\qquad |\,5> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix}1\\0\\2i\end{pmatrix}\,.$$

$$P(0) = \left| \frac{1}{\sqrt{5}}(-2i,\ 0,\ 1)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{70}}(-2i+3)\right|^2 = \frac{1}{70}(3-2i)(3+2i) = \frac{9+4}{70} = \frac{13}{70}.$$

$$P(1) = \left|(0,\ 1,\ 0)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{14}}(2)\right|^2 = \frac{4}{14} = \frac{20}{70}.$$

$$P(5) = \left| \frac{1}{\sqrt{5}}(1,\ 0,\ 2i)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{70}}(1+6i)\right|^2 = \frac{1}{70}(1+6i)(1-6i) = \frac{1+36}{70} = \frac{37}{70}.$$

Postscript: Notice that the sum of the probabilities is 1.

2–7. For $|\psi> = \begin{pmatrix}3i\\2\end{pmatrix}$, $\mathcal{C} \to \begin{pmatrix}3 & 4i\\-4i & 3\end{pmatrix}$, and $\mathcal{H} \to \begin{pmatrix}1 & 0 & -2i\\0 & 1 & 0\\2i & 0 & 4\end{pmatrix}$, what measurements can be made, and what are the probabilities of each possible result?

The given $|\psi>$ and $\mathcal{H}$ are not in the same space, thus a measurement of "$\mathcal{H}$–ness" is not possible. $|\psi>$ and $\mathcal{C}$ are in the same space, so measuring "$\mathcal{C}$–ness" is possible.

The normalized eigenvectors and eigenvalues of $\mathcal{C}$ from problem 1–21 of chapter 1 are

$$|-1> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \qquad |7> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}.$$

This is a different state vector than used in the previous five problems and is not yet normalized. Per the probability postulate, the state vector need not be normalized. This problem is completed without normalization of the state vector for demonstration purposes.

$$P(-1) = \frac{\left|\frac{1}{\sqrt{2}}(1,\ -i)\begin{pmatrix}3i\\2\end{pmatrix}\right|^2}{(-3i,\ 2)\begin{pmatrix}3i\\2\end{pmatrix}} = \frac{\frac{1}{2}|3i-2i|^2}{9+4} = \frac{(i)(-i)}{26} = \frac{1}{26}.$$

$$P(7) = \frac{\left|\frac{1}{\sqrt{2}}(1,\ i)\begin{pmatrix}3i\\2\end{pmatrix}\right|^2}{(-3i,\ 2)\begin{pmatrix}3i\\2\end{pmatrix}} = \frac{\frac{1}{2}|3i+2i|^2}{9+4} = \frac{(5i)(-5i)}{26} = \frac{25}{26}.$$

Postscript: Using unnormalized eigenvectors with an unnormalized state vector, division by both $<\psi|\psi>$ and $<\alpha|\alpha>$ is required.

2–8. Find the expectation values of $\mathcal{A}$, $\mathcal{B}$, $\mathcal{L}_y$, $\mathcal{C}$, and $\mathcal{H}$ using the eigenvalues and probabilities of problems 2–2 through 2–7.

An **expectation value** is the anticipated average of many measurements made on an ensemble of identical systems. An expectation value is defined

$$< \mathcal{A} >_\psi \;=\; \sum_i P\,(\alpha_i)\,\alpha_i\,.$$

It is the sum of the products of the eigenvalue and the probability of measuring that eigenvalue. An expectation value is simply a weighted average.

$$< \mathcal{A} >_\psi \;=\; \sum_i P\,(\alpha_i)\,\alpha_i \;=\; \frac{1}{14}\,(3) \;+\; \frac{4}{14}\,(4) \;+\; \frac{9}{14}\,(5) \;=\; \frac{3}{14} + \frac{16}{14} + \frac{45}{14} \;=\; \frac{64}{14} \;=\; 4\,\frac{4}{7}\,.$$

$$< \mathcal{B} >_\psi \;=\; \sum_i P\,(\beta_i)\,\beta_i \;=\; \frac{2}{28}\,(2) \;+\; \frac{25}{28}\,(3) \;+\; \frac{1}{28}\,(1) \;=\; \frac{4}{28} + \frac{75}{28} + \frac{1}{28} \;=\; \frac{80}{28} \;=\; 2\,\frac{6}{7}\,.$$

$$< \mathcal{L}_y >_\psi \;=\; \frac{3}{14}\,(-\sqrt{2}\,) \;+\; \frac{8}{14}\,(0) \;+\; \frac{3}{14}\,(\sqrt{2}\,) \;=\; 0\,.$$

$$< \mathcal{C} >_\psi \;=\; \frac{1}{26}\,(-1) \;+\; \frac{25}{26}\,(7) \;=\; -\frac{1}{26} + \frac{175}{26} \;=\; \frac{174}{26} \;=\; 6\,\frac{9}{13}\,.$$

$$< \mathcal{H} >_\psi \;=\; \frac{13}{70}\,(0) \;+\; \frac{20}{70}\,(1) \;+\; \frac{37}{70}(5) \;=\; 0 + \frac{20}{70} + \frac{185}{70} \;=\; \frac{205}{70} \;=\; 2\,\frac{13}{14}\,.$$

Postscript: Probabilities are dependent upon the state vector, therefore, expectation values that are computed using probabilities are also dependent upon the state vector. The expectation value symbols have been subscripted with ψ to emphasize this dependence.

The field of statistics uses the terminology "expected value" while physics generally uses the term "expectation value." They are mathematically identical. An expected value or expectation value is the prediction of an overall weighted average taken on a statistical sample.

2–9. Show that $<\psi\,|\,\mathcal{D}\,|\,\psi>$ yields the five expectation values calculated previously.

The expression $<\psi\,|\,\mathcal{D}\,|\,\psi>$ is an alternate method of calculating an expectation value having the advantage that eigenvalues and probabilities are not required. It can thus be applied without having to solve the eigenvalue/eigenvector problem or calculating probabilities.

Remember that an expectation value is dependent upon the state vector. Use the state vector $|\,\psi> \;=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$ for $\mathcal{A}$, $\mathcal{B}$, $\mathcal{L}_y$, and $\mathcal{H}$, and $|\,\psi> \;=\; \frac{1}{\sqrt{13}}\begin{pmatrix}3i\\2\end{pmatrix}$ for $\mathcal{C}$.

$$< \mathcal{A} >_\psi \;=\; <\psi\,|\,\mathcal{A}\,|\,\psi> \;=\; \frac{1}{\sqrt{14}}\,(1,\;2,\;3)\begin{pmatrix}3&0&0\\0&4&0\\0&0&5\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$$

$$= \;\frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}3\\8\\15\end{pmatrix} \;=\; \frac{1}{14}\,(3+16+45) \;=\; \frac{64}{14} \;=\; 4\,\frac{4}{7}\,.$$

$$< \mathcal{B} >_\psi \;=\; <\psi\,|\,\mathcal{B}\,|\,\psi> \;=\; \frac{1}{\sqrt{14}}\,(1,\;2,\;3)\begin{pmatrix}2&0&0\\0&2&1\\0&1&2\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$$

$$= \;\frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}2\\4+3\\2+6\end{pmatrix} \;=\; \frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}2\\7\\8\end{pmatrix} \;=\; \frac{1}{14}\,(2+14+24) \;=\; \frac{40}{14} \;=\; 2\,\frac{6}{7}\,.$$

$$< \mathcal{L}_y >_\psi \;=\; <\psi\,|\,\mathcal{L}_y\,|\,\psi> \;=\; \frac{1}{\sqrt{14}}\,(1,\;2,\;3)\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$$

$$= \;\frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}-2i\\i-3i\\2i\end{pmatrix} \;=\; \frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}-2i\\-2i\\2i\end{pmatrix} \;=\; \frac{1}{14}\,(-2i-4i+6i) \;=\; 0\,.$$

$$< \mathcal{C} > \;=\; \frac{1}{\sqrt{13}}(-3i\,,\;\;2)\begin{pmatrix}3&4i\\-4i&3\end{pmatrix}\frac{1}{\sqrt{13}}\begin{pmatrix}3i\\2\end{pmatrix} \;=\; \frac{1}{13}(-3i\,,\;\;2)\begin{pmatrix}9i+8i\\12+6\end{pmatrix}$$

$$= \;\frac{1}{13}(-3i\,,\;\;2)\begin{pmatrix}17i\\18\end{pmatrix} \;=\; \frac{1}{13}(51+36) \;=\; \frac{87}{13} \;=\; 6\,\frac{9}{13}\,.$$

$$< \mathcal{H} > \;=\; \frac{1}{\sqrt{14}}\,(1,\;2,\;3)\begin{pmatrix}1&0&-2i\\0&1&0\\2i&0&4\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$$

$$= \;\frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}1-6i\\2\\12+2i\end{pmatrix} \;=\; \frac{1}{14}\,(1-6i+4+36+6i) \;=\; \frac{41}{14} \;=\; 2\,\frac{13}{14}\,.$$

Postscript: The expectation value of $\mathcal{A}$ conventionally appears as $< \mathcal{A} >$, without a subscript ψ as illustrated in the last two examples. Further, $< \mathcal{A} >$ is seen more frequently than $<\psi\,|\,\mathcal{A}\,|\,\psi>$, also per the last two calculations. Remember, nevertheless, that an expectation value is dependent upon a state vector.

That $\sum P_{\mathcal{A}}\,(\alpha_i)\,\alpha_i \;=\; <\psi\,|\,\mathcal{A}\,|\,\psi>$ is addressed in problem 2–25 and exercise 2–37.

2–10. Find the uncertainty of $\mathcal{A} \;=\; \begin{pmatrix}3&0&0\\0&4&0\\0&0&5\end{pmatrix}$ given $|\,\psi> \;=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$.

Two measures of central tendency are frequently encountered in quantum mechanics. The first is the previously discussed expectation value. The other is **uncertainty** or **standard deviation**.

Uncertainty, or standard deviation, is defined in terms of the expectation value,

$$\triangle \mathcal{A}_\psi \;=\; <\psi\,|\left(\mathcal{A} - <\mathcal{A}>\mathcal{I}\right)^2|\,\psi>^{1/2},$$

where the uncertainty on the left is subscripted because it is dependent on the state vector $|\,\psi>$. A state vector is needed to calculate the expectation value, therefore, a state vector is needed to calculate the uncertainty. The expectation value times the identity operator means

$$<\mathcal{A}>\mathcal{I} \;=\; 4\frac{4}{7}\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix} \;=\; \begin{pmatrix}4\frac{4}{7}&0&0\\0&4\frac{4}{7}&0\\0&0&4\frac{4}{7}\end{pmatrix} \quad \text{for the operator } \mathcal{A}\text{, for example.}$$

$$\begin{aligned}
\left(\triangle \mathcal{A}_\psi\right)^2 \;&=\; <\psi\,|\left(\mathcal{A} - <\mathcal{A}>\mathcal{I}\right)^2|\,\psi> \\
&=\; \frac{1}{\sqrt{14}}\,(1,\;2,\;3)\left[\begin{pmatrix}3&0&0\\0&4&0\\0&0&5\end{pmatrix} - \begin{pmatrix}4\frac{4}{7}&0&0\\0&4\frac{4}{7}&0\\0&0&4\frac{4}{7}\end{pmatrix}\right]^2 \frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \\
&=\; \frac{1}{14}\,(1,\;2,\;3)\left[\begin{pmatrix}-1\frac{4}{7}&0&0\\0&-\frac{4}{7}&0\\0&0&\frac{3}{7}\end{pmatrix}\right]^2 \begin{pmatrix}1\\2\\3\end{pmatrix} \\
&=\; \frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}-\frac{11}{7}&0&0\\0&-\frac{4}{7}&0\\0&0&\frac{3}{7}\end{pmatrix}\begin{pmatrix}-\frac{11}{7}&0&0\\0&-\frac{4}{7}&0\\0&0&\frac{3}{7}\end{pmatrix}\begin{pmatrix}1\\2\\3\end{pmatrix} \\
&=\; \frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}-\frac{11}{7}&0&0\\0&-\frac{4}{7}&0\\0&0&\frac{3}{7}\end{pmatrix}\begin{pmatrix}-11/7\\-8/7\\9/7\end{pmatrix} \;=\; \frac{1}{14}\,(1,\;2,\;3)\begin{pmatrix}121/49\\32/49\\27/49\end{pmatrix} \\
&=\; \frac{1}{14}\left(121/49 + 64/49 + 81/49\right) \;=\; \frac{1}{14}\,\frac{266}{49} \;=\; \frac{2\cdot 7\cdot 19}{2\cdot 7^3} \;=\; \frac{19}{49} \;\approx\; 0.39 \\
\Rightarrow \quad \triangle \mathcal{A}_\psi \;&=\; \frac{\sqrt{19}}{7} \;\approx\; 0.62\,.
\end{aligned}$$

Postscript: The term "uncertainty" has the same meaning in quantum mechanics as the term "standard deviation" does in statistics for discrete systems. The two terms are closely related for continuous systems. Two uncertainties are multiplied in the **Heisenberg uncertainty principle**.

The conventional way to write the definition of uncertainty is $\triangle \mathcal{A} \;=\; <\left(\mathcal{A} - <\mathcal{A}>\right)^2>^{1/2}$, where the state vector and identity operator are implicit.

Variance is the square of standard deviation, or $\left(\triangle \mathcal{A}_\psi\right)^2 \;=\; <\psi\,|\left(\mathcal{A} - <\mathcal{A}>\mathcal{I}\right)^2|\,\psi>$. Variance is often a convenient intermediate result in a calculation of uncertainty or standard deviation having the advantage that it avoids the square root.

2–11. Show that $\triangle \mathcal{A}_\psi = <\psi\,|\,\mathcal{A}^2 - <\mathcal{A}>^2\,\mathcal{I}\,|\,\psi>^{1/2}$.

This alternative is often the most direct way to calculate an uncertainty. A useful theorem from probability and statistics is that $<\mathcal{A}+\mathcal{B}> = <\mathcal{A}> + <\mathcal{B}>$. See Meyer[1] or another reference for depth concerning this theorem.

Work with variance and take a square root as the last step to obtain uncertainty. That $<\mathcal{A}+\mathcal{B}> = <\mathcal{A}> + <\mathcal{B}>$ is used twice. That $<\psi\,|\,\mathcal{A}<\mathcal{A}>\mathcal{I}\,|\,\psi> = <\psi|\,<\mathcal{A}>^2\,\mathcal{I}\,|\,\psi>$ is not obvious, however,

$$\begin{aligned}<\psi\,|\,\mathcal{A}<\mathcal{A}>\mathcal{I}\,|\,\psi> &= <\psi\,|\,\mathcal{A}<\mathcal{A}>\,|\,\psi> = <\mathcal{A}><\psi\,|\,\mathcal{A}\,|\,\psi> = <\mathcal{A}><\mathcal{A}> \\ &= <\mathcal{A}>^2 = <\mathcal{A}>^2<\psi\,|\,\psi> = <\psi|\,<\mathcal{A}>^2\,|\,\psi> = <\psi|\,<\mathcal{A}>^2\,\mathcal{I}\,|\,\psi>\end{aligned}$$

where $<\psi\,|\,\psi>$ is multiplication by a convenient form of one given a normalized $|\,\psi>$.

$$\begin{aligned}\left(\triangle \mathcal{A}_\psi\right)^2 &= <\psi\,|\left(\mathcal{A} - <\mathcal{A}>\mathcal{I}\right)^2|\,\psi> \\ &= <\psi\,|\left(\mathcal{A} - <\mathcal{A}>\mathcal{I}\right)\left(\mathcal{A} - <\mathcal{A}>\mathcal{I}\right)|\,\psi> \\ &= <\psi\,|\,\mathcal{A}^2 - \mathcal{A}<\mathcal{A}>\mathcal{I} - <\mathcal{A}>\mathcal{I}\mathcal{A} + <\mathcal{A}>^2\mathcal{I}\,|\,\psi> \qquad (1) \\ &= <\psi\,|\,\mathcal{A}^2 - 2\mathcal{A}<\mathcal{A}>\mathcal{I} + <\mathcal{A}>^2\mathcal{I}\,|\,\psi> \qquad (2) \\ &= <\psi\,|\,\mathcal{A}^2\,|\,\psi> - <\psi\,|\,2\mathcal{A}<\mathcal{A}>\mathcal{I}\,|\,\psi> + <\psi|\,<\mathcal{A}>^2\,\mathcal{I}\,|\,\psi> \qquad (3) \\ &= <\psi\,|\,\mathcal{A}^2\,|\,\psi> - 2<\psi|\,<\mathcal{A}>^2\,\mathcal{I}\,|\,\psi> + <\psi|\,<\mathcal{A}>^2\,\mathcal{I}\,|\,\psi> \qquad (4) \\ &= <\psi\,|\,\mathcal{A}^2\,|\,\psi> - <\psi|\,<\mathcal{A}>^2\,\mathcal{I}\,|\,\psi> \\ &= <\psi\,|\,\mathcal{A}^2 - <\mathcal{A}>^2\,\mathcal{I}\,|\,\psi> \qquad (5) \\ \Rightarrow \quad \triangle \mathcal{A}_\psi &= <\psi\,|\,\mathcal{A}^2 - <\mathcal{A}>^2\,\mathcal{I}\,|\,\psi>^{1/2}.\end{aligned}$$

Line (1) uses the fact that $\mathcal{I}^2 = \mathcal{I}$. An operator $\mathcal{A}$ commutes with the scalar $<\mathcal{A}>$ and the identity operator in line (2). Line (3) uses $<\mathcal{A}+\mathcal{B}> = <\mathcal{A}> + <\mathcal{B}>$. Equation (4) depends on the fact that $<\psi\,|\,\mathcal{A}<\mathcal{A}>\mathcal{I}\,|\,\psi> = <\psi|\,<\mathcal{A}>^2\,\mathcal{I}\,|\,\psi>$. Line (5) uses the identity $<\mathcal{A}> + <\mathcal{B}> = <\mathcal{A}+\mathcal{B}>$ again.

Postscript: Uncertainty is often written $\triangle \mathcal{A} = \left(\mathcal{A}^2 - <\mathcal{A}>^2\right)^{1/2}$, where the state vector and the identity operator are both implied.

2–12. Calculate the uncertainty of $\mathcal{A}$ from problem 2–10 using the result of problem 2–11.

The state vector $|\,\psi>$ must be the same used in problem 2–10 to obtain the same result.

---

[1] Meyer *Introductory Probability and Statistical Applications* (Addison-Wesley Publishing Co., Reading, Massachusetts, 1970), pp.123–136.

$$
\begin{aligned}
\mathcal{A}^2 - <\mathcal{A}>^2 \mathcal{I} &= \begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix}^2 - \left(\frac{32}{7}\right)^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix} \begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix} - \frac{1024}{49} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} 9 & 0 & 0 \\ 0 & 16 & 0 \\ 0 & 0 & 25 \end{pmatrix} - \begin{pmatrix} 1024/49 & 0 & 0 \\ 0 & 1024/49 & 0 \\ 0 & 0 & 1024/49 \end{pmatrix} \\
&= \begin{pmatrix} 441/49 & 0 & 0 \\ 0 & 784/49 & 0 \\ 0 & 0 & 1225/49 \end{pmatrix} - \begin{pmatrix} 1024/49 & 0 & 0 \\ 0 & 1024/49 & 0 \\ 0 & 0 & 1024/49 \end{pmatrix} \\
&= \begin{pmatrix} -583/49 & 0 & 0 \\ 0 & -240/49 & 0 \\ 0 & 0 & 201/49 \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
\Rightarrow \quad \triangle \mathcal{A}_\psi &= <\psi\,|\,\mathcal{A}^2 - <\mathcal{A}>^2 \mathcal{I}\,|\,\psi>^{1/2} \\
&= \left[\frac{1}{\sqrt{14}}\,(1,\ 2,\ 3) \begin{pmatrix} -583/49 & 0 & 0 \\ 0 & -240/49 & 0 \\ 0 & 0 & 201/49 \end{pmatrix} \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}\right]^{1/2} \\
&= \left[\frac{1}{14}\,(1,\ 2,\ 3) \begin{pmatrix} -583/49 \\ -480/49 \\ 603/49 \end{pmatrix}\right]^{1/2} = \left[\frac{1}{14 \cdot 49}(-583 - 960 + 1809)\right]^{1/2} \\
&= \sqrt{\frac{266}{2 \cdot 7^3}} = \sqrt{\frac{2 \cdot 7 \cdot 19}{2 \cdot 7^3}} = \sqrt{\frac{19}{49}} = \frac{\sqrt{19}}{7}\,.
\end{aligned}
$$

2–13. Find the uncertainty for $|\psi> = \begin{pmatrix} 3i \\ 2 \end{pmatrix}$, $\mathcal{C} = \begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}$ using both formulations.

This example features a non-diagonal operator with imaginary components. The normalized state vector is $|\psi> = \frac{1}{\sqrt{13}} \begin{pmatrix} 3i \\ 2 \end{pmatrix}$ and the expectation value is $\frac{87}{13}$. Obtain uncertainty as a last step by taking the square root of variance.

$$
\begin{aligned}
(\triangle \mathcal{C})^2 &= \frac{1}{\sqrt{13}}(-3i\,,\ \ 2) \left[\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} - \begin{pmatrix} \frac{87}{13} & 0 \\ 0 & \frac{87}{13} \end{pmatrix}\right]^2 \frac{1}{\sqrt{13}} \begin{pmatrix} 3i \\ 2 \end{pmatrix} \\
&= \frac{1}{13}(-3i\,,\ \ 2) \left[\begin{pmatrix} \frac{39}{13} & \frac{52}{13}i \\ -\frac{52}{13}i & \frac{39}{13} \end{pmatrix} - \begin{pmatrix} \frac{87}{13} & 0 \\ 0 & \frac{87}{13} \end{pmatrix}\right]^2 \begin{pmatrix} 3i \\ 2 \end{pmatrix} \\
&= \frac{1}{13}(-3i\,,\ \ 2) \left[\begin{pmatrix} -\frac{48}{13} & \frac{52}{13}i \\ -\frac{52}{13}i & -\frac{48}{13} \end{pmatrix}\right]^2 \begin{pmatrix} 3i \\ 2 \end{pmatrix}
\end{aligned}
$$

$$= \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} -48 & 52i \\ -52i & -48 \end{pmatrix}\begin{pmatrix} -48 & 52i \\ -52i & -48 \end{pmatrix}\begin{pmatrix} 3i \\ 2 \end{pmatrix}$$

$$= \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} -48 & 52i \\ -52i & -48 \end{pmatrix}\begin{pmatrix} -144i+104i \\ 156-96 \end{pmatrix}$$

$$= \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} -48 & 52i \\ -52i & -48 \end{pmatrix}\begin{pmatrix} -40i \\ 60 \end{pmatrix} = \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} 1920i+3120i \\ -2080-2880 \end{pmatrix}$$

$$= \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} 5040i \\ -4960 \end{pmatrix} = \frac{1}{13^3}(15120-9920) = \frac{5200}{13^3} = \frac{400}{13^2} \quad \Rightarrow \quad \triangle\mathcal{C} = \frac{20}{13}.$$

$$(\triangle\mathcal{C})^2 = \frac{1}{\sqrt{13}}(-3i,\ 2)\left[\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}^2 - \begin{pmatrix} \frac{87}{13} & 0 \\ 0 & \frac{87}{13} \end{pmatrix}^2\right]\frac{1}{\sqrt{13}}\begin{pmatrix} 3i \\ 2 \end{pmatrix}$$

$$= \frac{1}{13}(-3i,\ 2)\left[\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix} - \begin{pmatrix} \frac{87}{13} & 0 \\ 0 & \frac{87}{13} \end{pmatrix}\begin{pmatrix} \frac{87}{13} & 0 \\ 0 & \frac{87}{13} \end{pmatrix}\right]\begin{pmatrix} 3i \\ 2 \end{pmatrix}$$

$$= \frac{1}{13}(-3i,\ 2)\left[\begin{pmatrix} 25 & 24i \\ -24i & 25 \end{pmatrix} - \begin{pmatrix} \frac{7569}{169} & 0 \\ 0 & \frac{7569}{169} \end{pmatrix}\right]\begin{pmatrix} 3i \\ 2 \end{pmatrix}$$

$$= \frac{1}{13^3}(-3i,\ 2)\left[\begin{pmatrix} 4225 & 4056i \\ -4056i & 4225 \end{pmatrix} - \begin{pmatrix} 7569 & 0 \\ 0 & 7569 \end{pmatrix}\right]\begin{pmatrix} 3i \\ 2 \end{pmatrix}$$

$$= \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} -3344 & 4056i \\ -4056i & -3344 \end{pmatrix}\begin{pmatrix} 3i \\ 2 \end{pmatrix} = \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} -10032i+8112i \\ 12168-6688 \end{pmatrix}$$

$$= \frac{1}{13^3}(-3i,\ 2)\begin{pmatrix} -1920i \\ 5480 \end{pmatrix} = \frac{1}{13^3}(-5760+10960) = \frac{5200}{13^3} = \frac{400}{13^2} \Rightarrow \triangle\mathcal{C} = \frac{20}{13}.$$

2–14. Given that $|v> \rightarrow \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$ and $<w| \rightarrow (3,\ 4,\ 5)$, find $|v><w|$.

$|v><w|$ is an **outer product**. If $|v> \rightarrow \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix}$ and $<w| \rightarrow (w_1,\ w_2,\ w_3,\ \cdots)$,

then $$|v><w| = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix}(w_1,\ w_2,\ w_3,\ \cdots) = \begin{pmatrix} v_1w_1 & v_1w_2 & v_1w_3 & \cdots \\ v_2w_1 & v_2w_2 & v_2w_3 & \cdots \\ v_3w_1 & v_3w_2 & v_3w_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

is the outer product, sometimes called a **dyad**. The outer product of two vectors is an operator.

$$|v><w| = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}(3,\ 4,\ 5) = \begin{pmatrix} 1\cdot3 & 1\cdot4 & 1\cdot5 \\ 2\cdot3 & 2\cdot4 & 2\cdot5 \\ 3\cdot3 & 3\cdot4 & 3\cdot5 \end{pmatrix} = \begin{pmatrix} 3 & 4 & 5 \\ 6 & 8 & 10 \\ 9 & 12 & 15 \end{pmatrix}$$

Postscript: Outer products will be used to form **projection operators** and to express **completeness relations**.

2–15. (a) Find the projection operator for the ket $|2>$ in the basis of unit vectors where $|1>$ is the first unit vector.

(b) Apply this projection operator to an arbitrary ket.

(c) Apply this projection operator to an arbitrary bra.

The projection operator is defined $\mathcal{P}_i = |i><i|$ for the ket $|i>$, where $|i>$ and $<i|$ are corresponding unit vectors. Here, $|2> = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$. Use $|v> = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix}$ as the arbitrary ket.

(a) $$|2><2| = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} (0,\ 1,\ 0,\ \cdots) = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

(b) $$|2><2|v> = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 \\ v_2 \\ 0 \\ \vdots \end{pmatrix}.$$

(c) $$<v|2><2| = (v_1,\ v_2,\ v_3,\ \cdots) \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = (0,\ v_2,\ 0,\ \cdots).$$

Postscript: The projection operator $|2><2|$ selects the second component from any ket or bra. It "projects" the second component from the original vector. The result of operation with the projection operator $|2><2|$ is a vector of the original type with the original second component and all other components zero. Similarly, $\mathcal{P}_4$ will project the fourth component from any vector, and $\mathcal{P}_i$ will project the i^{th} component from any vector.

2–16. What is the meaning of the consecutive projection operators $\mathcal{P}_i \mathcal{P}_j$?

Let the operator $\mathcal{P}_i \mathcal{P}_j$ act on a ket to the right, for instance, $\mathcal{P}_i \mathcal{P}_j |v>$. Then $\mathcal{P}_j$ selects the j^{th} component, and all other components are zero. So $\mathcal{P}_i$ operates on a vector with one non-zero component. If the non-zero component is in the i^{th} place in the vector, the operation with $\mathcal{P}_i$ will return the same ket with one non-zero component. If the non-zero component is in other than the i^{th} place in the vector, the operation with $\mathcal{P}_i$ will return the zero vector. This reduction illustrates the use of Dirac notation and the Kronecker delta, and assumes orthonormality.

$$\mathcal{P}_i \mathcal{P}_j = |i><i|j><j| = |i>\,\delta_{ij}\,<j| = |i><j|\,\delta_{ij} = |i><i| = \mathcal{P}_i.$$

Postscript: $< i \,|\, j > \;=\; \delta_{ij}$ is the assumption of orthonormality. The eigenvectors of any Hermitian operator are orthogonal, so can be made orthonormal through a normalization process. Orthonormality is essentially a necessary condition for many quantum mechanical calculations.

Notice that $< j \,|\, \delta_{ij} \;=\; < i \,|$. It says that the only condition under which this product is non-zero is when $i = j$. Should $i \neq j$, the result is zero. A state vector that is zero indicates the absence of a system which is generally not of interest so cases that are zero are usually ignored.

The problem could be finished $|\, i > \delta_{ij} \; < j \,| \;=\; |\, j >< j \,| \;=\; \mathcal{P}_j$ because $i = j \;\Leftrightarrow\; j = i$.

2–17. Express the completeness relation in three dimensions.

In any given space, there are as many projection operators as the dimension of the space. Add them all to obtain an identity operator, that is

$$\sum_i \mathcal{P}_i \;=\; \sum_i |\, i >< i \,| \;=\; \mathcal{I}$$

which is the **completeness relation**. It is a **resolution of the identity**, or another form of an identity operator. The completeness relation can be expressed in arbitrary or infinite dimensions.

$$\sum_{i=1}^{3} \mathcal{P}_i \;=\; \sum_{i=1}^{3} |\, i >< i \,| \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 1, & 0, & 0 \end{pmatrix} \;+\; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0, & 1, & 0 \end{pmatrix} \;+\; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \begin{pmatrix} 0, & 0, & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathcal{I} \,.$$

Postscript: An identity operator is the analogy of the real number "1" in its space. Just as multiplying by any form of 1 does not change the magnitude of a quantity, operating with $\mathcal{I}$ does not change an object in a vector space. The identity operator can be inserted in any expression in any place in any form including the completeness relation without affecting the meaning of other objects in the expression. Then as some portions operate to the left and other portions operate to the right, forms may emerge that may be illuminating.

2–18. Expand $|\, \psi > \;=\; \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$ in the eigenbases of (a) $\mathcal{A} \;=\; \begin{pmatrix} 3 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix}$ and (b) $\mathcal{L}_y \;=\; \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$.

(c) Check your expansions by calculating the probabilities of measuring each eigenvalue using the expansion coefficients.

A vector may be expressed in any eigenbasis that spans the appropriate space. The eigenvectors of Hermitian operators can therefore be used to represent any vector of the same dimension.

The first step is to obtain the eigenvectors by solving the eigenvalue/eigenvector problem, and that has been previously completed for both of the given operators. Next, consider

$$|\,\psi> \;=\; \mathcal{I}\,|\,\psi> \;=\; \left(\sum_{i=1}^{n} |\,\alpha_i><\alpha_i\,|\right)|\,\psi> \;=\; \sum_{i=1}^{n} |\,\alpha_i>\left(<\alpha_i\,|\,\psi>\right) \;=\; \sum_{i=1}^{n} c_i\,|\,\alpha_i>,$$

where the c_i are complex numbers that are the inner product of each $<\alpha_i\,|\,\psi>$. The process described by this equation is known as **expansion in an eigenbasis** and the c_i are called both **expansion coefficients** and **probability amplitudes**.

Per the eigenvalue and probability postulates, eigenvalues are measured with the probabilities

$$P\,(\alpha_i) \;=\; \left|<\alpha_i\,|\,\psi>\right|^2 \;=\; \left|\,c_i\,\right|^2,$$

given that the eigenvectors and the state vector are normalized. The eigenvectors of $\mathcal{A}$ are unit vectors that are inherently of unit length. The eigenvectors of $\mathcal{L}_y$, however, contain normalization constants of $1/2$ and $1/\sqrt{2}$ that cannot be absorbed into the expansion coefficients in part (b).

(a) The expansion can be done by inspection when the eigenvectors are unit vectors, nevertheless,

$$\begin{aligned}
|\,\psi> \;&=\; \sum_{i=1}^{3} |\,\alpha_i><\alpha_i\,|\,\psi> \\
&=\; \begin{pmatrix}1\\0\\0\end{pmatrix}(1,\;0,\;0)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}(0,\;1,\;0)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} + \begin{pmatrix}0\\0\\1\end{pmatrix}(0,\;0,\;1)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \\
&=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\0\\0\end{pmatrix}(1+0+0) \;+\; \frac{1}{\sqrt{14}}\begin{pmatrix}0\\1\\0\end{pmatrix}(0+2+0) \;+\; \frac{1}{\sqrt{14}}\begin{pmatrix}0\\0\\1\end{pmatrix}(0+0+3) \\
&=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\0\\0\end{pmatrix} \;+\; \frac{2}{\sqrt{14}}\begin{pmatrix}0\\1\\0\end{pmatrix} \;+\; \frac{3}{\sqrt{14}}\begin{pmatrix}0\\0\\1\end{pmatrix},
\end{aligned}$$

where the last expression is the expansion of the state vector in the eigenbasis of $\mathcal{A}$.

(b) The expansion of the state vector in the eigenbasis of $\mathcal{L}_y$ is

$$\begin{aligned}
|\,\psi> \;&=\; \sum_{i=1}^{3} |\,\alpha_i><\alpha_i\,|\,\psi> \\
&=\; \left[\frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\,i\\-1\end{pmatrix}\right]\frac{1}{2}\,(1,\;\sqrt{2}\,i,\;-1)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} + \left[\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}\right]\frac{1}{\sqrt{2}}\,(1,\;0,\;1)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \\
&\qquad\qquad + \left[\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\,i\\-1\end{pmatrix}\right]\frac{1}{2}\,(1,\;-\sqrt{2}\,i,\;-1)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \\
&=\; \left[\frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\,i\\-1\end{pmatrix}\right]\frac{1}{2\sqrt{14}}\,(1+2\sqrt{2}\,i-3) \;+\; \left[\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}\right]\frac{1}{\sqrt{28}}\,(1+0+3)
\end{aligned}$$

$$+ \left[\frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2}\,i \\ -1 \end{pmatrix}\right] \frac{1}{2\sqrt{14}}\left(1 - 2\sqrt{2}\,i - 3\right)$$

$$= \frac{-1+\sqrt{2}\,i}{\sqrt{14}}\left[\frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2}\,i \\ -1 \end{pmatrix}\right] + \frac{4}{\sqrt{28}}\left[\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}\right] + \frac{-1-\sqrt{2}\,i}{\sqrt{14}}\left[\frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2}\,i \\ -1 \end{pmatrix}\right].$$

(c) The six probabilities are

$$P(3) = \left|\frac{1}{\sqrt{14}}\right|^2 = \frac{1}{14}, \quad P(4) = \left|\frac{2}{\sqrt{14}}\right|^2 = \frac{4}{14}, \quad P(5) = \left|\frac{3}{\sqrt{14}}\right|^2 = \frac{9}{14} \quad \text{for } \mathcal{A}, \text{ and}$$

$$P(-\sqrt{2}) = \left|\frac{-1+\sqrt{2}i}{\sqrt{14}}\right|^2 = \left(\frac{-1-\sqrt{2}i}{\sqrt{14}}\right)\left(\frac{-1+\sqrt{2}i}{\sqrt{14}}\right) = \frac{1+2}{14} = \frac{3}{14},$$

$$P(0) = \left|\frac{4}{\sqrt{28}}\right|^2 = \frac{16}{28} = \frac{8}{14},$$

$$P(\sqrt{2}) = \left|\frac{-1-\sqrt{2}i}{\sqrt{14}}\right|^2 = \left(\frac{-1+\sqrt{2}i}{\sqrt{14}}\right)\left(\frac{-1-\sqrt{2}i}{\sqrt{14}}\right) = \frac{1+2}{14} = \frac{3}{14}, \quad \text{for } \mathcal{L}_y.$$

Postscript: Combining all the constants in the last line of part (b) yields a simpler expression, but the simpler expression hides the expansion coefficients $c_i = <\alpha_i\,|\,\psi>$, and the capability to calculate probabilities from the simpler expression is compromised.

Using expansion coefficients to calculate probabilities is dominantly the most efficient method for some of the problems that will be encountered. The other reason to introduce the technique of expansion in an eigenbasis is that it is essential to the **time evolution** of the **stationary states** that are the solutions to the time-dependent Schrodinger equation.

2–19. (a) Write the basis-independent Hamiltonian for a free particle.

(b) Write the basis-independent Hamiltonian for a simple harmonic oscillator (SHO).

(c) Write the Hamiltonian for a free particle in position space.

(d) Write the Hamiltonian for a simple harmonic oscillator in position space.

(e) Write the Hamiltonian for an unknown potential in position space.

(f) Write the Hamiltonian for a free particle in momentum space.

(g) Write the Hamiltonian for a simple harmonic oscillator in momentum space.

The Hamiltonian operator is intrinsic to the Schrodinger postulate. This problem is an intermediate step to writing the Schrodinger equation for systems under the influence of various potentials.

The classical Hamiltonian is $H = T + V$. The non-relativistic kinetic energy term is $T = p^2/2m$. The free particle is not influenced by any potential so the potential energy term for

a free particle is $V(x) = 0$. The potential energy function for a simple harmonic oscillator is $V(x) = kx^2/2$. The dynamic variables of classical mechanics become quantum mechanical operators, $x \to \mathcal{X}$ and $p \to \mathcal{P}$ as $H \to \mathcal{H}$, all in Hilbert space. A quantum mechanical Hamiltonian $\mathcal{H}$ expressed in terms of the basis-independent operators $\mathcal{X}$ and $\mathcal{P}$ is basis-independent.

Transitioning from Hilbert space is the act of **representation**. In the position basis in one spatial dimension, $\mathcal{X} \to x$ and $\mathcal{P} \to -i\hbar \dfrac{d}{dx}$. In the momentum basis, $\mathcal{P} \to p$, $\mathcal{X} \to i\hbar \dfrac{d}{dp}$. Substitute these differential operators in the basis-independent Hamiltonian operators of parts (a) and (b) to obtain the basis-dependent Hamiltonian operators for parts (c) through (g).

(a) $\mathcal{H} = \dfrac{\mathcal{P}^2}{2m}$ for a free particle in Hilbert space.

(b) $\mathcal{H} = \dfrac{\mathcal{P}^2}{2m} + \dfrac{1}{2}k\mathcal{X}^2$ for an SHO in Hilbert space.

(c) $\mathcal{H} = \dfrac{\mathcal{P}^2}{2m} \to -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2}$ for a free particle in position space.

(d) $\mathcal{H} = \dfrac{\mathcal{P}^2}{2m} + \dfrac{1}{2}k\mathcal{X}^2 \to -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2} + \dfrac{1}{2}kx^2$ for an SHO in position space.

(e) $\mathcal{H} = \dfrac{\mathcal{P}^2}{2m} + \mathcal{V}(\mathcal{X}) \to -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2} + V(x)$ for an unknown potential in position space.

(f) $\mathcal{H} = \dfrac{\mathcal{P}^2}{2m} \to \dfrac{p^2}{2m}$ for a free particle in momentum space.

(g) $\mathcal{H} = \dfrac{\mathcal{P}^2}{2m} + \dfrac{1}{2}k\mathcal{X}^2 \to \dfrac{p^2}{2m} - \dfrac{\hbar^2}{2}k\dfrac{d^2}{dp^2}$ for an SHO in momentum space.

Postscript: Explanations for $\mathcal{X} \to x$ and $\mathcal{P} \to -i\hbar \dfrac{d}{dx}$ in position space are provided in chapter 5. Accept that these and the momentum based representations are correct and use them. These representations are much more useful than the details that are necessary to derive them.

Notice that each potential is, or is assumed to be in part (e), a function of position only; that $\mathcal{H} \neq \mathcal{H}(t)$. This leads to the **time-independent Schrodinger equation**.

2–20. Discuss how the time-independent Schrodinger equation, $\mathcal{H}\,|\,E_i> = E_i\,|\,E_i>$, follows from the time-dependent Schrodinger equation stated in the Schrodinger postulate.

A time-dependent quantum mechanical Hamiltonian, $\mathcal{H} = \mathcal{H}(t)$, has matrix elements that are functions of time. A Schrodinger equation in which the Hamiltonian is independent of time is known as a **time-independent Schrodinger equation**. When $\mathcal{H} \neq \mathcal{H}(t)$, the time-dependence becomes simple and probabilities, expectation values, and uncertainties are time-independent.

Total energy is represented $\mathcal{E} \to i\hbar \dfrac{d}{dt}$. The differential operator form is seen in the time-dependent Schrodinger equation.

The Hamiltonian is the total energy operator. Energy is an observable quantity so the Hamiltonian is necessarily a Hermitian operator per the observables postulate. Any state vector can be expanded in terms of the eigenvectors of the Hermitian Hamiltonian. The eigenvectors of the Hamiltonian are the energy eigenvectors, represented $|\,E_i>$, and the eigenvalues of the Hamiltonian are the energy eigenvalues, denoted E_i. Thus,

$$\mathcal{H}\,|\,\psi> \;=\; i\hbar\frac{d}{dt}\,|\,\psi> \;\longrightarrow\; \mathcal{H}\,|\,\psi> \;=\; \mathcal{E}\,|\,\psi> \;\longrightarrow\; \mathcal{H}\,|\,E_i> = \;\mathcal{E}\,|\,E_i>,$$

and assuming that $\mathcal{H} \neq \mathcal{H}(t)$, the last equation is simply an eigenvalue/eigenvector equation so that $\mathcal{E}$ can be nothing other than the energy eigenvalues, or $\mathcal{H}\,|\,E_i> \;=\; E_i\,|\,E_i>$.

Postscript: The time-dependent Schrodinger equation must be used when $\mathcal{H} = \mathcal{H}(t)$, and it is often difficult or impossible to solve analytically. The usual approach to a Schrodinger equation with a weakly time-dependent Hamiltonian is to find a time-independent solution and then model the time dependence as a perturbation. A numerical solution is often the only recourse if the Hamiltonian is strongly time dependent.

The representations for position and momentum presented in problem 2–19 will be supported while developing continuous systems in chapter 5. Time is a parameter with which no quantum mechanical operator is associated[2], and other than to point to the Schrodinger postulate, the representation $\mathcal{E} \rightarrow i\hbar\,\dfrac{d}{dt}$ is beyond our scope. Time is a scalar quantity in this text.

2–21. Show that $|\,E_i\,(t)> \;=\; e^{-iE_it/\hbar}\,|\,E_i>$ for a system having a time-independent Hamiltonian.

This problem is an introduction to **time evolution**. It is concurrently an introduction to **stationary states**. Stationary states are the energy eigenstates $|\,E_i>$ of a time-independent Hamiltonian and the solutions to the time-independent Schrodinger equation. The stationary states evolve in time proportionally to the exponential of the energy eigenvalue.

Use the condition of time-independence of the Hamiltonian in the time-dependent Schrodinger equation to reason that

$$i\hbar\,\frac{d}{dt}\,|\,E_i\,(t)> \;=\; E_i\,|\,E_i\,(t)>$$

for individual eigenstates of $\mathcal{H}$. This is a variables separable differential equation, so separate the variables and integrate both sides from 0 to t. The last step is to substitute the conventional notation $|\,E_i>$ for $|\,E_i\,(0)>$.

The time-dependent Schrodinger equation is $i\hbar\,\dfrac{d}{dt}\,|\,\psi\,(t)\,> \;=\; \mathcal{H}\,|\,\psi\,(t)\,>$, where the time-dependence of the state vector is indicated explicitly. The state vector can be expanded into a linear combination of the eigenvectors (state vector postulate) of the total energy operator $\mathcal{H}$. Denote the energy eigenstates for the total energy operator $|\,E_i\,(t)>$. The eigenstates must be functions

[2] Cohen-Tannoudji, Diu, & Laloe, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), 4th ed., pp. 252.

of time if the state vector is a function of time. A state vector can be an individual eigenstate, therefore the time-dependent Schrodinger equation applies to each eigenstate individually. If the Hamiltonian is time-independent, the eigenvalues are time-independent (eigenvalues are determined solely by the operator), and $\mathcal{H}\,|\,E_i> \;=\; E_i\,|\,E_i>$ from the last problem. Therefore,

$$i\hbar\frac{d}{dt}\,|\,E_i\,(t)> \;=\; E_i\,|\,E_i(t)>\,,$$

where the eigenvalues are constants and not functions of time, again, because the Hamiltonian is independent of time. This is a variables separable differential equation that can be arranged

$$\frac{d\,|\,E_i\,(t)>}{|\,E_i\,(t)>} \;=\; \frac{E_i}{i\hbar}\,dt \qquad \Rightarrow \qquad \int_0^t \frac{d\,|\,E_i\,(t')>}{|\,E_i\,(t')>} \;=\; \frac{E_i}{i\hbar}\int_0^t dt'$$

where the independent variable is primed to differentiate it from the upper limit of integration. Multiplying numerator and denominator of the right side by i, the last equation implies

$$\begin{aligned}
&\ln\Big(\,|\,E_i\,(t')>\Big)\Big|_0^t \;=\; \frac{-iE_i}{\hbar}\,t'\,\Big|_0^t \\
&\Rightarrow \qquad \ln|\,E_i\,(t)> - \;\ln|\,E_i\,(0)> \;=\; -iE_it/\hbar \\
&\Rightarrow \qquad \ln\left(\frac{|\,E_i\,(t)>}{|\,E_i\,(0)>}\right) \;=\; -iE_it/\hbar \\
&\Rightarrow \qquad \frac{|\,E_i\,(t)>}{|\,E_i\,(0)>} \;=\; e^{-iE_it/\hbar} \\
&\Rightarrow \qquad |\,E_i\,(t)> \;=\; e^{-iE_it/\hbar}\,|\,E_i\,(0)> \;=\; e^{-iE_it/\hbar}\,|\,E_i>
\end{aligned}$$

after substituting $|\,E_i>$ for $|\,E_i\,(0)>$ as is conventional.

Postscript: The time evolution of an energy eigenstate is described by the product of $e^{-iE_it/\hbar}$ and that energy eigenstate. The state vector is a superposition of all the eigenstates, so

$$|\,\psi> \;=\; \sum_i c_i\,|\,E_i> \qquad \Rightarrow \qquad |\,\psi\,(t)> \;=\; \sum_i c_i\,|\,E_i>\,e^{-iE_it/\hbar}$$

where $\mathcal{H} \neq \mathcal{H}\,(t)$. The energy eigenstates $|\,E_i>$ are known as stationary states. The probability of a measurement for a state vector which is a function of time is unaffected when $\mathcal{H} \neq \mathcal{H}\,(t)$; the probabilities are the same as the time-independent case. The probabilities are "stationary" as time advances, and probability density is independent of time. Stationary states are the result of time being separable from other observable quantities. The prerequisite for time being separable from other observables is a time-independent Hamiltonian.

This problem explicitly uses time as an independent variable within ket vectors. Time is the only quantity that can be used this way. Time is not an observable quantity in the same sense as position and momentum. Time is intrinsic to all spaces. The notation $|\,\psi\,(t)>$ says only that time moves forward (or backward) in every space.

2–22. (a) Find the time-dependent state vector for

$$|\,\psi(t=0)\!> \;=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} \qquad \text{where} \qquad \mathcal{H} \;=\; \begin{pmatrix}3&0&0\\0&4&0\\0&0&5\end{pmatrix}.$$

(b) Calculate the probability of each possible result of a measurement of energy as the state vector evolves in time.

First, notice that $\mathcal{H} \neq \mathcal{H}(t)$. Part (a) requires you to apply the expansion of problem 2–18. Remember that $|\,\psi(t)\!>$ is a superposition of all time-evolving eigenstates, in this case

$$|\,\psi(t)\!> \;=\; \sum_{i=1}^{3} c_i\,|\,E_i\!>\, e^{-iE_it/\hbar}\,.$$

Having expanded this state vector in the eigenbasis of this operator previously, there is little to do for part (a) except to write the answer. Part (b) is a numerical example illustrating the fact that the time evolution of stationary states does not affect calculations of probabilities.

(a) The energy eigenvalues corresponding to the energy eigenvectors are $E_i = 3,\ 4,$ and 5, so

$$|\,\psi(t)\!> \;=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\0\\0\end{pmatrix}e^{-i3t/\hbar} \;+\; \frac{2}{\sqrt{14}}\begin{pmatrix}0\\1\\0\end{pmatrix}e^{-i4t/\hbar} \;+\; \frac{3}{\sqrt{14}}\begin{pmatrix}0\\0\\1\end{pmatrix}e^{-i5t/\hbar} \;=\; \frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\2\,e^{-i4t/\hbar}\\3\,e^{-i5t/\hbar}\end{pmatrix}$$

which is the time-dependent state vector exhibiting time evolution.

(b) The probabilities are

$$\begin{aligned}
P(E=3) \;&=\; \left|\,(1,\ 0,\ 0)\frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\2\,e^{-i4t/\hbar}\\3\,e^{-i5t/\hbar}\end{pmatrix}\right|^2 \;=\; \frac{1}{14}\left|\;e^{-i3t/\hbar}\;\right|^2 \\
&=\; \frac{1}{14}\left(e^{-i3t/\hbar}\right)\left(e^{+i3t/\hbar}\right) \;=\; \frac{1}{14}\,e^0 \;=\; \frac{1}{14}\,. \\
P(E=4) \;&=\; \left|\,(0,\ 1,\ 0)\frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\2\,e^{-i4t/\hbar}\\3\,e^{-i5t/\hbar}\end{pmatrix}\right|^2 \;=\; \frac{1}{14}\left|\,2\,e^{-i4t/\hbar}\,\right|^2 \\
&=\; \frac{1}{14}\left(2\,e^{-i4t/\hbar}\right)\left(2\,e^{+i4t/\hbar}\right) \;=\; \frac{4}{14}\,e^0 \;=\; \frac{4}{14}\,. \\
P(E=5) \;&=\; \left|\,(0,\ 0,\ 1)\frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\2\,e^{-i4t/\hbar}\\3\,e^{-i5t/\hbar}\end{pmatrix}\right|^2 \;=\; \frac{1}{14}\left|\,3\,e^{-i5t/\hbar}\,\right|^2 \\
&=\; \frac{1}{14}\left(3\,e^{-i5t/\hbar}\right)\left(3\,e^{+i5t/\hbar}\right) \;=\; \frac{9}{14}\,e^0 \;=\; \frac{9}{14}\,.
\end{aligned}$$

The probabilities are independent of time and are the same probabilities obtained in problem 2–2 when time evolution was not considered.

2–23. Consider a system described by the Hamiltonian

$$\mathcal{H} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 7 \end{pmatrix}, \quad \text{which at} \quad t = 0 \quad \text{is in the state} \quad |\psi(0)> = \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix}.$$

(a) If the energy is measured, what results can be obtained, and with what probabilities will these results be obtained?

(b) Calculate the expectation value $< \mathcal{H} > = < \psi(0) | \mathcal{H} | \psi(0) >$. Then show that your expectation value agrees with your calculations from part (a) using $< \mathcal{H} > = \sum P(E_i) E_i$.

(c) Expand the initial state vector $|\psi(0)>$ in the energy eigenbasis to calculate the time dependent state vector $|\psi(t)>$.

(d) If the energy is measured at time t, what results can be obtained, and with what probabilities will these results be obtained? Compare your answers with the $t = 0$ case of part (a). Explain why these probabilities are independent of time even though the state vector is time dependent.

(e) Suppose that you measure the energy of the system at $t = 0$ and you find $E = 7$. What is the state vector of the system immediately after your measurement? Now let the system evolve without any additional measurements until $t = 10$. What is the state vector $|\psi(10)>$ at $t = 10$? What energies will you measure if you repeat the energy measurement at $t = 10$?

The eigenvalue postulate addresses the possibilities and the probability postulate determines the respective probabilities for part (a). Notice that the given state vector is normalized. You must find that $< \psi(0) | \mathcal{H} | \psi(0) > = \sum P(E_i) E_i$ for part (b). Use the procedures of problem 2–18 to expand the state vector in the energy eigenbasis. Use the result of problem 2–21 illustrated in problem 2–22 for part (c). The eigenvalue postulate addresses the possibilities and the probability postulate determines the probabilities for part (d), without regard to time dependence. Probability calculations must agree with part (a). When you find $E = 7$ for part (e), the state vector changes in accordance with the eigenvector postulate, so $|\psi(0)> \rightarrow |E = 7>$. There is one possible result with a probability of 1, and the otherwise two possible results have probability zero.

(a) Possible results of a measurement of energy are the energy eigenvalues 3, 5, and 7.

$$P(E_i = 3) = \left| (1,\ 0,\ 0) \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{14}} (1) \right|^2 = \frac{1}{14},$$

$$P(E_i = 5) = \left| (0,\ 1,\ 0) \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{14}} (3) \right|^2 = \frac{9}{14},$$

$$P(E_i = 7) = \left| (0,\ 0,\ 1) \frac{1}{\sqrt{14}} \begin{pmatrix} 1 \\ 3 \\ 2 \end{pmatrix} \right|^2 = \left| \frac{1}{\sqrt{14}} (2) \right|^2 = \frac{4}{14}.$$

Notice that the sum of the probabilities is 1.

(b) The $t = 0$ expectation value of the energy is

$$\begin{aligned} <\mathcal{H}> &= <\psi(0)\,|\,\mathcal{H}\,|\,\psi(0)> = \frac{1}{\sqrt{14}}\begin{pmatrix}1,\ 3,\ 2\end{pmatrix}\begin{pmatrix}3&0&0\\0&5&0\\0&0&7\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\3\\2\end{pmatrix} \\ &= \frac{1}{14}\begin{pmatrix}1,\ 3,\ 2\end{pmatrix}\begin{pmatrix}3\\15\\14\end{pmatrix} = \frac{1}{14}\begin{pmatrix}3+45+28\end{pmatrix} = \frac{76}{14} = \frac{38}{7} \approx 5.43\,, \quad \text{and} \\ \sum_i P(E_i)\,E_i &= \frac{1}{14}3 + \frac{9}{14}5 + \frac{4}{14}7 = \frac{3+45+28}{14} = \frac{76}{14} = \frac{38}{7} \approx 5.43\,. \end{aligned}$$

(c) Expanding the state vector in the energy eigenbasis,

$$\begin{aligned} |\,\psi(0)> &= \sum_i |\,E_i><E_i\,|\,\psi(0)> \\ &= \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}1,\ 0,\ 0\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\3\\2\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0,\ 1,\ 0\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\3\\2\end{pmatrix} + \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0,\ 0,\ 1\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}1\\3\\2\end{pmatrix} \\ &= \frac{1}{\sqrt{14}}\begin{pmatrix}1\\0\\0\end{pmatrix} + \frac{3}{\sqrt{14}}\begin{pmatrix}0\\1\\0\end{pmatrix} + \frac{2}{\sqrt{14}}\begin{pmatrix}0\\0\\1\end{pmatrix}. \end{aligned}$$

With the time zero expansion, we can then write the complete time-dependent state vector

$$\begin{aligned} |\,\psi(t)> &= \sum_i |\,E_i><E_i\,|\,\psi(0)>\, e^{-iE_it/\hbar} \\ &= \frac{1}{\sqrt{14}}\begin{pmatrix}1\\0\\0\end{pmatrix}e^{-i3t/\hbar} + \frac{3}{\sqrt{14}}\begin{pmatrix}0\\1\\0\end{pmatrix}e^{-i5t/\hbar} + \frac{2}{\sqrt{14}}\begin{pmatrix}0\\0\\1\end{pmatrix}e^{-i7t/\hbar} = \frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\3\,e^{-i5t/\hbar}\\2\,e^{-i7t/\hbar}\end{pmatrix}. \end{aligned}$$

(d) At any time, the only possible results of a measurement of energy are the eigenenergies of the system, which are $3,\ 5\,,$ and $7\,.$ The "time-dependent" probabilities are

$$\begin{aligned} P(3) &= \left|\begin{pmatrix}1,\ 0,\ 0\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\3\,e^{-i5t/\hbar}\\2\,e^{-i7t/\hbar}\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{14}}\,e^{-i3t/\hbar}\right|^2 = \frac{1}{14}\,e^{+i3t/\hbar}\,e^{-i3t/\hbar} = \frac{1}{14}\,e^0 = \frac{1}{14}\,, \\ P(5) &= \left|\begin{pmatrix}0,\ 1,\ 0\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\3\,e^{-i5t/\hbar}\\2\,e^{-i7t/\hbar}\end{pmatrix}\right|^2 = \left|\frac{3}{\sqrt{14}}\,e^{-i5t/\hbar}\right|^2 = \frac{9}{14}\,e^{+i5t/\hbar}\,e^{-i5t/\hbar} = \frac{9}{14}\,e^0 = \frac{9}{14}\,, \\ P(7) &= \left|\begin{pmatrix}0,\ 0,\ 1\end{pmatrix}\frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i3t/\hbar}\\3\,e^{-i5t/\hbar}\\2\,e^{-i7t/\hbar}\end{pmatrix}\right|^2 = \left|\frac{2}{\sqrt{14}}\,e^{-i7t/\hbar}\right|^2 = \frac{4}{14}\,e^{+i7t/\hbar}\,e^{-i7t/\hbar} = \frac{4}{14}\,e^0 = \frac{4}{14}\,. \end{aligned}$$

These are exactly the same probabilities obtained in part (a). There is no time dependence in the probabilities because the eigenvectors of the Hamiltonian have only a time-dependent phase that

"cancels" in the sense that $e^0 = 1$ in these calculations. Time dependency will "cancel" in one way or another in all cases that the Hamiltonian is independent of time, *i.e.*, $\mathcal{H} \neq \mathcal{H}(t)$. The probabilities are "stationary" in time, which is the meaning of the term "stationary states."

(e) An energy measurement with the result $E = 7$ forces the system into the energy eigenstate

$$|\psi(t>0)> \;=\; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} e^{-i7t/\hbar} \qquad \Rightarrow \qquad |\psi(t=10)> \;=\; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} e^{-i7(10)/\hbar},$$

so the probability of measuring $E = 7$ at $t = 10$ is

$$\left| \begin{pmatrix} 0, & 0, & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} e^{-i70/\hbar} \right|^2 \;=\; (0+0+1)\, e^{(i70-i70)/\hbar} \;=\; 1 \cdot e^0 \;=\; 1\,,$$

and the probability of measuring any other eigenenergy is zero since

$$\left| \begin{pmatrix} 1, & 0, & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} e^{-i70/\hbar} \right|^2 \;=\; \left| \begin{pmatrix} 0, & 1, & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} e^{-i70/\hbar} \right|^2 \;=\; 0\,.$$

2–24. Consider a system described by the Hamiltonian

$$\mathcal{H} \;=\; \begin{pmatrix} 1 & 3 \\ 3 & 1 \end{pmatrix}, \quad \text{which at} \quad t = 0 \quad \text{is in the state} \quad |\psi(0)> \;=\; \frac{1}{\sqrt{13}} \begin{pmatrix} 2 \\ 3 \end{pmatrix}.$$

(a) Is $\mathcal{H}$ Hermitian?

(b) Solve the eigenvalue/eigenvector problem to obtain the eigenvalues and eigenvectors of $\mathcal{H}$.

(c) If the energy is measured, what results can be obtained, and with what probabilities will these results be obtained?

(d) Calculate the expectation value of the Hamiltonian using both

$$<\mathcal{H}> \;=\; <\psi(0)\,|\,\mathcal{H}\,|\,\psi(0)> \qquad \text{and} \qquad <\mathcal{H}> \;=\; \sum P(E_i)\, E_i\,.$$

(e) Calculate the time dependent state vector $|\psi(t)>$.

(f) If the energy is measured at time t, what results can be obtained, and with what probabilities will these results be obtained? Compare your answer with the $t = 0$ case in part (c).

(g) Diagonalize $\mathcal{H}$ using a unitary transformation. Transform $|\psi(0)>$ and both eigenvectors to be consistent with this unitary transformation.

(h) Find $|\psi(t)>$ and both $t > 0$ probabilities in the basis in which $\mathcal{H}$ is diagonal.

(i) Suppose that you measure the energy of the system at $t = 0$ and you find $E = -2$. Find the state vector of the system immediately after your measurement and at time $t = 10$ in both the basis in which $\mathcal{H}$ is diagonal and in the basis of part (b). What energies will you measure if you repeat the energy measurement at $t = 10$?

This problem emphasizes the postulates and their applications using a Hamiltonian that is not diagonal. Parts (c) through (f) may be more interesting than similar calculations using diagonal matrices because the off-diagonal elements contribute cross terms. Diagonalize the Hamiltonian for part (g). Understanding diagonalization is the initial step to understanding simultaneous diagonalization, and simultaneous diagonalization is the foundation underlying the essential concept of a complete set of commuting observables.

Expand the state vector in the energy eigenbasis using $|\psi(0)> = \sum_j |E_j><E_j|\psi(0)>$ where $|E_j>$ are the normalized eigenvectors of the Hamiltonian matrix for part (e). The only time dependence is that of the energy eigenvectors $|E_j(t)> = \exp(-iE_jt/\hbar)|E_j(0)>$, per previous problems. The probabilities for part (f) are identical to those from part (c). Transform $\mathcal{H}$ using $\mathcal{U}^\dagger \mathcal{H} \mathcal{U}$ for part (g). Form $\mathcal{U}$ from the eigenvectors of $\mathcal{H}$ as done in chapter 1. Transform kets $\mathcal{U}^\dagger|i>$ to establish them in the same basis as $\mathcal{U}^\dagger \mathcal{H} \mathcal{U}$ (see problem 3–6). Of course, probabilities for part (h) are identical to those found in parts (c) and (f). Notice that the calculations done in the basis in which the Hamiltonian is diagonal are much more straightforward.

(a) $$\mathcal{H}^\dagger = \left[\begin{pmatrix}1 & 3\\ 3 & 1\end{pmatrix}^{\mathrm{T}*}\right]^* = \left[\begin{pmatrix}1 & 3\\ 3 & 1\end{pmatrix}\right]^* = \begin{pmatrix}1^* & 3^*\\ 3^* & 1^*\end{pmatrix} = \begin{pmatrix}1 & 3\\ 3 & 1\end{pmatrix} = \mathcal{H},$$

therefore, $\mathcal{H}$ is Hermitian. The observables postulate says that this is necessary for a Hamiltonian.

(b) To obtain the eigenvalues, $\det\begin{pmatrix}1-\alpha & 3\\ 3 & 1-\alpha\end{pmatrix} = (1-\alpha)^2 - 9 = 0$

$$\Rightarrow \quad 1 - 2\alpha + \alpha^2 - 9 = 0 \quad \Rightarrow \quad \alpha^2 - 2\alpha - 8 = 0 \quad \Rightarrow \quad (\alpha - 4)(\alpha + 2) = 0,$$

$\Rightarrow$ $\alpha = -2,\ 4,$ are the eigenvalues of the Hamiltonian operator. For $\alpha = -2$,

$$\begin{pmatrix}1 & 3\\ 3 & 1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = -2\begin{pmatrix}a\\ b\end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} a & + & 3b & = & -2a \\ 3a & + & b & = & -2b \end{array} \quad \Rightarrow \quad \begin{array}{l} b = -a \\ a = -b \end{array}$$

$$\Rightarrow \quad |-2> = \mathrm{A}\begin{pmatrix}1\\ -1\end{pmatrix} \quad \Rightarrow \quad |-2> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}$$

is the normalized eigenvector. The eigenvector corresponding to the eigenvalue 4 is

$$\begin{pmatrix}1 & 3\\ 3 & 1\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} = 4\begin{pmatrix}a\\ b\end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcl} a & + & 3b & = & 4a \\ 3a & + & b & = & 4b \end{array} \quad \Rightarrow \quad \begin{array}{l} b = a \\ a = b \end{array}$$

$$\Rightarrow \quad |4> = \mathrm{A}\begin{pmatrix}1\\ 1\end{pmatrix} \quad \Rightarrow \quad |4> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix} \quad \text{is the normalized eigenvector.}$$

(c) We can now address the $t = 0$ probabilities which are

$$P(-2) = \left|\frac{1}{\sqrt{2}}(1,\ -1)\frac{1}{\sqrt{13}}\begin{pmatrix}2\\ 3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{26}}(2-3)\right|^2 = \left|\frac{-1}{\sqrt{26}}\right|^2 = \frac{1}{26},$$

$$P(4) = \left|\frac{1}{\sqrt{2}}(1,\ 1)\frac{1}{\sqrt{13}}\begin{pmatrix}2\\ 3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{26}}(2+3)\right|^2 = \left|\frac{5}{\sqrt{26}}\right|^2 = \frac{25}{26}.$$

The probabilities sum to 1, as they must.

(d) The expectation value is

$$< \mathcal{H} > \;=\; <\psi(0)\,|\,\mathcal{H}\,|\,\psi(0)> \;=\; \frac{1}{\sqrt{13}}\,(2,\;3)\begin{pmatrix}1 & 3\\ 3 & 1\end{pmatrix}\frac{1}{\sqrt{13}}\begin{pmatrix}2\\ 3\end{pmatrix} \;=\; \frac{1}{13}\,(2,\;3)\begin{pmatrix}2+9\\ 6+3\end{pmatrix}$$
$$= \;\frac{1}{13}\,(2,\;3)\begin{pmatrix}11\\ 9\end{pmatrix} \;=\; \frac{1}{13}\,(22+27) \;=\; \frac{49}{13} \;\approx\; 3.77\,.$$

$$< \mathcal{H} > \;=\; \sum_i P\,(E_i)\,E_i \;=\; \frac{1}{26}\,(-2) \;+\; \frac{25}{26}\,4 \;=\; -\frac{2}{26} \;+\; \frac{100}{26} \;=\; \frac{98}{26} \;=\; \frac{49}{13} \;\approx\; 3.77\,.$$

One advantage of using a second procedure is that it is a check for all previous calculations.

(e) The expansion of the $t = 0$ state vector in the energy basis is

$$|\,\psi(0)> \;=\; \sum_i\,|\,E_i><E_i\,|\,\psi(0)>$$
$$= \;\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}\frac{1}{\sqrt{2}}(1,\;-1)\,\frac{1}{\sqrt{13}}\begin{pmatrix}2\\ 3\end{pmatrix} \;+\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix}\frac{1}{\sqrt{2}}(1,\;1)\,\frac{1}{\sqrt{13}}\begin{pmatrix}2\\ 3\end{pmatrix}$$
$$= \;\frac{1}{2\sqrt{13}}\begin{pmatrix}1\\ -1\end{pmatrix}(2-3) \;+\; \frac{1}{2\sqrt{13}}\begin{pmatrix}1\\ 1\end{pmatrix}(2+3) \;=\; \frac{-1}{2\sqrt{13}}\begin{pmatrix}1\\ -1\end{pmatrix} \;+\; \frac{5}{2\sqrt{13}}\begin{pmatrix}1\\ 1\end{pmatrix}$$
$$\Rightarrow \;\;|\,\psi(t)> \;=\; -\frac{1}{2\sqrt{13}}\begin{pmatrix}1\\ -1\end{pmatrix}e^{i2t/\hbar} \;+\; \frac{5}{2\sqrt{13}}\begin{pmatrix}1\\ 1\end{pmatrix}e^{-i4t/\hbar} \;=\; \frac{1}{2\sqrt{13}}\begin{pmatrix}-e^{i2t/\hbar}+5\,e^{-i4t/\hbar}\\ e^{i2t/\hbar}+5\,e^{-i4t/\hbar}\end{pmatrix}.$$

(f) Considering time-dependence, the probabilities are

$$P\,(-2) \;=\; \left|\,\frac{1}{\sqrt{2}}\,(1,\;-1)\,\frac{1}{2\sqrt{13}}\begin{pmatrix}-e^{i2t/\hbar}+5\,e^{-i4t/\hbar}\\ e^{i2t/\hbar}+5\,e^{-i4t/\hbar}\end{pmatrix}\right|^2$$
$$= \;\left|\frac{1}{2\sqrt{26}}\left(-e^{i2t/\hbar} \;+\; 5\,e^{-i4t/\hbar} \;-\; e^{i2t/\hbar} \;-\; 5\,e^{-i4t/\hbar}\right)\right|^2$$
$$= \;\left|\frac{1}{2\sqrt{26}}\left(-2e^{i2t/\hbar}\right)\right|^2 \;=\; \frac{1}{26}\left(-e^{-i2t/\hbar}\right)\left(-e^{i2t/\hbar}\right) \;=\; \frac{1}{26}$$

$$P\,(4) \;=\; \left|\,\frac{1}{\sqrt{2}}\,(1,\;1)\,\frac{1}{2\sqrt{13}}\begin{pmatrix}-e^{i2t/\hbar}+5\,e^{-i4t/\hbar}\\ e^{i2t/\hbar}+5\,e^{-i4t/\hbar}\end{pmatrix}\right|^2$$
$$= \;\left|\frac{1}{2\sqrt{26}}\left(-e^{i2t/\hbar} \;+\; 5\,e^{-i4t/\hbar} \;+\; e^{i2t/\hbar} \;+\; 5\,e^{-i4t/\hbar}\right)\right|^2$$
$$= \;\left|\frac{1}{2\sqrt{26}}\left(10e^{-i4t/\hbar}\right)\right|^2 \;=\; \frac{1}{26}\left(5e^{i4t/\hbar}\right)\left(5e^{-i4t/\hbar}\right) \;=\; \frac{25}{26}$$

(g) Placing the eigenvector corresponding to the smaller eigenvalue on the left and the eigenvector corresponding to larger eigenvalue on the right yields the unitary transformation matrix,

$$\mathcal{U} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix} \qquad \Rightarrow \qquad \mathcal{U}^\dagger \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}$$

$$\Rightarrow \quad \mathcal{U}^\dagger\,\mathcal{H}\mathcal{U} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 3\\ 3 & 1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix} \;=\; \frac{1}{2}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\begin{pmatrix}-2 & 4\\ 2 & 4\end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix}-2-2 & 4-4\\ -2+2 & 4+4\end{pmatrix} \;=\; \begin{pmatrix}-2 & 0\\ 0 & 4\end{pmatrix}.$$

A consistent unitary transformation for the kets is found using

$$<i\,|\,\mathcal{H}\,|\,i> \;=\; <i\,|\,\mathcal{I}\,|\,\mathcal{H}\,|\,\mathcal{I}\,|\,i> \;=\; <i\,|\,\mathcal{U}\mathcal{U}^\dagger\,|\,\mathcal{H}\,|\,\mathcal{U}\mathcal{U}^\dagger\,|\,i> \;=\; \Big(<i\,|\,\mathcal{U}\Big)\Big(\mathcal{U}^\dagger\,\mathcal{H}\mathcal{U}\Big)\Big(\mathcal{U}^\dagger\,|\,i>\Big),$$

operators transforming as $\mathcal{U}^\dagger\,\mathcal{H}\mathcal{U}$ require kets transform as $\mathcal{U}^\dagger\,|\,i>$. The state vector is

$$\mathcal{U}^\dagger\,|\,\psi(0)> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\frac{1}{\sqrt{13}}\begin{pmatrix}2\\ 3\end{pmatrix} \;=\; \frac{1}{\sqrt{26}}\begin{pmatrix}2-3\\ 2+3\end{pmatrix} \;=\; \frac{1}{\sqrt{26}}\begin{pmatrix}-1\\ 5\end{pmatrix}.$$

The eigenvectors are easily found by inspection but notice that they also transform correctly,

$$\mathcal{U}^\dagger\,|\,-2> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix} \;=\; \frac{1}{2}\begin{pmatrix}1+1\\ 1-1\end{pmatrix} \;=\; \frac{1}{2}\begin{pmatrix}2\\ 0\end{pmatrix} \;=\; \begin{pmatrix}1\\ 0\end{pmatrix},$$

$$\mathcal{U}^\dagger\,|\,4> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 1\end{pmatrix} \;=\; \frac{1}{2}\begin{pmatrix}1-1\\ 1+1\end{pmatrix} \;=\; \frac{1}{2}\begin{pmatrix}0\\ 2\end{pmatrix} \;=\; \begin{pmatrix}0\\ 1\end{pmatrix}.$$

(h) The $t=0$ expansion is

$$|\,\psi(0)> \;=\; \begin{pmatrix}1\\ 0\end{pmatrix}(1,\;0)\,\frac{1}{\sqrt{26}}\begin{pmatrix}-1\\ 5\end{pmatrix} \;+\; \begin{pmatrix}0\\ 1\end{pmatrix}(0,\;1)\,\frac{1}{\sqrt{26}}\begin{pmatrix}-1\\ 5\end{pmatrix}$$
$$= \frac{1}{\sqrt{26}}\begin{pmatrix}1\\ 0\end{pmatrix}(-1+0) \;+\; \frac{1}{\sqrt{26}}\begin{pmatrix}0\\ 1\end{pmatrix}(0+5) \;=\; -\frac{1}{\sqrt{26}}\begin{pmatrix}1\\ 0\end{pmatrix} \;+\; \frac{5}{\sqrt{26}}\begin{pmatrix}0\\ 1\end{pmatrix},$$
$$\Rightarrow \quad |\,\psi(t)> \;=\; -\frac{1}{\sqrt{26}}\begin{pmatrix}1\\ 0\end{pmatrix}e^{i2t/\hbar} \;+\; \frac{5}{\sqrt{26}}\begin{pmatrix}0\\ 1\end{pmatrix}e^{-i4t/\hbar} \;=\; \frac{1}{\sqrt{26}}\begin{pmatrix}-e^{i2t/\hbar}\\ 5\,e^{-i4t/\hbar}\end{pmatrix}.$$

Probabilities are

$$P(-2) \;=\; \left|(1,\;0)\,\frac{1}{\sqrt{26}}\begin{pmatrix}-e^{i2t/\hbar}\\ 5\,e^{-i4t/\hbar}\end{pmatrix}\right|^2 \;=\; \left|\frac{-1}{\sqrt{26}}\left(e^{i2t/\hbar}\right)\right|^2 \;=\; \frac{1}{26}\left(e^{-i2t/\hbar}\right)\left(e^{+i2t/\hbar}\right) \;=\; \frac{1}{26},$$

$$P(4) \;=\; \left|(0,\;1)\,\frac{1}{\sqrt{26}}\begin{pmatrix}-e^{i2t/\hbar}\\ 5\,e^{-i4t/\hbar}\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{26}}\left(5\,e^{-i4t/\hbar}\right)\right|^2 = \frac{1}{26}\left(5\,e^{+i4t/\hbar}\right)\left(5\,e^{-i4t/\hbar}\right) = \frac{25}{26}.$$

(i) Per the eigenvector postulate, measuring $E=-2$ changes the $t=0$ state vector to

$$|\,\psi'(0)> \;=\; \begin{pmatrix}1\\ 0\end{pmatrix} \qquad \Rightarrow \qquad |\,\psi'(t)> \;=\; \begin{pmatrix}1\\ 0\end{pmatrix}e^{i2t/\hbar},$$

in the basis in which $\mathcal{H}$ is diagonal. In the original non-diagonal basis, the state vector is

$$|\,\psi'(0)> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix} \qquad \Rightarrow \qquad |\,\psi'(t)> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -1\end{pmatrix}e^{i2t/\hbar}.$$

Identical probabilities necessarily follow, that is

$$P(-2) = \left| (1,\ 0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i2t/\hbar} \right|^2 = \left| (1+0)\, e^{i2t/\hbar} \right|^2 = \left(e^{+i2t/\hbar} \right) \left(e^{-i2t/\hbar} \right) = 1\,,$$

$$P(4) = \left| (0,\ 1) \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{i2t/\hbar} \right|^2 = \left| (0+0)\, e^{i2t/\hbar} \right|^2 = 0\,,$$

$$P(-2) = \left| \frac{1}{\sqrt{2}} (1,\ -1) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{i2t/\hbar} \right|^2 = \left| \frac{1}{2} (1+1)\, e^{i2t/\hbar} \right|^2 = \left(e^{+i2t/\hbar} \right) \left(e^{-i2t/\hbar} \right) = 1\,,$$

$$P(4) = \left| \frac{1}{\sqrt{2}} (1,\ 1) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{i2t/\hbar} \right|^2 = \left| \frac{1}{2} (1-1)\, e^{i2t/\hbar} \right|^2 = 0\,.$$

2–25. Show that $\sum P_{\mathcal{A}}(\alpha_i)\, \alpha_i = <\psi\,|\,\mathcal{A}\,|\,\psi>$.

Individual probabilities are $P_{\mathcal{A}}(\alpha_i) = \left| <\alpha_i\,|\,\psi> \right|^2$. The operator $\mathcal{A}$ is an observable quantity, therefore, it is Hermitian. All Hermitian operators can be diagonalized. $\mathcal{A}$ is assumed to be in diagonal form, or $\mathcal{A} = \mathcal{U}^{\dagger} \mathcal{A}' \mathcal{U}$ where $\mathcal{A}'$ is a non-diagonal form of $\mathcal{A}$. A diagonal $\mathcal{A}$ has eigenvalues on the main diagonal and eigenvectors that are unit vectors.

$$\sum P_{\mathcal{A}}(\alpha_i)\, \alpha_i = \sum \left| <\alpha_i\,|\,\psi> \right|^2 \alpha_i$$

$$= \left| <\alpha_1\,|\,\psi> \right|^2 \alpha_1 + \left| <\alpha_2\,|\,\psi> \right|^2 \alpha_2 + \left| <\alpha_3\,|\,\psi> \right|^2 \alpha_3 + \cdots$$

$$= <\psi\,|\,\alpha_1><\alpha_1\,|\,\psi>\, \alpha_1 + <\psi\,|\,\alpha_2><\alpha_2\,|\,\psi>\, \alpha_2 + <\psi\,|\,\alpha_3><\alpha_3\,|\,\psi>\, \alpha_3 + \cdots$$

$$= <\psi\,|\left(|\,\alpha_1><\alpha_1\,|\,\alpha_1 + |\,\alpha_2><\alpha_2\,|\,\alpha_2 + |\,\alpha_3><\alpha_3\,|\,\alpha_3 + \cdots \right) |\,\psi> =$$

$$<\psi\,|\left(\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} (1,\ 0,\ 0,\ \ldots)\, \alpha_1 + \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} (0,\ 1,\ 0,\ \ldots)\, \alpha_2 + \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \end{pmatrix} (0,\ 0,\ 1,\ \ldots)\, \alpha_3 + \cdots \right) |\,\psi>$$

$$= <\psi\,|\left(\begin{pmatrix} \alpha_1 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & \alpha_2 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \cdots \\ 0 & 0 & \alpha_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} + \cdots \right) |\,\psi>$$

$$= <\psi\,|\begin{pmatrix} \alpha_1 & 0 & 0 & \cdots \\ 0 & \alpha_2 & 0 & \cdots \\ 0 & 0 & \alpha_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} |\,\psi> = <\psi\,|\,\mathcal{A}\,|\,\psi>$$

having recognized the diagonal form of $\mathcal{A}$ with eigenvalues on the principal diagonal.

Postscript: Inherent in equations involving probabilities and vectors is that $|\,\psi>$ and all $|\,\alpha>$ are normalized. Relations involving probabilities and vectors are proportionalities rather than equalities if the vectors are not normalized.

Exercises

2–26. The "$\mathcal{A}$–ness" of a particle or system in the state

$$|\psi> \rightarrow \begin{pmatrix} 4 \\ 2 \\ 1 \end{pmatrix} \qquad \text{where} \qquad \mathcal{A} \rightarrow \begin{pmatrix} 2 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 6 \end{pmatrix} \qquad \text{is measured.}$$

(a) Normalize $|\psi>$.

(b) What is the probability of a measurement of 4?

(c) What are the possible outcomes of a measurement of the "$\mathcal{A}$–ness" of $|\psi>$?

(d) Calculate the probability of each possibility.

(e) Show that the sum of the probabilities is 1.

(f) A measurement of the "$\mathcal{A}$–ness" of $|\psi>$ yields the value 6. A second measurement of the "$\mathcal{A}$–ness" of $|\psi>$ is then made. What are the possibilities and probabilities of the outcomes of this second measurement?

The preponderance of 2 X 2 and 3 X 3 operators intend to expose the substance of non-relativistic quantum mechanics in an accessible fashion. The postulates can be understood in this context, and then generalized to apply to more complex systems.

See problem 2–2 for the processes and precise rationale for this exercise.

2–27. What are the possible results and the probability of obtaining each possible result of a measurement of the "$\mathcal{B}$–ness" of a system where

$$\mathcal{B} \rightarrow \begin{pmatrix} 1 & 0 & -3 \\ 0 & 3 & 0 \\ -3 & 0 & 1 \end{pmatrix} \qquad \text{and the state is} \qquad |\psi> \rightarrow \begin{pmatrix} 4 \\ 2 \\ 1 \end{pmatrix}?$$

$$|-2> \; = \; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \qquad |3> \; = \; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \text{and} \qquad |4> \; = \; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

are the eigenvalues and eigenvectors.

See problem 2–3. Remember to normalize the state vector.

2–28. The operator $\mathcal{A}$ is as given in exercise 2–26 and the operator $\mathcal{B}$ is as given in exercise 2–27. The state vector of the system is initially $|\psi> = \begin{pmatrix} 4 \\ 2 \\ 1 \end{pmatrix}$ for the following questions.

(a) If we measure a value of 5 for $\mathcal{A}$, what are the possible values of successive measurements of $\mathcal{B}$, $\mathcal{A}$, $\mathcal{B}$, etc., and their respective probabilities?

(b) If we measure $\mathcal{A}$ and get 2, what are the possible values of a subsequent measurement of $\mathcal{B}$ and the probabilities of each possibility?

(c) Having measured a value of 6 for $\mathcal{A}$, and then measured a value of -2 for $\mathcal{B}$, what are the possible values of another measurement of $\mathcal{A}$ and their respective probabilities?

(d) Having measured a value of 6 for $\mathcal{A}$, and then measured a value of 4 for $\mathcal{B}$, what are the possible values of a measurement of $\mathcal{A}$ and their respective probabilities?

(e) If we measure 4 for $\mathcal{B}$, what are the possible values of subsequent measurements of $\mathcal{A}$ and their respective probabilities?

See problem 2–4. The state vector becomes the eigenvector of the eigenvalue measured.

2–29. Given $|\psi> = \begin{pmatrix} 3i \\ 2 \end{pmatrix}$, $\mathcal{D} \rightarrow \begin{pmatrix} 1 & 2i \\ -2i & 4 \end{pmatrix}$, and $\mathcal{F} \rightarrow \begin{pmatrix} 5 & 2i & 1 \\ -2i & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$,

what measurements can be made, and what are the probabilities of each possible result?

A self consistent description must have objects from the same space. You solved the eigenvalue/eigenvector problem for both operators in exercise 1–44. See problems 2–6 and 2–7.

2–30. Given $|\psi> = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$, $\mathcal{D} \rightarrow \begin{pmatrix} 1 & 2i \\ -2i & 4 \end{pmatrix}$, and $\mathcal{F} \rightarrow \begin{pmatrix} 5 & 2i & 1 \\ -2i & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$,

what measurements can be made, and what are the probabilities of each possible result? Ensure your probabilities sum to 1.

This is similar to the previous exercise and problems 2–6 and 2–7.

2–31. Find $\sum P(\alpha_i)\,\alpha_i$ for the $\mathcal{A}$, $\mathcal{B}$, $\mathcal{D}$, and $\mathcal{F}$ used in the previous 5 exercises.

Use the probabilities and eigenvalues from exercises 2–26 through 2–30. See problem 2–8.

2–32. Find $<\psi\,|\,\mathcal{A}\,|\,\psi>$ for $\mathcal{A}$, $\mathcal{B}$, $\mathcal{D}$, and $\mathcal{F}$.

Using the appropriate state vector (three different state vectors for the four parts of this exercise), the expectation values must be the same as the previous exercise. The two techniques offer a method to double check an expectation value calculation.

2–33. Find $\triangle\mathcal{A}$ for $\mathcal{A} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 6 \end{pmatrix}$ where $|\,\psi> = \begin{pmatrix} 4 \\ 2 \\ 1 \end{pmatrix}$ using both formulations.

Problems 2–10 and 2–12 and the previous two exercises pertain.

$$\triangle\mathcal{A}_\psi = <\psi\,|\left(\mathcal{A} - <\mathcal{A}>\mathcal{I}\right)^2|\,\psi>^{1/2} \qquad \text{and} \qquad \triangle\mathcal{A}_\psi = <\psi\,|\,\mathcal{A}^2 - <\mathcal{A}>^2\,\mathcal{I}\,|\,\psi>^{1/2}$$

are the two referenced formulations. Remember to use a normalized state vector. Avoid square roots within work using variance and obtain uncertainty with a square root as the last step.

2–34. Find the uncertainty for $|\,\psi> = \begin{pmatrix} 3i \\ 2 \end{pmatrix}$, $\mathcal{D} = \begin{pmatrix} 1 & 2i \\ -2i & 4 \end{pmatrix}$ using both formulations.

Smaller than the previous exercise but non-diagonal and with complex components. You should have the normalized state vector and the expectation value from previous exercises. Again, finding variance and obtaining uncertainty by taking a square root in the last step is recommended.

2–35. Consider a system described by the Hamiltonian

$$\mathcal{H} = \begin{pmatrix} -2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 4 \end{pmatrix}, \quad \text{which at} \quad t = 0 \quad \text{is in the state} \quad |\,\psi(0)> = \frac{1}{\sqrt{17}}\begin{pmatrix} 2 \\ 3 \\ -2 \end{pmatrix}.$$

(a) Find the possibilities for a measurement of energy and the probability of each possibility.

(b) Calculate $<\mathcal{H}>$ using both $<\mathcal{H}> = <\psi(0)\,|\,\mathcal{H}\,|\,\psi(0)>$ and $<\mathcal{H}> = \sum_i P(E_i)\,E_i$.

(c) Obtain the time dependent state vector $|\,\psi(t)>$ in the energy eigenbasis.

(d) If the energy is measured at time t what results can be obtained and with what probabilities will these results be obtained? Compare your probabilities with the $t = 0$ case in part (a).

(e) Suppose that you measure the energy of the system at $t = 0$ and you find $E = -1$. What is the state vector of the system immediately after your measurement? What is the state vector $|\,\psi(10)>$ at $t = 10$? What energies will you measure at $t = 10$?

See problems 2–22 and 2–23.

2–36. Consider a system described by the Hamiltonian

$$\mathcal{H} \;=\; \begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}, \qquad \text{which at} \quad t = 0 \quad \text{is in the state} \qquad |\,\psi(0)> \;=\; \frac{1}{\sqrt{29}} \begin{pmatrix} 2 \\ 5 \end{pmatrix}.$$

(a) Is $\mathcal{H}$ Hermitian?

(b) Obtain the eigenvalues and eigenvectors of $\mathcal{H}$ by solving the eigenvalue/eigenvector problem.

(c) If the energy is measured what results can be obtained and with what probabilities will these results be obtained?

(d) Calculate the expectation value of the Hamiltonian using both

$$<\mathcal{H}>_{\psi(0)} \;=\; <\psi(0)\,|\,\mathcal{H}\,|\,\psi(0)> \qquad \text{and} \qquad <\mathcal{H}> \;=\; \sum_i P(E_i)\,E_i\,.$$

(e) Obtain the time dependent state vector $|\,\psi(t)>$ in the energy eigenbasis.

(f) If the energy is measured at time t, what results can be obtained and with what probabilities will these results be obtained? Compare your answer with the $t = 0$ case in part (c).

(g) Diagonalize $\mathcal{H}$ using a unitary transformation. Transform $|\,\psi(0)>$ and both eigenvectors to be consistent with this unitary transformation.

(h) Calculate $|\,\psi(t)>$ and both $t > 0$ probabilities in the basis in which $\mathcal{H}$ is diagonal.

(i) Suppose that you measure the energy of the system at $t = 0$ and you find $E = 2$. Find the state vector of the system immediately after your measurement and at time $t = 10$ in both the basis in which $\mathcal{H}$ is diagonal and in the basis of part (b). What energies will you measure if you repeat the energy measurement at $t = 10$?

See problem 2–24. Transform kets $\mathcal{U}^\dagger\,|\,i>$ to establish them in the same basis as $\mathcal{U}^\dagger\,\mathcal{H}\,\mathcal{U}$.

2–37. Given the arbitrary diagonal operator and the arbitrary state vector

$$\Omega \;=\; \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \qquad \text{and} \qquad |\,\psi> \;=\; \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \text{show that} \quad <\psi\,|\,\Omega\,|\,\psi> \;=\; \sum_i P(\omega_i)\,\omega_i\,.$$

The two methods of calculating expectation values yield identical results. First, normalize the state vector to find that $1/\sqrt{|\,x\,|^2 + |\,y\,|^2 + |\,z\,|^2}$ is the normalization constant. Then calculate $<\psi\,|\,\Omega\,|\,\psi>$. Calculate the probabilities for each eigenvalue using the unit vectors appropriate to a diagonal operator. You then have the probabilities and the eigenvalues to calculate $\sum_i P(\omega_i)\,\omega_i$. This problem is relatively simple in the basis of a diagonal operator. Thinking about how this would be done in general may help you to appreciate more fully the utility of diagonal operators.

2–38. Consider the operator

$$\Omega \;=\; \begin{pmatrix} 0 & 4i & 0 \\ -4i & 0 & -3i \\ 0 & 3i & 0 \end{pmatrix} \qquad \text{and the state vector} \qquad |\,\psi> \;=\; \begin{pmatrix} 1 \\ i \\ -1 \end{pmatrix}.$$

(a) Verify that the eigenvalues and eigenvectors of Ω are

$$|\,\omega=-5> \;=\; \frac{4}{5\sqrt{2}} \begin{pmatrix} 1 \\ i5/4 \\ 3/4 \end{pmatrix}, \qquad |\,\omega=0> \;=\; \frac{3}{5} \begin{pmatrix} 1 \\ 0 \\ -4/3 \end{pmatrix}, \qquad |\,\omega=5> \;=\; \frac{4}{5\sqrt{2}} \begin{pmatrix} 1 \\ -i5/4 \\ 3/4 \end{pmatrix}.$$

Using Ω, $|\,\psi>$, and the given eigenvalues and eigenvectors,

(b) find the probabilities of each possibility,

(c) find the expectation value using both $<\psi\,|\,\Omega\,|\,\psi>$ and $\sum_i P\,(\omega_i)\,\omega_i$,

(d) calculate the uncertainty using $\triangle\,\Omega_\psi \;=\; <\psi\,|\left(\Omega - <\Omega>\mathcal{I}\right)^2|\,\psi>^{1/2}$,

(e) and calculate the uncertainty using $\triangle\,\Omega_\psi \;=\; <\psi\,|\,\Omega^2 - <\Omega>^2\,\mathcal{I}\,|\,\psi>^{1/2}$.

Part (a) intends that you show $\Omega\,|\,\omega_i> \;=\; \omega_i\,|\,\omega_i>$ for the eigenvalues and eigenvectors given. You should see that the three eigenvectors given are scaled by -5, 0, and 5. The meaning of an eigenvalue/eigenvector equation is that the "direction" of the eigenvector is unchanged, only its length or norm is affected.

Parts (b) through (d) should be straightforward. Of course, the answers to parts (d) and (e) must be the same. Uncertainty for a discrete system is the same as standard deviation. The uncertainties being calculated are those to be used in the Heisenberg uncertainty principle. Compute variance and then take a square root to obtain uncertainty to find $\triangle\,\Omega \;=\; \sqrt{74}\,/3$.

2–39. The diagonal form of the Ω operator used in the last problem is $\Omega \;=\; \begin{pmatrix} -5 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 5 \end{pmatrix}$.

(a) Transform $|\,\psi> \;=\; \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ i \\ -1 \end{pmatrix}$ used in the previous problem to the diagonal basis.

(b) Calculate the probability of each possibility of a measurement of Ω.

(c) Calculate the expectation value using both $<\psi\,|\,\Omega\,|\,\psi>$ and $\sum_i P\,(\omega_i)\,\omega_i$.

(d) Calculate the uncertainty using $\triangle\,\Omega_\psi \;=\; <\psi\,|\left(\Omega - <\Omega>\mathcal{I}\right)^2|\,\psi>^{1/2}$.

(e) Calculate the uncertainty using $\triangle\,\Omega_\psi \;=\; <\psi\,|\,\Omega^2 - <\Omega>^2\,\mathcal{I}\,|\,\psi>^{1/2}$.

The calculations of the last exercise are simpler in the diagonal basis. Transform the state vector $\mathcal{U}^\dagger \,|\, \psi >$ to change it to the same basis as the diagonal Ω. Use the eigenvectors given in the previous exercise to form $\mathcal{U}$ so that

$$\mathcal{U}^\dagger \;=\; \begin{pmatrix} 4/5\sqrt{2} & -i/\sqrt{2} & 3/5\sqrt{2} \\ 3/5 & 0 & -4/5 \\ 4/5\sqrt{2} & i/\sqrt{2} & 3/5\sqrt{2} \end{pmatrix}.$$

The probabilities of measuring any eigenvalue, the expectation value, and the uncertainty must be the same as the last exercise.

2–40. Find the possible outcomes of a measurement, the probabilities of each possible outcome, the expectation value, and the uncertainty for

$$\sigma_y \;=\; \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \text{given that} \qquad |\,\psi> \;=\; \begin{pmatrix} 2 \\ i \end{pmatrix}.$$

Support your answers with alternative calculations or consistency checks where possible.

The operator is one of the Pauli spin matrices. This exercise is posed without parts per a real world situation. The multi-part problems attempts to highlight the necessary path.

Normalize the state vector, solve the eigenvalue/eigenvector problem, and use the eigenvectors and the state vector to obtain probabilities. The sum of the probabilities must be 1. Calculate $< \sigma_y > \;=\; <\psi \,|\, \sigma_y \,|\, \psi>$ and check using $< \sigma_y > \;=\; \sum P\,(\sigma_{y_i})\,\sigma_{y_i}$. Calculate the uncertainty $\triangle \sigma_{y_\psi} = <\psi \,|\, \Big(\sigma_y - < \sigma_y > \mathcal{I}\Big)^2 \,|\, \psi>^{1/2}$ and check with $\triangle \sigma_{y_\psi} = <\psi \,|\, \sigma_y^2 - < \sigma_y >^2 \mathcal{I} \,|\, \psi>^{1/2}$.

2–41. Consider the operator $\Lambda \;=\; \begin{pmatrix} 1 & 1 \\ -2 & 4 \end{pmatrix}$, which has eigenvalues and normalized eigenvectors

$|\,\lambda = 2> \;=\; \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $|\,\lambda = 3> \;=\; \dfrac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$. For the state vector $|\,\psi> \;=\; \dfrac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix}$,

the square of the inner product $\Big| <\lambda \,|\, \psi> \Big|^2$ is $9/10$ using the eigenvector that corresponds to 2, and $16/25$ for the eigenvector that corresponds to 3. It seems these should be probabilities, but their sum is not 1. There is, in fact, an error present. Can you determine what the error is?

This counter example is meant to highlight an error and thus increase the chance that you will avoid it. If you perform the mathematical mechanics you will find that the error is not in the given information. Consider the observables postulate. Also, are these eigenvectors orthogonal?

Chapter 3

Discrete Systems II A Complete Set of Commuting Observables

Each operator encountered to this point has readily distinguishable eigenvalues, and thus, readily associated eigenvectors. Should an operator be degenerate, meaning that it has one or more duplicate eigenvalues, a second measurement is necessary to uniquely determine the eigenstate. The two operators together then form a **complete set of commuting observables**.

A preferred method of lifting a degeneracy is simultaneous diagonalization. All Hermitian operators can be diagonalized by an appropriate unitary transformation. Unitary operators play a central role in diagonalization and simultaneous diagonalization. Operators must have the same eigenbasis to both be diagonalized by the same transformation, which means they must commute.

Proof that the eigenvalues of a Hermitian operator are real has been provided earlier, and there are two more proofs in this chapter. Claims that the eigenvectors of a Hermitian operator are orthogonal, that all Hermitian operators can be diagonalized, and that the eigenvectors of Hermitian operators form a basis are supported in this chapter following further development of unitary operators and unitary transformations.

The transition from $\mathbb{C}^2$ and $\mathbb{C}^3$ to $\mathbb{C}^\infty$ was embedded in a few examples in the last chapter. The transition is more prevalent in this chapter, which includes numerous examples of operator algebra without reference to any specific space. Numerical examples in $\mathbb{C}^2$ and $\mathbb{C}^3$ are plentiful, but a significant number of results of this chapter are applicable to $\mathbb{C}^\infty$.

3–1. What is a degenerate operator and why are degenerate operators a concern?

A **degenerate operator** is an operator with at least one duplicate eigenvalue. The concern is that should a measurement return one of the duplicate eigenvalues, the eigenstate is not known uniquely. For instance, the operator $\mathcal{H} = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ has duplicate eigenvalues of 1. Should a measurement return 1 for this operator, the eigenstate is unknown; it could be $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ or $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$. $\mathcal{H}$ is a degenerate operator and a measurement of 1 does not uniquely identify the eigenstate.

3–2. How is degeneracy lifted?

A method to lift the degeneracy is to find an operator like $\mathcal{K} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$ with which $\mathcal{H}$ commutes, measure $\mathcal{K}$ after measuring 1 for $\mathcal{H}$, and if 2 is the result, the eigenstate is $|1, 2> = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, but if 3 is the result, the eigenstate is $|1, 3> = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ and the degeneracy is lifted. $\mathcal{H}$ and $\mathcal{K}$ together constitute a **complete set of commuting observables**.

Postscript: Problem 3–1 is an example of the difficulty degeneracy presents and problem 3–2 highlights a method of resolution. The clarity of diagonal operators has been employed in these two problems to expose concepts applicable to all Hermitian operators.

3–3. Show that $\left(\mathcal{A}\mathcal{B}\right)^{-1} = \mathcal{B}^{-1}\mathcal{A}^{-1}$.

The inverse of an operator $\mathcal{T}$ is an operator $\mathcal{T}^{-1}$ such that

$$\mathcal{T}\mathcal{T}^{-1} = \mathcal{T}^{-1}\mathcal{T} = \mathcal{I}.$$

This problem addresses yet other forms of **resolution** and **insertion of the identity**. The identity operator is so named because anything upon which it operates remains identical. Use of the identity operator is analogous to multiplication by 1 in the real number system. The real utility of any identity operator (or any identity element including the number 1 in the real number system) is that it has an infinite number of different forms, $\mathcal{A}\mathcal{A}^{-1}$, $\mathcal{B}\mathcal{B}^{-1}$, and $\left(\mathcal{A}\mathcal{B}\right)^{-1}\left(\mathcal{A}\mathcal{B}\right)$ to name just the three resolutions/forms that are employed in this problem.

This problem also establishes the fact that the inverse of the product of two operators is the reverse order of the product of the two inverses, which parallels the more useful fact that the adjoint of the product of two operators is the reverse order of the product of the two adjoints.

$\mathcal{I}$	$= \mathcal{A}\mathcal{A}^{-1}$	statement of the identity
$\mathcal{I}$	$= \mathcal{A}\mathcal{I}\mathcal{A}^{-1}$	insertion of the identity
$\mathcal{I}$	$= \mathcal{A}\mathcal{B}\mathcal{B}^{-1}\mathcal{A}^{-1}$	resolution of the identity $\mathcal{I} = \mathcal{B}\mathcal{B}^{-1}$
$\mathcal{I}$	$= \left(\mathcal{A}\mathcal{B}\right)\mathcal{B}^{-1}\mathcal{A}^{-1}$	associative property
$\left(\mathcal{A}\mathcal{B}\right)^{-1}\mathcal{I}$	$= \left(\mathcal{A}\mathcal{B}\right)^{-1}\left(\mathcal{A}\mathcal{B}\right)\mathcal{B}^{-1}\mathcal{A}^{-1}$	operate from the left with $\left(\mathcal{A}\mathcal{B}\right)^{-1}$
$\left(\mathcal{A}\mathcal{B}\right)^{-1}\mathcal{I}$	$= \mathcal{I}\mathcal{B}^{-1}\mathcal{A}^{-1}$	resolution of the identity $\mathcal{I} = \left(\mathcal{A}\mathcal{B}\right)^{-1}\left(\mathcal{A}\mathcal{B}\right)$
$\left(\mathcal{A}\mathcal{B}\right)^{-1}$	$= \mathcal{B}^{-1}\mathcal{A}^{-1}$	operation by the identity

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Postscript: A short comment on lines 5 and 6 may be helpful. Remember that the product of two operators is another operator, so $\left(\mathcal{A}\mathcal{B}\right)$ is an operator, and its inverse is denoted $\left(\mathcal{A}\mathcal{B}\right)^{-1}$.

If $\det\mathcal{A} = 0$, $\mathcal{A}$ is a **singular operator**, for which an inverse does not exist.

3–4. Show that if $\mathcal{A}$ and $\mathcal{B}$ are two-dimensional operators, $\left(\mathcal{A}\,\mathcal{B}\right)^{\dagger} = \mathcal{B}^{\dagger}\mathcal{A}^{\dagger}$.

This is a limited but definitive proof for two-dimensional operators. Use

$$\mathcal{A} \rightarrow \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad \text{and} \qquad \mathcal{B} \rightarrow \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix},$$

for instance. Simply form the matrix products of the left and right side of $\left(\mathcal{A}\,\mathcal{B}\right)^\dagger = \mathcal{B}^\dagger\,\mathcal{A}^\dagger$, the adjoint of the product and the product of the adjoints in the reverse order, compare them, and they will be the same. This proof can be extended to higher dimension.

$$\left(\mathcal{A}\,\mathcal{B}\right)^\dagger = \left[\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}\right]^\dagger = \left[\begin{pmatrix} a_{11}b_{11} + a_{12}b_{21} & a_{11}b_{12} + a_{12}b_{22} \\ a_{21}b_{11} + a_{22}b_{21} & a_{21}b_{12} + a_{22}b_{22} \end{pmatrix}\right]^\dagger$$

$$= \begin{pmatrix} a_{11}^* b_{11}^* + a_{12}^* b_{21}^* & a_{21}^* b_{11}^* + a_{22}^* b_{21}^* \\ a_{11}^* b_{12}^* + a_{12}^* b_{22}^* & a_{21}^* b_{12}^* + a_{22}^* b_{22}^* \end{pmatrix}.$$

The product of the adjoints in the opposite order is

$$\mathcal{B}^\dagger\,\mathcal{A}^\dagger = \left[\begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}\right]^\dagger\left[\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}\right]^\dagger = \begin{pmatrix} b_{11}^* & b_{21}^* \\ b_{12}^* & b_{22}^* \end{pmatrix}\begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix}$$

$$= \begin{pmatrix} a_{11}^* b_{11}^* + a_{12}^* b_{21}^* & a_{21}^* b_{11}^* + a_{22}^* b_{21}^* \\ a_{11}^* b_{12}^* + a_{12}^* b_{22}^* & a_{21}^* b_{12}^* + a_{22}^* b_{22}^* \end{pmatrix}.$$

This is, in fact, the same as the first expansion, therefore $\left(\mathcal{A}\,\mathcal{B}\right)^\dagger = \mathcal{B}^\dagger\,\mathcal{A}^\dagger$.

3–5. (a) Show that the adjoint of a non-singular unitary operator is equal to its inverse.

(b) Show that the product of unitary operators is unitary.

(c) Use operator algebra to show that if $\mathcal{A}$ and $\mathcal{B}$ are unitary, $\left(\mathcal{A}\,\mathcal{B}\right)^\dagger = \mathcal{B}^\dagger\,\mathcal{A}^\dagger$.

This problem is intended to illustrate operator algebra. All three parts are intended to be completed without the use of an explicit matrix. You can operate on both sides of an equation with the same operator if you operate from the same side. Operation must be from the left on both sides or from the right on both sides because operators do not generally commute. Operator algebra allows insertion of the operator $\mathcal{I}$ in any form and in any circumstance that is convenient.

Part (a) is an application of the definitions of unitary and inverse relations, $\mathcal{A}\,\mathcal{A}^\dagger = \mathcal{I}$, and $\mathcal{A}\,\mathcal{A}^{-1} = \mathcal{I}$, for instance. To show that the product of any two unitary operators is unitary, start with the product of two arbitrary unitary operators, say $\mathcal{A}\,\mathcal{B} = \mathcal{C}$. Operate on both sides with appropriate operators to show that $\mathcal{C}\,\mathcal{C}^\dagger = \mathcal{I}$. Remember that $\left(\mathcal{A}\mathcal{B}\right)^\dagger = \mathcal{B}^\dagger\mathcal{A}^\dagger$ from chapter 1 and the previous problem. Part (c) is a more elegant determination of this fact for unitary operators. Start with $\mathcal{A}\,\mathcal{A}^\dagger = \mathcal{I}$ and insert the identity between the two operators. It is likely $\mathcal{B}\,\mathcal{B}^\dagger$ will be a convenient form. The result of part (b) helps clarify part (c).

(a) If $\mathcal{A}$ is unitary, $\mathcal{A}\,\mathcal{A}^\dagger = \mathcal{I}$. $\mathcal{A}\,\mathcal{A}^{-1} = \mathcal{I}$ for all non-singular operators, so

$$\begin{aligned} \mathcal{A}\,\mathcal{A}^\dagger &= \mathcal{A}\,\mathcal{A}^{-1} && \text{because both are equal to } \mathcal{I} \\ \mathcal{A}^{-1}\,\mathcal{A}\,\mathcal{A}^\dagger &= \mathcal{A}^{-1}\,\mathcal{A}\,\mathcal{A}^{-1} && \text{operate from the left with } \mathcal{A}^{-1} \\ \mathcal{I}\,\mathcal{A}^\dagger &= \mathcal{I}\,\mathcal{A}^{-1} && \text{because } \mathcal{A}^{-1}\,\mathcal{A} = \mathcal{I} \\ \mathcal{A}^\dagger &= \mathcal{A}^{-1} && \text{which is the desired result.} \end{aligned}$$

(b) If $\mathcal{A}$ and $\mathcal{B}$ are unitary, then $\mathcal{A}\mathcal{A}^\dagger = \mathcal{B}\mathcal{B}^\dagger = \mathcal{I}$. Consider their product

$$\begin{aligned}
\mathcal{A}\,\mathcal{B} &= \mathcal{C} && \text{the product of two operators is an operator} \\
\mathcal{A}\mathcal{B}\mathcal{B}^\dagger &= \mathcal{C}\,\mathcal{B}^\dagger && \text{operate from the right with } \mathcal{B}^\dagger \\
\mathcal{A}\mathcal{I} = \mathcal{A} &= \mathcal{C}\,\mathcal{B}^\dagger && \text{because } \mathcal{B}\mathcal{B}^\dagger = \mathcal{I} \\
\mathcal{A}\mathcal{A}^\dagger &= \mathcal{C}\,\mathcal{B}^\dagger\mathcal{A}^\dagger && \text{operate from the right with } \mathcal{A}^\dagger \\
\mathcal{I} &= \mathcal{C}\,\mathcal{B}^\dagger\mathcal{A}^\dagger && \text{because } \mathcal{A}\mathcal{A}^\dagger = \mathcal{I} \\
\mathcal{I} &= \mathcal{C}\,(\mathcal{A}\mathcal{B})^\dagger && \text{use of } (\mathcal{A}\mathcal{B})^\dagger = \mathcal{B}^\dagger\mathcal{A}^\dagger \\
\mathcal{I} &= \mathcal{C}\,\mathcal{C}^\dagger && \text{definition of } \mathcal{C}
\end{aligned}$$

or $\mathcal{C}\mathcal{C}^\dagger = \mathcal{I}$, and therefore, the product of unitary operators is unitary.

(c) Given that $\mathcal{A}$ and $\mathcal{B}$ are unitary,

$$\begin{aligned}
\mathcal{A}\mathcal{A}^\dagger &= \mathcal{I} && \text{definition of unitary} \\
\mathcal{A}\mathcal{I}\mathcal{A}^\dagger &= \mathcal{I} && \text{insertion of the identity} \\
\mathcal{A}\mathcal{B}\mathcal{B}^\dagger\mathcal{A}^\dagger &= \mathcal{I} && \text{use of the form } \mathcal{I} = \mathcal{B}\mathcal{B}^\dagger \\
(\mathcal{A}\mathcal{B})\,\mathcal{B}^\dagger\mathcal{A}^\dagger &= \mathcal{I} && \text{associative property} \\
(\mathcal{A}\mathcal{B})^\dagger\,(\mathcal{A}\mathcal{B})\,\mathcal{B}^\dagger\,\mathcal{A}^\dagger &= (\mathcal{A}\mathcal{B})^\dagger\,\mathcal{I} && \text{operation from the left with } (\mathcal{A}\mathcal{B})^\dagger \\
\mathcal{I}\,\mathcal{B}^\dagger\,\mathcal{A}^\dagger &= (\mathcal{A}\mathcal{B})^\dagger && \text{because } (\mathcal{A}\mathcal{B})^\dagger(\mathcal{A}\mathcal{B}) = \mathcal{I} \text{ from part (b)} \\
\mathcal{B}^\dagger\,\mathcal{A}^\dagger &= (\mathcal{A}\mathcal{B})^\dagger && \text{or} \quad (\mathcal{A}\mathcal{B})^\dagger = \mathcal{B}^\dagger\,\mathcal{A}^\dagger .
\end{aligned}$$

3–6. Show how the unitary transformation $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ determines the transformation of vectors.

The transformation of kets was indicated to be $\mathcal{U}^\dagger\,|\,v>$ in the last chapter. This problem explains why. It also is intended to convey that Dirac notation is independent of basis.

An inner product is a scalar. An operator acting on a vector, such as $\mathcal{A}\,|\,v>$ is a vector, $\mathcal{A}\,|\,v> = |\,v'>$ for instance. Since $<w\,|\,\mathcal{A}\,|\,v> = <w\,|\,v'>$, it follow that $<w\,|\,\mathcal{A}\,|\,v>$ is a scalar because $<w\,|\,v'>$ is a scalar. We will encounter numerous brakets where a bra and a ket sandwich an operator. This type of braket is a scalar, just as an inner product is a scalar.

When conducting a unitary transformation on an operator, any associated bras and kets also require transformation. Insert the identity in the braket $<w\,|\,\mathcal{A}\,|\,v>$ to the immediate left and right of $\mathcal{A}$, use the fact that the identity can be expressed $\mathcal{U}\mathcal{U}^\dagger = \mathcal{I}$, and examine pieces.

$$\begin{aligned}
<w\,|\,\mathcal{A}\,|\,v> &= <w\,|\,\mathcal{I}\mathcal{A}\mathcal{I}\,|\,v> \\
&= <w|\;\mathcal{U}\mathcal{U}^\dagger\,\mathcal{A}\;\mathcal{U}\mathcal{U}^\dagger\;|\,v> \\
&= \underbrace{\Big(<w\,|\,\mathcal{U}\Big)}_{\text{transform bras}}\quad \overbrace{\Big(\mathcal{U}^\dagger\mathcal{A}\mathcal{U}\Big)}^{\text{transform operators}}\quad \underbrace{\Big(\mathcal{U}^\dagger\,|\,v>\Big)}_{\text{transform kets}} .
\end{aligned}$$

The object in the center set of parenthesis is our unitary transformation. For general $<w|$ and $|v>$, the last equation says we must transform a bra as $<w|\mathcal{U}$ and a ket as $\mathcal{U}^\dagger|v>$ to be consistent with the form of the unitary transformation chosen.

Postscript: Notice that if $\mathcal{U}\mathcal{A}\mathcal{U}^\dagger$ is chosen as the unitary transformation, $<w|\mathcal{U}^\dagger$ would be the correct method to transform a bra and $\mathcal{U}|v>$ would be the correct manner to transform a ket. Our convention of $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ is precisely that, a convention, rather than a mathematical necessity. Be aware that other conventions are possible.

3–7. Show that the inner product $<q|k>$ where $|q> \rightarrow \begin{pmatrix} 4i \\ 3 \end{pmatrix}$ and $|k> \rightarrow \begin{pmatrix} -6 \\ 2-3i \end{pmatrix}$, is invariant under the unitary transformation that diagonalizes $\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}$.

First, the inner product is

$$<q|k> \;=\; (-4i,\;\; 3)\begin{pmatrix} -6 \\ 2-3i \end{pmatrix} \;=\; 24i+6-9i \;=\; 6+15i$$

The unitary transformation found to diagonalize $\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}$ was found in chapter 1 to be

$$\mathcal{U} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \qquad \Rightarrow \qquad \mathcal{U}^\dagger \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}.$$

Transform the bra as $<q|\mathcal{U}$ and the ket as $\mathcal{U}^\dagger|k>$.

$$<q|\mathcal{U} \;=\; (-4i,\;\; 3)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \;=\; \frac{1}{\sqrt{2}}(-4i+3i,\;\; -4i-3i) \;=\; \frac{1}{\sqrt{2}}(-i,\;\; -7i) \;=\; <q'|$$

$$\mathcal{U}^\dagger|k> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} -6 \\ 2-3i \end{pmatrix} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} -6-2i-3 \\ -6+2i+3 \end{pmatrix} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} -9-2i \\ -3+2i \end{pmatrix} \;=\; |k'>$$

$$<q'|k'> \;=\; \frac{1}{\sqrt{2}}(-i,\;\; -7i)\frac{1}{\sqrt{2}}\begin{pmatrix} -9-2i \\ -3+2i \end{pmatrix} \;=\; \frac{1}{2}(9i-2+21i+14)$$

$$=\; \frac{1}{2}(12+30i) \;=\; 6+15i \;=\; <q|k>\;.$$

3–8. Show that the inner product $<g|5>$ where $|g> \rightarrow \begin{pmatrix} 2 \\ 3-i \\ -i \end{pmatrix}$ and $|5> \rightarrow \begin{pmatrix} -1-5i \\ 4 \\ -2i \end{pmatrix}$, is invariant under the unitary transformation that diagonalizes $\begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix}$.

Like 3–7 except in $\mathbb{C}^3$. The appropriate unitary transformation from chapter 1 is

$$\mathcal{U} \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix} 2i & 0 & 1 \\ 0 & \sqrt{5} & 0 \\ 1 & 0 & 2i \end{pmatrix} \qquad \Rightarrow \qquad \mathcal{U}^\dagger \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix} -2i & 0 & 1 \\ 0 & \sqrt{5} & 0 \\ 1 & 0 & -2i \end{pmatrix}.$$

Transform the bra as $<g\,|\mathcal{U}$ and the ket as $\mathcal{U}^\dagger\,|\,5>$.

$$<g\,|\,5> \;=\; \big(\,2\,,\;\; 3+i\,,\;\; i\big)\begin{pmatrix} -1-5i \\ 4 \\ -2i \end{pmatrix} \;=\; -2-10i+12+4i+2 \;=\; 12-6i$$

$$<g\,|\mathcal{U} \;=\; \big(\,2\,,\;\; 3+i\,,\;\; i\big)\frac{1}{\sqrt{5}}\begin{pmatrix} 2i & 0 & 1 \\ 0 & \sqrt{5} & 0 \\ 1 & 0 & 2i \end{pmatrix} \;=\; \frac{1}{\sqrt{5}}\big(4i+i\,,\;\; 3\sqrt{5}+\sqrt{5}\,i\,,\;\; 2-2\big)$$

$$=\; \frac{1}{\sqrt{5}}\big(5i\,,\;\; 3\sqrt{5}+\sqrt{5}\,i\,,\;\; 0\big) \;=\; <g'\,|$$

$$\mathcal{U}^\dagger\,|\,5> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix} -2i & 0 & 1 \\ 0 & \sqrt{5} & 0 \\ 1 & 0 & -2i \end{pmatrix}\begin{pmatrix} -1-5i \\ 4 \\ -2i \end{pmatrix} \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix} 2i-10-2i \\ 4\sqrt{5} \\ -1-5i-4 \end{pmatrix}$$

$$=\; \frac{1}{\sqrt{5}}\begin{pmatrix} -10 \\ 4\sqrt{5} \\ -5-5i \end{pmatrix} \;=\; |\,5'>$$

$$<g'\,|\,5'> \;=\; \frac{1}{\sqrt{5}}\big(5i\,,\;\; 3\sqrt{5}+\sqrt{5}\,i\,,\;\; 0\big)\frac{1}{\sqrt{5}}\begin{pmatrix} -10 \\ 4\sqrt{5} \\ -5-5i \end{pmatrix} \;=\; \frac{1}{5}\big(-50i+60+20i+0\big)$$

$$=\; \frac{1}{5}\big(60-30i\big) \;=\; 12-6i\,.$$

3–9. Show that a unitary transformation preserves an inner product in general.

$<x\,|\mathcal{U} = <x'\,|\,,\;\; \mathcal{U}^\dagger\,|\,y> = \;|\,y'>\;\; \Rightarrow \;\; <x'\,|\,y'> = <x\,|\mathcal{U}\mathcal{U}^\dagger\,|\,y> = <x\,|\mathcal{I}\,|\,y> = <x\,|\,y>\,.$

Postscript: This is occasionally expressed $<\mathcal{U}x\,|\,\mathcal{U}y> \;=\; <x\,|\,y>$.

Our definition is that an operator $\mathcal{U}$ is unitary if $\mathcal{U}\mathcal{U}^\dagger \;=\; \mathcal{U}^\dagger\mathcal{U} \;=\; \mathcal{I}$. From our method of constructing $\mathcal{U}$ and this definition it follows that (1) the column vectors composing a unitary operator are orthogonal, that operation with a unitary operator on vectors (2) preserves lengths/norms, (3) preserves angles/angle analogs, and (4) preserves inner products, and that a unitary transformation (5) preserves eigenvalues. All five properties are proven in this and other problems and exercises that follow. There is mathematical latitude in the definition of a unitary operator. Occasionally $\mathcal{A}^\dagger \;=\; \mathcal{A}^{-1}$ is the defining equation. Other treatments use a variety of the five listed properties as defining characteristics.

Another alternate view is that if $<x\,|\,\mathcal{U}^\dagger = <x'\,|$ and $\mathcal{U}\,|\,y> = |\,y'>$, can the operator $\mathcal{U}$ be defined such that $<x\,|\,y> = <x'\,|\,y'>$? In other words, can an operator $\mathcal{U}$ be defined such that it requires preservation of an inner product? Simply substituting the two equations in the top line of this paragraph into the inner product of the primed vectors,

$$<x'\,|\,y'> \;=\; <x\,|\,\mathcal{U}^\dagger\mathcal{U}\,|\,y> \;=\; <x\,|\,y>$$

if and only if $\mathcal{U}^\dagger\mathcal{U} = \mathcal{I}$, so preservation of an inner product can define a unitary operator.

3–10. Show that $|\,g>$ and $|\,g'>$ from problem 3–8 have the same norm.

This is numerical evidence that a unitary transformation preserves a vector's norm.

$$\big|\,|\,g>\,\big|^2 = <g\,|\,g> \;=\; \big(2\,,\;\; 3+i\,,\;\; i\big)\begin{pmatrix} 2 \\ 3-i \\ -i \end{pmatrix} = 4+9+1+1 \;=\; 15 \quad\Rightarrow\quad \big|\,|\,g>\,\big| \;=\; \sqrt{15}\,.$$

$$\big|\,|\,g'>\,\big|^2 = <g'\,|\,g'> \;=\; \frac{1}{\sqrt{5}}\big(5i\,,\;\; 3\sqrt{5}+\sqrt{5}\,i\,,\;\; 0\big)\frac{1}{\sqrt{5}}\begin{pmatrix} -5i \\ 3\sqrt{5}-\sqrt{5}\,i \\ 0 \end{pmatrix}$$

$$= \;\frac{1}{5}\big(25+45+5+0\big) \;=\; \frac{1}{5}\,75 \;=\; 15 \quad\Rightarrow\quad \big|\,|\,g'>\,\big| \;=\; \sqrt{15}\,.$$

Postscript: The proof in general is left as exercise 3–36, however, consider the choice of $<x\,|$ and $|\,x>$ instead of $<x\,|$ and $|\,y>$ in problem 3–9 for a proof in general.

3–11. Show that a unitary transformation preserves angles.

This problem supports an important property of a unitary transformation and is intended to prompt some thought about the meaning of angles/angle analogs in a higher dimensional space. "Angle" is the accepted terminology though "angle analog" may be a better description in $\mathbb{C}^n$.

An inner product is a generalization of a dot product. A dot or scalar product is defined

$$\vec{A}\cdot\vec{B} \;=\; |\,\vec{A}\,|\,|\,\vec{B}\,|\,\cos\theta$$

and is so defined because it is a projection of one vector onto another. Work, the usual initial introduction to the concept of energy, is the magnitude of a displacement in the direction of a force for which the dot/scalar product is useful. The fact that $\vec{A}\cdot\vec{B} = A_x\,B_x + A_y\,B_y + A_z\,B_z$ follows from the property of orthonormality. In fact, the actual trinomial multiplication is

$$\begin{aligned}\vec{A}\cdot\vec{B} \;=\;& A_x\,B_x\,\widehat{i}\cdot\widehat{i} \;+\; A_x\,B_y\,\widehat{i}\cdot\widehat{j} \;+\; A_x\,B_z\,\widehat{i}\cdot\widehat{k} \\ &+\; A_y\,B_x\,\widehat{j}\cdot\widehat{i} \;+\; A_y\,B_y\,\widehat{j}\cdot\widehat{j} \;+\; A_y\,B_z\,\widehat{j}\cdot\widehat{k} \\ &+\; A_z\,B_x\,\widehat{k}\cdot\widehat{i} \;+\; A_z\,B_y\,\widehat{k}\cdot\widehat{j} \;+\; A_z\,B_z\,\widehat{k}\cdot\widehat{k} \\ =\;& A_x\,B_x \;+\; A_y\,B_y \;+\; A_z\,B_z\end{aligned}$$

because $\widehat{i}\cdot\widehat{i} = \widehat{j}\cdot\widehat{j} = \widehat{k}\cdot\widehat{k} = 1$ and $\widehat{i}\cdot\widehat{j} = \widehat{i}\cdot\widehat{k} = \widehat{j}\cdot\widehat{i} = \widehat{j}\cdot\widehat{k} = \widehat{k}\cdot\widehat{i} = \widehat{k}\cdot\widehat{j} = 0$ in Cartesian coordinates, for instance. Thus, angles are

$$\theta \;=\; \cos^{-1}\frac{\vec{A}\cdot\vec{B}}{|\,\vec{A}\,|\,|\,\vec{B}\,|}$$

and are readily identifiable in $\mathbb{R}^2$ and $\mathbb{R}^3$. An interpretation is less clear in $\mathbb{R}^4$ though it is straightforward to write

$$\theta \;=\; \cos^{-1}\frac{A_1\,B_1 \;+\; A_2\,B_2 \;+\; A_3\,B_3 \;+\; A_4\,A_4}{|\,\vec{A}\,|\,|\,\vec{B}\,|}\,.$$

This may have meaning in a hyperbolic space, but is better pictured as an abstraction for quantum mechanical purposes. The generalization to $\mathbb{C}^n$, where abstraction is necessary, is straightforward.

The generalization

$$\theta \;=\; \cos^{-1}\frac{<A\,|\,B>}{|\,|\,A>\,|\,|\,|\,B>\,|}$$

applies to $\mathbb{C}^n$. Under a unitary transformation, the inner product of two vectors is preserved (problem 3–9), and the norm of each vector is preserved (problem 3–10 and exercise 3–36 which resembles problem 3–9). Therefore, the angle θ must remain identical, or is preserved, under a unitary transformation.

3–12. Show that the eigenvectors of non-degenerate Hermitian operators are orthogonal.

This is a claim made in the first problem of chapter 1 which has been repeated numerous times. Remember Hermitian means $\mathcal{A} \;=\; \mathcal{A}^{\dagger}$.

Let $|\,x>$ and $|\,y>$ be any two eigenvectors of $\mathcal{A}$. Then

$$\begin{aligned}
<x\,|\,\mathcal{A}\,|\,y> \;&=\; <x\,|\,\mathcal{A}\,|\,y> && \text{trivial statement}\\
0 \;&=\; <x\,|\,\mathcal{A}\,|\,y> \;-\; <x\,|\,\mathcal{A}\,|\,y> && \text{subtraction to obtain a homogeneous equation}\\
0 \;&=\; \big(<x\,|\,\mathcal{A}\big)\,|\,y> \;-\; <x\,|\,\big(\mathcal{A}\,|\,y>\big) && \text{associative property}\\
0 \;&=\; \big(\mathcal{A}^{\dagger}\,|\,x>\big)^{\dagger}\,|\,y> \;-\; <x\,|\,\big(\mathcal{A}\,|\,y>\big) && \text{adjoint of product is reverse of product of adjoints}\\
0 \;&=\; \big(\mathcal{A}\,|\,x>\big)^{\dagger}\,|\,y> \;-\; <x\,|\,\big(\mathcal{A}\,|\,y>\big) && \text{Hermitian property}\\
0 \;&=\; \big(\alpha_x\,|\,x>\big)^{\dagger}\,|\,y> \;-\; <x\,|\,\big(\alpha_y\,|\,y>\big) && \text{eigenvalue/eigenvector equations}\\
0 \;&=\; \alpha_x\big(\,|\,x>\big)^{\dagger}\,|\,y> \;-\; \alpha_y\,<x\,|\,\big(\,|\,y>\big) && \text{eigenvalues are scalars}\\
0 \;&=\; \alpha_x\,<x\,|\,y> \;-\; \alpha_y\,<x\,|\,y> && \text{bra is adjoint of ket}\\
0 \;&=\; \big(\alpha_x \;-\; \alpha_y\big)\,<x\,|\,y> && \text{distributive property}
\end{aligned}$$

but $\alpha_x \neq \alpha_y$ because $\mathcal{A}$ is given to be non-degenerate $\Rightarrow$ $<x\,|\,y> \;=\; 0$ which means $|\,x>$ and $|\,y>$ are orthogonal for all $|\,x> \;\neq\; |\,y>$.

Postscript: This can be modified to apply to degenerate Hermitian operators by adding a small Hermitian perturbation $\delta\mathcal{A}$ so that $\mathcal{A}+\delta\mathcal{A}$ is Hermitian with distinct eigenvalues, applying the same argument to $\mathcal{A}+\delta\mathcal{A}$, then letting $\delta\mathcal{A} \to 0$ during which it can be shown the eigenvectors do not lose the property of orthogonality.

Recall that the unitary operators that diagonalize a Hermitian operator are built from its normalized eigenvectors. Thus, this problem also constitutes a proof that unitary operators so built have columns of orthogonal and also orthonormal vectors.

3–13. Show that the eigenvalues of an operator are unchanged by a unitary transformation.

Some numerical examples for $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ were provided in chapter 1. A proof in general follows.

$$
\begin{aligned}
\mathcal{A}\,|\,a_i> \;&=\; \alpha_i\,|\,a_i> && \text{eigenvalue/eigenvector equation}\\
\mathcal{A}\mathcal{I}\,|\,a_i> \;&=\; \alpha_i\,|\,a_i> && \text{insertion of the identity}\\
\mathcal{A}\mathcal{U}\mathcal{U}^\dagger\,|\,a_i> \;&=\; \alpha_i\,|\,a_i> && \text{resolution of the identity } \mathcal{I} = \mathcal{U}\mathcal{U}^\dagger\\
\mathcal{U}^\dagger\mathcal{A}\mathcal{U}\mathcal{U}^\dagger\,|\,a_i> \;&=\; \mathcal{U}^\dagger\alpha_i\,|\,a_i> && \text{operation from the left with } \mathcal{U}^\dagger\\
(\mathcal{U}^\dagger\mathcal{A}\mathcal{U})\,\mathcal{U}^\dagger\,|\,a_i> \;&=\; \alpha_i\mathcal{U}^\dagger\,|\,a_i> && \text{associative law and commutivity of scalars}\\
\mathcal{U}^\dagger\mathcal{A}\mathcal{U}\;|\,a_i'> \;&=\; \alpha_i\,|\,a_i'> && \text{eigenvectors transformed by } \mathcal{U}^\dagger
\end{aligned}
$$

where the last line is the desired result indicating the operator is transformed as $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$, the eigenkets are transformed as $\mathcal{U}^\dagger\,|\,a_i> \;=\; |\,a_i'>$, but the eigenvalues, the α_i, are unchanged.

Postscript: This shows that the eigenvalues of any operator having a eigenvalue/eigenvector equation are unchanged by a unitary transformation. Though the postulates indicate the primary focus is on Hermitian operators, the condition of Hermiticity, $\mathcal{A} = \mathcal{A}^\dagger$, is not invoked.

All pertinent properties of unitary operators have been developed. Notice that problems 3–3, 3–5, 3–6, 3–9, 3–11, 3–12, and 3–13 with generic operators like $\mathcal{U}$ and $\mathcal{A}$, and generic vectors like $<w|$ and $|\,B>$, are completed without reference to space or basis. These results are applicable to any space including $\mathbb{C}^\infty$. These results apply in position space, momentum space, energy space, and any other space having a basis that spans the space.

In addition to the results developed, the seven problems listed in the above paragraph are examples of operator algebra. Since the dynamic variables of classical mechanics are described by operators in quantum mechanics, utility with operator algebra is quantum mechanically essential.

Problems 3–14 through 3–17 comprise one numerical example of simultaneous diagonalization.

3–14. (a) Is the Hamiltonian operator $\mathcal{H} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & -2i \\ 0 & 2i & 3 \end{pmatrix}$ Hermitian?

(b) Is $\mathcal{H}$ degenerate?

(c) If so, what are the implications of the degeneracy?

$\mathcal{H}$ is Hermitian because $\mathcal{H} = \mathcal{H}^\dagger$, using the explicit matrix representation

$$\mathcal{H} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & -2i \\ 0 & 2i & 3 \end{pmatrix} \quad \Rightarrow \quad \mathcal{H}^{\mathrm{T}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 2i \\ 0 & -2i & 3 \end{pmatrix} \quad \Rightarrow \quad \mathcal{H}^{\mathrm{T}*} = \mathcal{H}^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & -2i \\ 0 & 2i & 3 \end{pmatrix}$$

and part (a) is complete. The implication is that the operator $\mathcal{H}$ could represent an observable quantity (energy for a Hamiltonian operator). The fact that $\mathcal{H}$ is Hermitian also guarantees that it can be diagonalized. Part (b) requires solving the eigenvalue problem.

(b) $\det \begin{pmatrix} 1-\alpha & 0 & 0 \\ 0 & 3-\alpha & -2i \\ 0 & 2i & 3-\alpha \end{pmatrix} = (1-\alpha)(3-\alpha)^2 - 4(1-\alpha) = 9 - 15\alpha + 7\alpha^2 - \alpha^3 - 4 + 4\alpha$

$\Rightarrow \quad \alpha^3 - 7\alpha^2 + 11\alpha - 5 = 0$ is the characteristic equation which can be factored

$(\alpha - 5)(\alpha - 1)^2 = 0 \quad \Rightarrow \quad \alpha = 1\,,\ 1\,,\ 5$ are the eigenvalues. $\mathcal{H}$ is degenerate at $\alpha = 1$.

(c) Obtaining the eigenvectors is fruitless because a measurement of $\mathcal{H}$ returning 1 identifies two eigenstates. The eigenstate after a measurement of 1 cannot be uniquely determined.

3–15. Does $\mathcal{H}$ commute with $\mathcal{K} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}$?

The first step in lifting the degeneracy of $\mathcal{H}$ is to find a Hermitian operator with which it commutes.

$$\mathcal{H}\mathcal{K} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & -2i \\ 0 & 2i & 3 \end{pmatrix} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 4i \\ 0 & -4i & -1 \end{pmatrix}$$

$$\mathcal{K}\mathcal{H} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & -2i \\ 0 & 2i & 3 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 4i \\ 0 & -4i & -1 \end{pmatrix}$$

thus, $\big[\mathcal{H}\,,\mathcal{K}\big] = \mathcal{H}\mathcal{K} - \mathcal{K}\mathcal{H} = 0$ and these operators commute.

Postscript: That $\mathcal{K}$ is Hermitian is essential. The degeneracy of $\mathcal{H}$ is lifted by measurements of two observable quantities. A non-Hermitian $\mathcal{K}$ cannot represent an observable quantity, and "measurement" of a non-observable quantity is physically not possible.

That $\mathcal{H}$ and $\mathcal{K}$ commute means that the two operators share a common eigenbasis. Since both operators are Hermitian, they can both be diagonalized. And since they share a common eigenbasis, they can both be diagonalized by the same unitary transformation.

3–16. Solve the eigenvalue/eigenvector problem for $\mathcal{K}$.

The plan is to first ensure that $\mathcal{K}$ is not degenerate. If $\mathcal{K}$ is degenerate, it is acceptable only if the eigenstates can be identified uniquely. We find that $\mathcal{K}$ is not degenerate, so a unitary operator built from its eigenvectors will simultaneously diagonalize both $\mathcal{K}$ and $\mathcal{H}$.

$$\det\begin{pmatrix} 2-\alpha & 0 & 0 \\ 0 & 1-\alpha & 2i \\ 0 & -2i & 1-\alpha \end{pmatrix} = \big(2-\alpha\big)\big(1-\alpha\big)^2 - 4\big(2-\alpha\big) = 2-5\alpha+4\alpha^2-\alpha^3-8+4\alpha$$

$\Rightarrow \quad \alpha^3-4\alpha^2+\alpha+6 = 0$ is the characteristic equation which can be factored

$\big(\alpha+1\big)\big(\alpha-2\big)\big(\alpha-3\big) = 0 \quad \Rightarrow \quad \alpha = -1\,,\ 2\,,\ 3$ are the eigenvalues. $\mathcal{K}$ is a satisfactory operator from which to build an appropriate unitary operator. The eigenvectors are needed.

$$\mathcal{K}\,|\,a> \;=\; \alpha\,|\,a>$$

$$\Rightarrow \quad \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = -1\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} 2a &= -a \\ b+2ci &= -b \\ -2bi+c &= -c \end{aligned} \quad \Rightarrow \quad \begin{aligned} a &= 0 \\ ci &= -b \\ bi &= c \end{aligned}$$

$$\Rightarrow \quad a = 0\,,\ b = 1\,,\ c = i\,, \quad \Rightarrow \quad |-1> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix}$$

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 2\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} 2a &= 2a \\ b+2ci &= 2b \\ -2bi+c &= 2c \end{aligned} \quad \Rightarrow \quad \begin{aligned} a &= a \\ 2ci &= b \\ -2bi &= c \end{aligned}$$

$$\Rightarrow \quad a = 1\,,\ b = 0\,,\ c = 0\,, \quad \Rightarrow \quad |\,2> \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 3\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} 2a &= 3a \\ b+2ci &= 3b \\ -2bi+c &= 3c \end{aligned} \quad \Rightarrow \quad \begin{aligned} a &= 0 \\ ci &= b \\ -bi &= c \end{aligned}$$

$$\Rightarrow \quad a = 0\,,\ b = 1\,,\ c = -i\,, \quad \Rightarrow \quad |\,3> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix}$$

3–17. Simultaneously diagonalize $\mathcal{H}$ and $\mathcal{K}$.

Having two Hermitian operators that commute, form a unitary operator from the eigenvectors of the non-degenerate operator, and the unitary transformation $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ will diagonalize both.

$$\mathcal{U} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \\ i & 0 & -i \end{pmatrix} \quad \Rightarrow \quad \mathcal{U}^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & -i \\ \sqrt{2} & 0 & 0 \\ 0 & 1 & i \end{pmatrix}$$

$$\mathcal{U}^\dagger\mathcal{K}\mathcal{U} = \mathcal{U}^\dagger\begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \\ i & 0 & -i \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 0 & 1 & -i \\ \sqrt{2} & 0 & 0 \\ 0 & 1 & i \end{pmatrix}\begin{pmatrix} 0 & 2\sqrt{2} & 0 \\ -1 & 0 & 3 \\ -i & 0 & -3i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} -2 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 6 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

$$\mathcal{U}^\dagger\mathcal{H}\mathcal{U} = \mathcal{U}^\dagger\begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & -2i \\ 0 & 2i & 3 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \\ i & 0 & -i \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 0 & 1 & -i \\ \sqrt{2} & 0 & 0 \\ 0 & 1 & i \end{pmatrix}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 5 & 0 & 1 \\ 5i & 0 & -i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 10 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Postscript: The calculation $\mathcal{U}^\dagger\mathcal{K}\mathcal{U}$ was unnecessary. The unitary operator was built from left to right in the order of the eigenvector corresponding to the lowest eigenvalue to the eigenvector corresponding to the highest eigenvalue. Writing $\mathcal{K} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$ with the known eigenvalues in a diagonal basis by inspection is warranted. Similarly, had the unitary operator been built in the order of the eigenvector corresponding to the highest eigenvalue to the eigenvector corresponding to the lowest eigenvalue, writing $\mathcal{K} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ by inspection is warranted. Of course, should the unitary operator have been so built the operator $\mathcal{H} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 5 \end{pmatrix}$.

Suppose $\mathcal{K}$ was degenerate with eigenvalues of $2\,,\ 3\,,\ 3$. It would be acceptable only if eigenstates can be distinguished. If eigenstates were $|\,5\,,\ 2>,\ |\,1\,,\ 3>,$ and $|\,1\,,\ 3>$ the operator $\mathcal{K}$ is not acceptable. However, should the eigenstates be $|\,5\,,\ 3>,\ |\,1\,,\ 2>,$ and $|\,1\,,\ 3>$ eigenstates can be distinguished and $\mathcal{K}$ is acceptable.

The utility of the diagonal basis of unit vectors should be emphasized. The diagonal basis of unit vectors can make accessible the concepts of orthogonality, orthonormality, and basis. Consider

a diagonal basis in $\mathbb{C}^5$. The basis vectors are the unit vectors

$$|1> = \begin{pmatrix}1\\0\\0\\0\\0\end{pmatrix} \quad |2> = \begin{pmatrix}0\\1\\0\\0\\0\end{pmatrix} \quad |3> = \begin{pmatrix}0\\0\\1\\0\\0\end{pmatrix} \quad |4> = \begin{pmatrix}0\\0\\0\\1\\0\end{pmatrix} \quad |5> = \begin{pmatrix}0\\0\\0\\0\\1\end{pmatrix}.$$

That any vector in $\mathbb{C}^5$ can be expressed as a linear combination is straightforward, for instance

$$\begin{pmatrix}2i\\6\\3-4i\\i\sin(\pi/19)\\\sqrt{47}\end{pmatrix} = 2i\begin{pmatrix}1\\0\\0\\0\\0\end{pmatrix} + 6\begin{pmatrix}0\\1\\0\\0\\0\end{pmatrix} + (3-4i)\begin{pmatrix}0\\0\\1\\0\\0\end{pmatrix} + i\sin(\pi/19)\begin{pmatrix}0\\0\\0\\1\\0\end{pmatrix} + \sqrt{47}\begin{pmatrix}0\\0\\0\\0\\1\end{pmatrix}.$$

Any five component ket can be similarly expressed as a linear combination, thus the unit vectors span the space and constitute a basis in $\mathbb{C}^5$. The unit vectors are orthogonal and normalized by inspection, thus, they are orthonormal by inspection, or $<i\,|\,j> = \delta_{ij}$ by inspection. The eigenvalues of a diagonal operator are the elements on the principal diagonal so are obtained by inspection. Further, these advantages seem readily extensible to $\mathbb{C}^n$ for any n including ∞. These are some of the reasons diagonalization and simultaneous diagonalization are pursued.

3–18. (a) Find all possibilities for a measurement of the $\mathcal{H}$, $\mathcal{K}$ system.

(b) Find the probability of each possibility given $|\psi> = \frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$.

A measurement of a system of two operators is a set of two individual measurements, a measurement of $\mathcal{H}$ and a subsequent measurement of $\mathcal{K}$, for this complete set of commuting observables.

(a) Using $\mathcal{H} = \begin{pmatrix}5&0&0\\0&1&0\\0&0&1\end{pmatrix}$ and $\mathcal{K} = \begin{pmatrix}-1&0&0\\0&2&0\\0&0&3\end{pmatrix}$, a measurement of $\mathcal{H}$ yielding 5 collapses the state vector to $|\psi'> = \begin{pmatrix}1\\0\\0\end{pmatrix}$ and the only possible result of a measurement of $\mathcal{K}$ is -1. A measurement of $\mathcal{H}$ yielding 1 does not identify the new eigenstate. A subsequent measurement of $\mathcal{K}$ could yield 2 or 3, so $1,2$ is a second possibility, and $1,3$ is the third. The eigenstate is identified by the second measurement. The possibilities and eigenstates are

$$|5,\,-1> = \begin{pmatrix}1\\0\\0\end{pmatrix} \quad |1,\,2> = \begin{pmatrix}0\\1\\0\end{pmatrix} \quad |1,\,3> = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

after a measurement of the $\mathcal{H}$, $\mathcal{K}$ system.

$$\text{(b) } P(5,-1) \;=\; \big|<5,-1\,|\,\psi>\big|^2 = \left|\big(1\,,\;\;0\,,\;\;0\big)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{14}}(1+0+0)\right|^2 = \frac{1}{14}$$

$$P(1,2) \;=\; \big|<1,2\,|\,\psi>\big|^2 = \left|\big(0\,,\;\;1\,,\;\;0\big)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{14}}(0+2+0)\right|^2 = \frac{4}{14}$$

$$P(1,3) \;=\; \big|<1,3\,|\,\psi>\big|^2 = \left|\big(0\,,\;\;0\,,\;\;1\big)\,\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\right|^2 = \left|\frac{1}{\sqrt{14}}(0+0+3)\right|^2 = \frac{9}{14}$$

Postscript: Notice that both eigenvalues are required to uniquely identify each ket.

Notice also that the expectation value and the uncertainty of the $\mathcal{H}$, $\mathcal{K}$ system do not have meaning. $<\mathcal{H}>$, $<\mathcal{K}>$, $\triangle\mathcal{H}$, and $\triangle\mathcal{K}$ can be calculated, but $\sum P(\alpha_i)\,\alpha_i$ for the $\mathcal{H}$, $\mathcal{K}$ system is not possible because two eigenvalues correspond to each probability. The method $<\mathcal{A}> \;=\; <\psi\,|\,\mathcal{A}\,|\,\psi>$ also is dependent on a single eigenvalue per problem 2–25.

3–19. Calculate $<\mathcal{H}>$, $<\mathcal{K}>$, $\triangle\mathcal{H}$, and $\triangle\mathcal{K}$ given $\quad|\,\psi> \;=\; \dfrac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$.

The state vector is repeated to make clear that the probabilities of the previous problem apply.

$$<\mathcal{H}> \;=\; \sum P(\alpha_{\mathcal{H}})\,\alpha_{\mathcal{H}} \;=\; \frac{1}{14}\times 5 \;+\; \frac{4}{14}\times 1 \;+\; \frac{9}{14}\times 1 \;=\; \frac{5+4+9}{14} \;=\; \frac{18}{14} \;=\; \frac{9}{7}$$

$$<\mathcal{K}> \;=\; \sum P(\alpha_{\mathcal{K}})\,\alpha_{\mathcal{K}} \;=\; \frac{1}{14}\times(-1) \;+\; \frac{4}{14}\times 2 \;+\; \frac{9}{14}\times 3 \;=\; \frac{-1+8+27}{14} \;=\; \frac{34}{14} \;=\; \frac{17}{7}$$

$$\big(\triangle\mathcal{H}\big)^2 \;=\; \big(1\,,\;\;2\,,\;\;3\big)\frac{1}{\sqrt{14}}\left[\begin{pmatrix}5&0&0\\0&1&0\\0&0&1\end{pmatrix}^2 - \left(\frac{9}{7}\right)^2\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\right]\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}$$

$$= \;\frac{1}{14}\big(1\,,\;\;2\,,\;\;3\big)\left[\begin{pmatrix}25&0&0\\0&1&0\\0&0&1\end{pmatrix} - \begin{pmatrix}\frac{81}{49}&0&0\\0&\frac{81}{49}&0\\0&0&\frac{81}{49}\end{pmatrix}\right]\begin{pmatrix}1\\2\\3\end{pmatrix}$$

$$= \;\frac{1}{14}\big(1\,,\;\;2\,,\;\;3\big)\begin{pmatrix}\frac{1144}{49}&0&0\\0&-\frac{32}{49}&0\\0&0&-\frac{32}{49}\end{pmatrix}\begin{pmatrix}1\\2\\3\end{pmatrix} \;=\; \frac{1}{14\cdot 49}\big(1\,,\;\;2\,,\;\;3\big)\begin{pmatrix}1144\\-64\\-96\end{pmatrix}$$

$$= \;\frac{1}{2\cdot 7^3}\big(1144-128-288\big) \;=\; \frac{728}{2\cdot 7^3} \;=\; \frac{52}{7^2} \qquad\Rightarrow\qquad \triangle\mathcal{H} \;=\; \frac{\sqrt{52}}{7}$$

$$
\begin{aligned}
\left(\triangle\mathcal{K}\right)^2 &= \left(1,\ 2,\ 3\right)\frac{1}{\sqrt{14}}\left[\begin{pmatrix}-1&0&0\\0&2&0\\0&0&3\end{pmatrix}^2-\left(\frac{17}{7}\right)^2\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\right]\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\\
&= \frac{1}{14}\left(1,\ 2,\ 3\right)\left[\begin{pmatrix}1&0&0\\0&4&0\\0&0&9\end{pmatrix}-\begin{pmatrix}\frac{289}{49}&0&0\\0&\frac{289}{49}&0\\0&0&\frac{289}{49}\end{pmatrix}\right]\begin{pmatrix}1\\2\\3\end{pmatrix}\\
&= \frac{1}{14}\left(1,\ 2,\ 3\right)\begin{pmatrix}-\frac{240}{49}&0&0\\0&-\frac{93}{49}&0\\0&0&\frac{152}{49}\end{pmatrix}\begin{pmatrix}1\\2\\3\end{pmatrix} = \frac{1}{14\cdot 49}\left(1,\ 2,\ 3\right)\begin{pmatrix}-240\\-186\\456\end{pmatrix}\\
&= \frac{1}{2\cdot 7^3}\left(-240-372+1368\right) = \frac{756}{2\cdot 7^3} = \frac{54}{7^2} \quad\Rightarrow\quad \triangle\mathcal{K} = \frac{\sqrt{54}}{7}
\end{aligned}
$$

3–20. Find the time-dependent state vector for the $\mathcal{H}$, $\mathcal{K}$ system given

$$
|\,\psi\,(t=0)> \;=\; \frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}
$$

and that $\mathcal{H}$ is the total energy operator.

Time evolution of a system with a Hamiltonian operator such that $\mathcal{H} \neq \mathcal{H}(t)$ is determined by

$$
|\,\psi_i(t)> \;=\; |\,\psi_i(t=0)>\, e^{-iE_it/\hbar}
$$

where $|\,\psi_i(t=0)>$ are the system eigenvectors and E_i are the energy eigenvalues. The operator $\mathcal{K}$ shares the system eigenvectors with $\mathcal{H}$, but the eigenvalues of $\mathcal{K}$ are irrelevant to system's time evolution. The system's time evolution is dependent solely on the energy eigenvalues.

Expanding the state vector in the common eigenbasis,

$$
\begin{aligned}
|\,\psi\,(0)> &= \sum_i |\,E_i><E_i\,|\,\psi\,(0)>\\
&= \begin{pmatrix}1\\0\\0\end{pmatrix}\left(1,\ 0,\ 0\right)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\left(0,\ 1,\ 0\right)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix} + \begin{pmatrix}0\\0\\1\end{pmatrix}\left(0,\ 0,\ 1\right)\frac{1}{\sqrt{14}}\begin{pmatrix}1\\2\\3\end{pmatrix}\\
&= \frac{1}{\sqrt{14}}\begin{pmatrix}1\\0\\0\end{pmatrix} + \frac{2}{\sqrt{14}}\begin{pmatrix}0\\1\\0\end{pmatrix} + \frac{3}{\sqrt{14}}\begin{pmatrix}0\\0\\1\end{pmatrix}.
\end{aligned}
$$

With the time zero expansion, we can then write the complete time-dependent state vector

$$
\begin{aligned}
|\,\psi\,(t)> &= \sum_i |\,E_i><E_i\,|\,\psi\,(0)>\, e^{-iE_it/\hbar}\\
&= \frac{1}{\sqrt{14}}\begin{pmatrix}1\\0\\0\end{pmatrix}e^{-i(5)t/\hbar} + \frac{2}{\sqrt{14}}\begin{pmatrix}0\\1\\0\end{pmatrix}e^{-i(1)t/\hbar} + \frac{3}{\sqrt{14}}\begin{pmatrix}0\\0\\1\end{pmatrix}e^{-i(1)t/\hbar} = \frac{1}{\sqrt{14}}\begin{pmatrix}e^{-i5t/\hbar}\\2\,e^{-it/\hbar}\\3\,e^{-it/\hbar}\end{pmatrix}.
\end{aligned}
$$

Postscript: Should the eigenbasis be other than the unit vectors, the expansion is necessary. When the eigenbasis is the unit vectors, however, the expansion is likely unnecessary and simply writing the answer, the final expression in this problem, is warranted.

3–21. A researcher is interested in a system with a total energy operator $\mathcal{H} = \begin{pmatrix} 1 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 1 \end{pmatrix}$, but is disappointed to find that $\mathcal{H}$ is degenerate. The system also has observable quantities $\mathcal{A} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 2 & i \\ 0 & -i & 2 \end{pmatrix}$ and $\mathcal{B} = \begin{pmatrix} 2 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 2 \end{pmatrix}$. Design a measurement for the researcher, then find all appropriate values and functions given the state function $|\psi(0)> = \begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix}$.

This problem is the numerical culmination of the first three chapters and chapter 3 in particular. It marks the passage from discrete systems to continuous systems. The ideas presented in the first three chapters apply in $\mathbb{C}^\infty$, though they are likely most accessible in $\mathbb{C}^2$ and $\mathbb{C}^3$. Chapters 4 and beyond predominantly feature continuous systems ($\mathbb{C}^\infty$), nevertheless, the re-visitation of both the concepts and calculations of the first three chapters will occur frequently.

The postulates indicate that all that can be known quantum mechanically is simply not the same as what can be known classically. So what can be known quantum mechanically? Possibilities, probabilities, expectation values, uncertainties, and time evolution are appropriate values and functions. The first step is to find a complete set of commuting observables.

Notice that $\mathcal{H}$, $\mathcal{A}$, and $\mathcal{B}$ are Hermitian.

The word "commuting" is explicit in the phrase "complete set of commuting observables." An operator that commutes with $\mathcal{H}$ is necessary.

$$\mathcal{H}\mathcal{A} = \begin{pmatrix} 1 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 1 \end{pmatrix} \begin{pmatrix} 4 & 0 & 0 \\ 0 & 2 & i \\ 0 & -i & 2 \end{pmatrix} = \begin{pmatrix} 4 & -1 & -2i \\ 0 & 4 & 2i \\ 4i & -i & 2 \end{pmatrix}$$

$$\mathcal{A}\mathcal{H} = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 2 & i \\ 0 & -i & 2 \end{pmatrix} \begin{pmatrix} 1 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 1 \end{pmatrix} = \begin{pmatrix} 4 & 0 & -4i \\ -1 & 4 & i \\ 2i & -2i & 2 \end{pmatrix}$$

thus, $\left[\mathcal{H}, \mathcal{A}\right] = \mathcal{H}\mathcal{A} - \mathcal{A}\mathcal{H} \neq 0$ and $\mathcal{A}$ does not share a common eigenbasis with $\mathcal{H}$ so is not acceptable to complete a set of commuting observables (notice that neither product of the non-commuting Hermitian operators is Hermitian). Examining $\mathcal{B}$,

$$\mathcal{H}\mathcal{B} = \begin{pmatrix} 1 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 1 \end{pmatrix} \begin{pmatrix} 2 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 2 \end{pmatrix} = \begin{pmatrix} 3 & 0 & -3i \\ 0 & 4 & 0 \\ 3i & 0 & 3 \end{pmatrix}$$

$$\mathcal{B}\mathcal{H} \;=\; \begin{pmatrix} 2 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 2 \end{pmatrix}\begin{pmatrix} 1 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 1 \end{pmatrix} \;=\; \begin{pmatrix} 3 & 0 & -3i \\ 0 & 4 & 0 \\ 3i & 0 & 3 \end{pmatrix}$$

thus, $\big[\mathcal{H}\,,\,\mathcal{B}\big] \;=\; \mathcal{H}\mathcal{B}-\mathcal{B}\mathcal{H} \;=\; 0$ and $\mathcal{B}$ does share a common eigenbasis with $\mathcal{H}$ so is acceptable to complete a set of commuting observables. (Notice that both products are Hermitian. The fact that products of <u>commuting</u> Hermitian operators must be a Hermitian operator is addressed as an exercise). Since $\mathcal{H}$ is known to be degenerate, solve the eigenvalue/eigenvector problem for $\mathcal{B}$.

$$\det\begin{pmatrix} 2-\lambda & 0 & -i \\ 0 & 2-\lambda & 0 \\ i & 0 & 2-\lambda \end{pmatrix} \;=\; \big(2-\lambda\big)^3 - 1\big(2-\lambda\big) \;\;=\;\; 8-12\lambda+6\lambda^2-\lambda^3-2+\lambda$$

$\Rightarrow\;\; \lambda^3-6\lambda^2+11\lambda-6 \;=\; 0$ is the characteristic equation. It is factored $\big(\lambda-1\big)\big(\lambda-2\big)\big(\lambda-3\big) \;=\; 0$ so the eigenvalues are $\lambda \;=\; 1\,,\;2\,,\;3\,,$ and $\mathcal{B}$ is not degenerate. This is good news because degeneracy would complicate the issue and may disqualify $\mathcal{B}$ from completing a set of commuting observables. The eigenvectors are found by solving $\mathcal{B}\,|\,v> \;=\; \beta\,|\,v>\,,$ meaning

$$\begin{pmatrix} 2 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 2 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} \;=\; 1\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad\Rightarrow\quad \begin{array}{rcl} 2a-ci &=& a \\ 2b &=& b \\ ai+2c &=& c \end{array} \quad\Rightarrow\quad \begin{array}{rcl} -ci &=& -a \\ b &=& 0 \\ ai &=& -c \end{array}$$

$$\Rightarrow\quad a \;=\; 1\,,\;\; b \;=\; 0\,,\;\; c \;=\; -i\,, \quad\Rightarrow\quad |\,1> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -i \end{pmatrix}.$$

$$\begin{pmatrix} 2 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 2 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} \;=\; 2\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad\Rightarrow\quad \begin{array}{rcl} 2a-ci &=& 2a \\ 2b &=& 2b \\ ai+2c &=& 2c \end{array} \quad\Rightarrow\quad \begin{array}{rcl} -ci &=& 0 \\ b &=& b \\ ai &=& 0 \end{array}$$

$$\Rightarrow\quad a \;=\; 0\,,\;\; b \;=\; 1\,,\;\; c \;=\; 0\,, \quad\Rightarrow\quad |\,2> \;=\; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

$$\begin{pmatrix} 2 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 2 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} \;=\; 3\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad\Rightarrow\quad \begin{array}{rcl} 2a-ci &=& 3a \\ 2b &=& 3b \\ ai+2c &=& 3c \end{array} \quad\Rightarrow\quad \begin{array}{rcl} -ci &=& a \\ b &=& 0 \\ ai &=& c \end{array}$$

$$\Rightarrow\quad a \;=\; 1\,,\;\; b \;=\; 0\,,\;\; c \;=\; i\,, \quad\Rightarrow\quad |\,3> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ i \end{pmatrix}.$$ A unitary operator built by placing these normalized eigenvectors from left to right in the order of the eigenvector corresponding to the lowest eigenvalue to the highest eigenvalue is

$$\mathcal{U} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ -i & 0 & i \end{pmatrix} \quad\Rightarrow\quad \mathcal{U}^\dagger \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & i \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -i \end{pmatrix}.$$ Then

$$\begin{aligned} \mathcal{U}^\dagger\mathcal{H}\mathcal{U} \;&=\; \mathcal{U}^\dagger\begin{pmatrix} 1 & 0 & -i \\ 0 & 2 & 0 \\ i & 0 & 1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ -i & 0 & i \end{pmatrix} \\ &=\; \frac{1}{2}\begin{pmatrix} 1 & 0 & i \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & -i \end{pmatrix}\begin{pmatrix} 0 & 0 & 2 \\ 0 & 2\sqrt{2} & 0 \\ 0 & 0 & 2i \end{pmatrix} \;=\; \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix} \;=\; \begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \end{aligned}$$

The representation of $\mathcal{B} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$ is per the postscript to problem 3–17, by inspection. Possibilities are the states $|\,0\,,\ 1\,>$ corresponding to the unit vector $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|\,2\,,\ 2\,>$ corresponding to the unit vector $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$, and $|\,2\,,\ 3\,>$ corresponding to the unit vector $\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$.

Probabilities require the state vector $|\,\psi(0)> \ = \begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix}$ which when normalized is

$$\big(-2i\,,\ 2\,,\ i\big)N^*\,N\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix} \ = \ \big|\,N\,\big|^2\big(4{+}4{+}1\big) \ = \ 1 \quad \Rightarrow \quad N \ = \ \frac{1}{3} \quad \Rightarrow \quad |\,\psi(0)> \ = \ \frac{1}{3}\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix}.$$

$$P\,(0,1) \ = \ \big|<0,1\,|\,\psi>\big|^2 = \ \left|\big(1\,,\ \ 0\,,\ \ 0\big)\,\frac{1}{3}\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix}\right|^2 = \ \left|\,\frac{1}{3}(2i+0+0)\,\right|^2 = \ \frac{(-2i)(2i)}{9} \ = \ \frac{4}{9}$$

$$P\,(2,2) \ = \ \big|<2,2\,|\,\psi>\big|^2 = \ \left|\big(0\,,\ \ 1\,,\ \ 0\big)\,\frac{1}{3}\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix}\right|^2 = \ \left|\,\frac{1}{3}(0+2+0)\,\right|^2 \ = \ \frac{4}{9}$$

$$P\,(2,3) \ = \ \big|<2,3\,|\,\psi>\big|^2 = \ \left|\big(0\,,\ \ 0\,,\ \ 1\big)\,\frac{1}{3}\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix}\right|^2 = \ \left|\,\frac{1}{3}(0+0-i)\,\right|^2 = \ \frac{(i)(-i)}{9} \ = \ \frac{1}{9}$$

$$<\mathcal{H}> \ = \ \sum P\,(\alpha_{\mathcal{H}})\,\alpha_{\mathcal{H}} \ = \ \frac{4}{9}\times 0 \ + \ \frac{4}{9}\times 2 \ + \ \frac{1}{9}\times 2 \ = \ \frac{0+8+2}{9} \ = \ \frac{10}{9}$$

$$<\mathcal{B}> \ = \ \sum P\,(\alpha_{\mathcal{B}})\,\alpha_{\mathcal{B}} \ = \ \frac{4}{9}\times 1 \ + \ \frac{4}{9}\times 2 \ + \ \frac{1}{9}\times 3 \ = \ \frac{4+8+3}{9} \ = \ \frac{15}{9} \ = \ \frac{5}{3}$$

$$\begin{aligned}
\big(\triangle\mathcal{H}\big)^2 \ &= \ \big(-2i\,,\ \ 2\,,\ \ i\big)\,\frac{1}{3}\left[\begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}^2 - \ \left(\frac{10}{9}\right)^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right]\frac{1}{3}\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix} \\
&= \ \frac{1}{9}\big(-2i\,,\ \ 2\,,\ \ i\big)\left[\begin{pmatrix} 0 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix} - \ \begin{pmatrix} \frac{100}{81} & 0 & 0 \\ 0 & \frac{100}{81} & 0 \\ 0 & 0 & \frac{100}{81} \end{pmatrix}\right]\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix} \\
&= \ \frac{1}{9}\big(-2i\,,\ \ 2\,,\ \ i\big)\begin{pmatrix} -\frac{100}{81} & 0 & 0 \\ 0 & \frac{224}{81} & 0 \\ 0 & 0 & \frac{224}{81} \end{pmatrix}\begin{pmatrix} 2i \\ 2 \\ -i \end{pmatrix} \ = \ \frac{1}{9^3}\big(-2i\,,\ \ 2\,,\ \ i\big)\begin{pmatrix} -200i \\ 448 \\ -224i \end{pmatrix} \\
&= \ \frac{1}{9^3}\big(-400+896+224\big) \ = \ \frac{720}{9^3} \ = \ \frac{80}{9^2} \quad \Rightarrow \quad \triangle\mathcal{H} \ = \ \frac{\sqrt{80}}{9}
\end{aligned}$$

$$
\begin{aligned}
\left(\triangle\mathcal{B}\right)^2 &= \left(-2i\,,\;\; 2\,,\;\; i\right)\frac{1}{3}\left[\begin{pmatrix}1&0&0\\0&2&0\\0&0&3\end{pmatrix}^2 - \left(\frac{5}{3}\right)^2\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}\right]\frac{1}{3}\begin{pmatrix}2i\\2\\-i\end{pmatrix} \\
&= \frac{1}{9}\left(-2i\,,\;\; 2\,,\;\; i\right)\left[\begin{pmatrix}1&0&0\\0&4&0\\0&0&9\end{pmatrix} - \begin{pmatrix}\frac{25}{9}&0&0\\0&\frac{25}{9}&0\\0&0&\frac{25}{9}\end{pmatrix}\right]\begin{pmatrix}2i\\2\\-i\end{pmatrix} \\
&= \frac{1}{9}\left(-2i\,,\;\; 2\,,\;\; i\right)\begin{pmatrix}-\frac{16}{9}&0&0\\0&\frac{11}{9}&0\\0&0&\frac{56}{9}\end{pmatrix}\begin{pmatrix}2i\\2\\-i\end{pmatrix} = \frac{1}{9^3}\left(-2i\,,\;\; 2\,,\;\; i\right)\begin{pmatrix}-32i\\22\\-56i\end{pmatrix} \\
&= \frac{1}{9^3}\left(-64+44+56\right) = \frac{36}{9^3} = \frac{4}{9^2} \qquad \Rightarrow \qquad \triangle\mathcal{B} = \frac{2}{9}
\end{aligned}
$$

$$
|\,\psi(t)> = \frac{2i}{3}\begin{pmatrix}1\\0\\0\end{pmatrix}e^{-i(0)t/\hbar} + \frac{2}{3}\begin{pmatrix}0\\1\\0\end{pmatrix}e^{-i(2)t/\hbar} - \frac{i}{3}\begin{pmatrix}0\\0\\1\end{pmatrix}e^{-i(2)t/\hbar} = \frac{1}{3}\begin{pmatrix}2i\\2\,e^{-i2t/\hbar}\\-i\,e^{-i2t/\hbar}\end{pmatrix}
$$

3–22. Show that the operator constructed from the normalized eigenvectors of a Hermitian operator is unitary such that $\mathcal{U}\mathcal{U}^\dagger = \mathcal{U}^\dagger\mathcal{U} = \mathcal{I}$.

Unitary operators and unitary transformations have been addressed and employed on numerous occasions. There are many ways to construct unitary operators which are not addressed in this text. This problem does, however, show that an operator that is constructed from the eigenvectors of a Hermitian operator by placing them in columns is unitary such that $\mathcal{U}\mathcal{U}^\dagger = \mathcal{U}^\dagger\mathcal{U} = \mathcal{I}$.

Problem 3–12 shows that the eigenvectors of a Hermitian operator are orthogonal, so when normalized, they are orthonormal. This problem requires imagination beyond mechanical mathematics and also requires that you recognize the normalized eigenvectors in columns in $\mathcal{U}$ and the normalized adjoint eigenvectors in rows in $\mathcal{U}^\dagger$.

Let $\mathcal{U} = \begin{pmatrix}a_1&b_1&c_1&\cdots\\a_2&b_2&c_2&\cdots\\a_3&b_3&c_3&\cdots\\\vdots&\vdots&\vdots&\ddots\end{pmatrix}$ where each column is a normalized eigenvector of $\mathcal{A}$ such that

$$
|\,a> = \begin{pmatrix}a_1\\a_2\\a_3\\\vdots\end{pmatrix}, \qquad |b> = \begin{pmatrix}b_1\\b_2\\b_3\\\vdots\end{pmatrix}, \qquad |c> = \begin{pmatrix}c_1\\c_2\\c_3\\\vdots\end{pmatrix}, \qquad \cdots, \qquad \text{then}
$$

$\mathcal{U}^\dagger = \begin{pmatrix}a_1^*&a_2^*&a_3^*&\cdots\\b_1^*&b_2^*&b_3^*&\cdots\\c_1^*&c_2^*&c_3^*&\cdots\\\vdots&\vdots&\vdots&\ddots\end{pmatrix}$ where each row is a transpose conjugate of a normalized eigenvector of $\mathcal{A}$ which is also normalized because $\left|\,<v\,|\,v>\,\right|^2 = 1 \qquad \Rightarrow \qquad \left|\,|\,v>\,\right| = 1$ and also that

$|<v|| = 1$. Then

$$\mathcal{U}^\dagger\mathcal{U} = \begin{pmatrix} a_1^* & a_2^* & a_3^* & \cdots \\ b_1^* & b_2^* & b_3^* & \cdots \\ c_1^* & c_2^* & c_3^* & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 & b_1 & c_1 & \cdots \\ a_2 & b_2 & c_2 & \cdots \\ a_3 & b_3 & c_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Rather than mechanical multiplication of elements, observe that the element in the first column, first row of the product operator is $<a\,|\,a>$, the element in the first column, second row is $<b\,|\,a>$, the element in the first column, third row is $<c\,|\,a>$, and so on so that the product matrix can be written

$$\mathcal{U}^\dagger\mathcal{U} = \begin{pmatrix} <a\,|\,a> & <a\,|\,b> & <a\,|\,c> & \cdots \\ <b\,|\,a> & <b\,|\,b> & <b\,|\,c> & \cdots \\ <c\,|\,a> & <c\,|\,b> & <c\,|\,c> & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

The eigenvectors of a Hermitian operator are orthogonal, so when normalized are orthonormal, thus $<i\,|\,j> = \delta_{ij}$, and

$$\mathcal{U}^\dagger\mathcal{U} = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \mathcal{I}. \quad \text{Then}$$

$$\mathcal{U}^\dagger\mathcal{U} = \mathcal{I} \;\Rightarrow\; \mathcal{U}\mathcal{U}^\dagger\mathcal{U} = \mathcal{U} \;\Rightarrow\; \mathcal{U}\mathcal{U}^\dagger\mathcal{U}\mathcal{U}^{-1} = \mathcal{U}\mathcal{U}^{-1} \;\Rightarrow\; \mathcal{U}\mathcal{U}^\dagger\mathcal{I} = \mathcal{I} \;\Rightarrow\; \mathcal{U}\mathcal{U}^\dagger = \mathcal{I}.$$

3–23. Show that the unitary transformation $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ diagonalizes Hermitian $\mathcal{A}$ placing eigenvalues on the diagonal, given that $\mathcal{U}$ is constructed from the normalized eigenvectors of $\mathcal{A}$.

Placing the normalized eigenvectors of $\mathcal{A}$ in columns ensures a unitary operator for which the unitary transformation $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ diagonalizes $\mathcal{A}$. The intent of this problem is to support the claim that all Hermitian operators can be diagonalized. That the eigenvalues of $\mathcal{A}$ are the diagonal elements is a necessary result, but that result is simply a bonus to the purpose.

Denote the unitary operator $\mathcal{U} = \begin{pmatrix} a_1 & b_1 & c_1 & \cdots \\ a_2 & b_2 & c_2 & \cdots \\ a_3 & b_3 & c_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$ where each column is an eigenvector of $\mathcal{A}$. Expressing each column in ket notation where

$$|\,a> = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}, \qquad |\,b> = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix}, \qquad |\,c> = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}, \qquad \cdots$$

the unitary operator can be written

$$\mathcal{U} \;=\; \Big(\, |\,a\!> \quad |\,b\!> \quad |\,c\!> \quad \cdots \Big)\,,$$

operating on this equation from the left with $\mathcal{U}^\dagger$,

$$\mathcal{U}^\dagger\mathcal{U} \;=\; \mathcal{I} \;=\; \Big(\mathcal{U}^\dagger\,|\,a\!> \quad \mathcal{U}^\dagger\,|\,b\!> \quad \mathcal{U}^\dagger\,|\,c\!> \quad \cdots\Big) \;=\; \left(\begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}\begin{pmatrix}0\\1\\0\\\vdots\end{pmatrix}\begin{pmatrix}0\\0\\1\\\vdots\end{pmatrix}\begin{matrix}\cdots\\\cdots\\\cdots\end{matrix}\right), \qquad (1)$$

where $\mathcal{U}^\dagger\mathcal{U} \;=\; \mathcal{I}$ on the right is written as assembled unit vectors. Operating on $\mathcal{U}$ with $\mathcal{A}$,

$$\mathcal{A}\mathcal{U} \;=\; \Big(\mathcal{A}\,|\,a\!> \quad \mathcal{A}\,|\,b\!> \quad \mathcal{A}\,|\,c\!> \quad \cdots\Big) \;=\; \Big(\alpha_1\,|\,a\!> \quad \alpha_2\,|\,b\!> \quad \alpha_3\,|\,c\!> \quad \cdots\Big) \qquad (2)$$

using the eigenvalue/eigenvector equation $\mathcal{A}\,|\,a_i\!> \;=\; \alpha_i\,|\,a_i\!>$. Operating on this with $\mathcal{U}^\dagger$,

$$\mathcal{U}^\dagger\mathcal{A}\mathcal{U} \;=\; \Big(\alpha_1\,\mathcal{U}^\dagger\,|\,a\!> \quad \alpha_2\,\mathcal{U}^\dagger\,|\,b\!> \quad \alpha_3\,\mathcal{U}^\dagger\,|\,c\!> \quad \cdots\Big)\,.$$

Comparing the right side of this equation with equation (1),

$$\mathcal{U}^\dagger\mathcal{A}\mathcal{U} \;=\; \left(\alpha_1\begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix} \quad \alpha_2\begin{pmatrix}0\\1\\0\\\vdots\end{pmatrix} \quad \alpha_3\begin{pmatrix}0\\0\\1\\\vdots\end{pmatrix}\begin{matrix}\cdots\\\cdots\\\cdots\end{matrix}\right) \;=\; \begin{pmatrix}\alpha_1 & 0 & 0 & \cdots\\ 0 & \alpha_2 & 0 & \cdots\\ 0 & 0 & \alpha_3 & \cdots\\ \vdots & \vdots & \vdots & \ddots\end{pmatrix}$$

which is a diagonal matrix with eigenvalues on the diagonal.

Postscript: This proof is limited to our method of constructing a unitary operator from the normalized eigenvectors of a Hermitian operator.

A brief extension of this argument again proves that the eigenvalues of a Hermitian operator must be real. If $\mathcal{A}$ is Hermitian, the diagonal $\mathcal{B} \;=\; \mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ is Hermitian (problem 1–27), and diagonal elements must be equal to their complex conjugates, $\alpha_i \;=\; \alpha_i^*$, to satisfy $\mathcal{B} \;=\; \mathcal{B}^\dagger$, thus, the diagonal elements which emerge as the eigenvalues in equation (2) must be real numbers.

3–24. Argue that the eigenvectors of a Hermitian operator span its space.

The operator $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ is given to be the diagonal form of $\mathcal{A}$.

A diagonal operator has unit vectors as basis vectors. Any vector in the space can be expressed as a linear combination of unit vectors, thus the unit vectors of $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ span the space. A unitary transformation preserves norms and angular relations between vectors because the inner product is invariant under a unitary transformation. The intrinsic orthonormality of a basis of unit vectors is thus preserved under a unitary transformation, so the fact that the eigenvectors of $\mathcal{U}^\dagger\mathcal{A}\mathcal{U}$ span the space means that the eigenvectors of a unitary transformation in the reverse of the usual order

$$\mathcal{U}\,(\mathcal{U}^\dagger\mathcal{A}\mathcal{U})\,\mathcal{U}^\dagger \;=\; \mathcal{U}\mathcal{U}^\dagger\mathcal{A}\mathcal{U}\mathcal{U}^\dagger \;=\; \mathcal{I}\mathcal{A}\mathcal{I} \;=\; \mathcal{A}$$

also span the space, form a basis, or are complete.

3–25. Show that every operator commutes with itself and powers of itself.

Though operator products are associative, they are not generally commutative. That an operator commutes with itself and powers of itself is important to the commutator algebra in the middle chapters. The proof is short and simple. Show that $\big[\mathcal{A},\ \mathcal{A}^n\big] = 0$, for all integral n. We solve this problem both intuitively and then by induction. The intuitive method is not a proof but the intent is that you believe the conjecture so may be more valuable. Expand the commutators $\big[\mathcal{A},\ \mathcal{A}^1\big]$, $\big[\mathcal{A},\ \mathcal{A}^2\big]$, $\big[\mathcal{A},\ \mathcal{A}^3\big]$, and observe a pattern that should satisfy your intuition that $\big[\mathcal{A},\ \mathcal{A}^n\big]$ must be zero because the pattern has to be identical regardless of n.

To show that $\big[\mathcal{A},\ \mathcal{A}^n\big] = 0$, first show that it is true for $n = 1$, meaning

$$\big[\mathcal{A},\ \mathcal{A}\big] = \mathcal{A}\mathcal{A} - \mathcal{A}\mathcal{A} = \mathcal{A}^2 - \mathcal{A}^2 = 0.$$

For $n = 2$ and $n = 3$,

$$\big[\mathcal{A},\ \mathcal{A}^2\big] = \mathcal{A}\mathcal{A}^2 - \mathcal{A}^2\mathcal{A} = \mathcal{A}^3 - \mathcal{A}^3 = 0,$$

$$\big[\mathcal{A},\ \mathcal{A}^3\big] = \mathcal{A}\mathcal{A}^3 - \mathcal{A}^3\mathcal{A} = \mathcal{A}^4 - \mathcal{A}^4 = 0.$$

The pattern does not change because the power changes so

$$\big[\mathcal{A},\ \mathcal{A}^n\big] = \mathcal{A}\mathcal{A}^n - \mathcal{A}^n\mathcal{A} = \mathcal{A}^{n+1} - \mathcal{A}^{n+1} = 0.$$

More formally, the induction hypothesis is $\big[\mathcal{A},\ \mathcal{A}^n\big] = 0$ and we have shown $\big[\mathcal{A},\ \mathcal{A}\big] = 0$, which is the $n = 1$ case. To relate the cases n and $n+1$,

$$\begin{aligned}\big[\mathcal{A},\ \mathcal{A}^{n+1}\big] &= \mathcal{A}\mathcal{A}^{n+1} - \mathcal{A}^{n+1}\mathcal{A} = \mathcal{A}\mathcal{A}\mathcal{A}^n - \mathcal{A}\mathcal{A}^n\mathcal{A} \\ &= \mathcal{A}\Big(\mathcal{A}\mathcal{A}^n - \mathcal{A}^n\mathcal{A}\Big) = \mathcal{A}\big[\mathcal{A},\ \mathcal{A}^n\big] = \mathcal{A}(0) = 0\end{aligned}$$

if the induction hypothesis is correct. The last line says that the commutator must be zero for the next power $n+1$ if the commutator is zero for an arbitrary power of n. Since the induction hypothesis is true for $n = 1$, it is necessarily true for all higher powers.

3–26. Show that the eigenvalues of a Hermitian operator are real using the eigenvalue/eigenvector equation and Dirac notation.

Here is a third proof that the eigenvalues of a Hermitian operator are real.

$$\mathcal{A}\,|\,a\!> = \alpha\,|\,a\!> \quad \Rightarrow \quad <\!a\,|\,\mathcal{A}^\dagger = <\!a\,|\,\alpha^* \quad \Rightarrow \quad <\!a\,|\,\mathcal{A} = <\!a\,|\,\alpha^*$$

because $\mathcal{A} = \mathcal{A}^\dagger$. Forming a braket of the last equation with $|\,a\!>$,

$$<\!a\,|\,\mathcal{A}\,|\,a\!> = <\!a\,|\,\alpha^*\,|\,a\!> \quad \Rightarrow \quad <\!a\,|\,\alpha\,|\,a\!> = <\!a\,|\,\alpha^*\,|\,a\!>$$

which is $\mathcal{A}\,|\,a\!> = \alpha\,|\,a\!>$ used on the left. Then since α and α^* are scalars,

$$\alpha <\!a\,|\,a\!> = \alpha^* <\!a\,|\,a\!> \quad \Rightarrow \quad \alpha = \alpha^*.$$

Exercises

3–27. (a) Show that the product of two diagonal operators with scalar elements is the diagonal operator composed of the scalar products of corresponding elements.

(b) Show that the square of a diagonal operator with scalar elements is the diagonal operator composed of the square of the elements.

(c) Show that all diagonal operators with scalar elements commute.

These are more convenient facts concerning diagonal operators.

Use two arbitrary diagonal operators like

$$\mathcal{A} = \begin{pmatrix} a_1 & 0 & 0 & \cdots \\ 0 & a_2 & 0 & \cdots \\ 0 & 0 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \qquad \mathcal{B} = \begin{pmatrix} b_1 & 0 & 0 & \cdots \\ 0 & b_2 & 0 & \cdots \\ 0 & 0 & b_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

where the non-zero elements are known to be scalars, and for part (c), that scalars commute.

That any Hermitian operator can be transformed into a diagonal form where the diagonal elements are not only scalars, but real scalars—that are eigenvalues—is a fact to be exploited. Working with diagonal operators has the potential to significantly reduce the degree of difficulty of numerous calculations, expectation values and uncertainties for instance, and has the additional advantage of the clarity of the unit vectors being the basis vectors.

3–28. Show that the product of two Hermitian operators that commute is a Hermitian operator.

Start with $\mathcal{A}\mathcal{B} = \mathcal{C}$ to show $\mathcal{C} = \mathcal{C}^\dagger$. That $\mathcal{A}$ and $\mathcal{B}$ commute means

$$\big[\mathcal{A},\ \mathcal{B}\big] = 0 \qquad \Rightarrow \qquad \mathcal{A}\mathcal{B} = \mathcal{B}\mathcal{A}.$$

3–29. Show that $\big(\mathcal{A}+\mathcal{B}\big)^\dagger = \mathcal{A}^\dagger + \mathcal{B}^\dagger$ in two dimensions.

That the adjoint of the sum is the same as the sum of the adjoints is not obvious but the fact is used frequently. The proof in two dimensions extends to arbitrary dimension. Use

$$\mathcal{A} \to \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad \text{and} \qquad \mathcal{B} \to \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}.$$

Calculate the adjoint of the sum and the sum of the adjoints. They will be the same.

3–30. Given that Ω and Λ are Hermitian operators, show that

(a) $\Omega\,\Lambda$ is not Hermitian,

(b) $\Omega\Lambda + \Lambda\Omega$ is Hermitian,

(c) $\big[\,\Omega,\,\Lambda\,\big]$ is anti-Hermitian, and

(d) $i\big[\,\Omega,\,\Lambda\,\big]$ is Hermitian.

We generally use upper case calligraphic letters to denote operators though many texts use Greek capital letters. All four parts use the result $\big(\,\Omega\,\Lambda\,\big)^\dagger \;=\; \Lambda^\dagger\,\Omega^\dagger$. Anti-Hermitian means $\Gamma \;=\; -\Gamma^\dagger$. As an example, Hermitian for part (d) means $\big(\,i\,\big[\,\Omega,\,\Lambda\,\big]\,\big)^\dagger \;=\; i\,\big[\,\Omega,\,\Lambda\,\big]$. To show this,

$$\begin{aligned}
\big(\,i\,\big[\,\Omega,\,\Lambda\,\big]\,\big)^\dagger \;&=\; (i)^*\,\big(\,\Omega\,\Lambda - \Lambda\,\Omega\,\big)^\dagger \;&=\; -i\,\Big(\,\big(\,\Omega\,\Lambda\,\big)^\dagger - \big(\,\Lambda\,\Omega\,\big)^\dagger\,\Big)\\
&=\; -i\,\big(\,\Lambda^\dagger\,\Omega^\dagger - \Omega^\dagger\,\Lambda^\dagger\,\big) \;&=\; -i\,\big(\,\Lambda\,\Omega - \Omega\,\Lambda\,\big)\\
&=\; -i\,\big(\,-\,\Omega\,\Lambda + \Lambda\,\Omega\,\big) \;&=\; i\,\big(\,\Omega\,\Lambda - \Lambda\,\Omega\,\big)\\
&=\; i\,\big[\,\Omega,\,\Lambda\,\big]\,, \quad \text{so it is Hermitian.}
\end{aligned}$$

Unlike exercise 3–28, assume non-commuting Λ and Ω.

3–31. Given a square operator $\mathcal{A}$, $\mathcal{B} \;=\; \dfrac{1}{2}\Big(\mathcal{A} + \mathcal{A}^\dagger\Big)$, and $\mathcal{C} \;=\; \dfrac{1}{2i}\Big(\mathcal{A} - \mathcal{A}^\dagger\Big)$, show that

(a) $\mathcal{A} \;=\; \mathcal{B} + i\mathcal{C}$,

(b) both $\mathcal{B}$ and $\mathcal{C}$ are Hermitian, but that $i\mathcal{C}$ is not.

(c) Show that $\big[\,\mathcal{B}\,,\,\mathcal{C}\,\big] \;=\; 0$ only if $\big[\,\mathcal{A}\,,\,\mathcal{A}^\dagger\,\big] \;=\; 0$.

Exercising straightforward operator algebra. The operator $\mathcal{A}$ must be square for the definitions of $\mathcal{B}$ and $\mathcal{C}$ to make sense. Notice that this exercise is not limited to Hermitian operators. This decomposition is an operator analog to a complex number with real and imaginary parts, where the real and imaginary parts are Hermitian.

3–32. (a) Show that $\mathcal{B}$ and $\mathcal{C}$ as defined in exercise 3–31 are Hermitian for $\mathcal{A} \;=\; \begin{pmatrix} 2i & 4+6i \\ 8 & 6-10i \end{pmatrix}$.

(b) Show that $\mathcal{A} \;=\; \mathcal{B} + i\mathcal{C}$ numerically for the given $\mathcal{A}$.

Small numerical examples may be useful to provide meaning and context. Notice that the given $\mathcal{A}$ is markedly non-Hermitian. For a complex number $z \;=\; a + bi$, the a and b are real numbers. The operator analogy for any square operator is $\mathcal{A} \;=\; \mathcal{B} + i\mathcal{C}$, where the $\mathcal{B}$ and $\mathcal{C}$ are as defined in the previous exercise and are Hermitian operators.

3–33. Show that the inner product $<c\,|\,g>$, where $|\,c> \;\rightarrow \begin{pmatrix} 5i \\ 2i \end{pmatrix}$ and $|\,g> \;\rightarrow \begin{pmatrix} 4 \\ 3+2i \end{pmatrix}$, is invariant under the unitary transformation that diagonalizes $\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}$.

The unitary transformation that diagonalizes $\begin{pmatrix} 3 & 4i \\ -4i & 3 \end{pmatrix}$ was found in chapter 1 to be

$$\mathcal{U} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \qquad \Rightarrow \qquad \mathcal{U}^{\dagger} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}.$$

Transform the bra as $<c\,|\mathcal{U}$ and the ket as $\mathcal{U}^{\dagger}\,|\,g>$. See problems 3–7 and 3–8.

3–34. Show that the inner product $<7\,|\,r>$, where $|\,7> \;\rightarrow \begin{pmatrix} 4i \\ 3 \\ -2i \end{pmatrix}$ and $|\,r> \;\rightarrow \begin{pmatrix} -3i \\ 6 \\ -5 \end{pmatrix}$, is invariant under the unitary transformation that diagonalizes $\begin{pmatrix} 1 & 0 & -2i \\ 0 & 1 & 0 \\ 2i & 0 & 4 \end{pmatrix}$.

The exercise in $\mathbb{C}^3$ like problems 3–7 and 3–8. The appropriate unitary transformation is

$$\mathcal{U} \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix} 2i & 0 & 1 \\ 0 & \sqrt{5} & 0 \\ 1 & 0 & 2i \end{pmatrix} \qquad \Rightarrow \qquad \mathcal{U}^{\dagger} \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix} -2i & 0 & 1 \\ 0 & \sqrt{5} & 0 \\ 1 & 0 & -2i \end{pmatrix}$$

from chapter 1. Transform the bra as $<7\,|\mathcal{U}$ and the ket as $\mathcal{U}^{\dagger}\,|\,r>$. The invariance of an inner product under a unitary transformation is an essential concept.

3–35. Show that the norms of $|\,q> \;\rightarrow \begin{pmatrix} 4i \\ 3 \end{pmatrix}$ and $|\,k> \;\rightarrow \begin{pmatrix} -6 \\ 2-3i \end{pmatrix}$ are preserved under the unitary transformation made in problem 3–7.

A unitary transformation is said to rotate basis vectors in $\mathbb{C}^n$. "Re-orient" may be a better description since "rotation" in $\mathbb{C}^n$ for $n > 3$ is difficult to picture, nevertheless, "rotate" is the accepted terminology. That a unitary transformation preserves lengths/norms, angles/angle analogs, inner products, and eigenvalues founds the usefulness of unitary transformations to quantum mechanics.

From problem 3–7, $\quad <q'\,| \;=\; \frac{1}{\sqrt{2}}\big(-i\,,\;\; -7i\big) \quad$ and $\quad |\,k'> \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} -9-2i \\ -3+2i \end{pmatrix}$,

and from chapter 1, $\;\big|\,|\,x>\,\big| \;=\; \big|\,<x\,|\,\big| \;=\; \sqrt{<x\,|\,x>}$. Problem 3–10 is an example in $\mathbb{C}^3$.

3–36. Show that a unitary transformation preserves a vector's norm in general,

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See problem 3–9 and the postscript of problem 3–10. This is a short proof.

3–37. Consider the two operators $\mathcal{H} = \begin{pmatrix} 2 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 2 \end{pmatrix}$ and $\mathcal{C} = \begin{pmatrix} 1 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 1 \end{pmatrix}$.

(a) Are these operators Hermitian?

(b) Is $\mathcal{H}$ degenerate?

(c) Do $\mathcal{H}$ and $\mathcal{C}$ commute?

(d) Simultaneously diagonalize both $\mathcal{H}$ and $\mathcal{C}$.

(e) List the possible eigenstates of the $\mathcal{H}$, $\mathcal{C}$ system.

The observables postulate indicates the fundamental importance of Hermiticity. Both $\mathcal{H}$ and $\mathcal{C}$ are Hermitian. $\mathcal{H}$ is degenerate with eigenvalues 1, 1, and 3. $\mathcal{H}$ and $\mathcal{C}$ do commute, which is necessary for simultaneous diagonalization. Should they not commute, they do not share a common eigenbasis so cannot be simultaneously diagonalized. This exercise requires finding the normalized eigenvectors of the non-degenerate operator to build the unitary operator. Part (e) intends that the possible eigenstates be identified in the basis that makes both $\mathcal{H}$ and $\mathcal{C}$ diagonal per problem 3–18 (a). Problems 3–14 through 3–17 are examples for parts (a) through (d).

3–38. Using $\mathcal{H}$ and $\mathcal{C}$ from the previous exercise and the state vector $|\psi> = \begin{pmatrix} 5i \\ 4 \\ 2-2i \end{pmatrix}$, find

(a) the probability of each possibility,

(b) both possible expectation values,

(c) both possible uncertainties,

(d) and the time-dependent state vector given that $\mathcal{H}$ is the total energy operator.

Normalize the state vector as a first step. The postulates do not require normalization, but the calculations for this problem become much more daunting without it. The probability postulate indicates how to complete the three calculations for part (a), where convenient unit vectors represent the three eigenstates. Possibilities and probabilities remain dominant through the whole of quantum mechanics. The associated statistical measures, expectation value and uncertainty which correspond to weighted average and standard deviation, follow from the possibilities and probabilities. The four parts of this exercise are the chapter 2 material involving a degenerate Hamiltonian requiring a second commuting operator to lift the degeneracy. See problems 3–18 through 3–20 for example calculations.

3–39. Check expectation values and uncertainties for exercise 3–38 using alternative calculations.

Recall from chapter 2 that

$$< \mathcal{A} >_\psi \;=\; \sum_i P(\alpha_i)\,\alpha_i \;=\; <\psi\,|\,\mathcal{A}\,|\,\psi> \quad \text{and}$$

$$\triangle \mathcal{A}_\psi \;=\; <\psi\,|\left(\mathcal{A} \;-\; < \mathcal{A} > \mathcal{I}\right)^2 |\,\psi>^{1/2} \;=\; <\psi\,|\,\mathcal{A}^2 - \,< \mathcal{A} >^2 \mathcal{I}\,|\,\psi>^{1/2} \;.$$

Thus, checks for expectation values and uncertainties are available.

3–40. Hermitian operator $\mathcal{H}$ has eigenvalues $2\,,\ 2\,,\ 5\,,$ and Hermitian operator $\mathcal{D}$ has eigenvalues $4\,,\ 4\,,\ 3\,,$ and $\left[\mathcal{H}\,,\mathcal{D}\right] \;=\; 0\,.$ Is it possible that these two degenerate operators can form a complete set of commuting observables? If so, under what conditions?

The answer to the first question is yes. Consider both $\mathcal{H}$ and $\mathcal{D}$ in the basis that diagonalizes both operators, though the unitary transformation that diagonalized both $\mathcal{H}$ and $\mathcal{D}$ is assumed. It is known to exist for commuting Hermitian operators, and does not need to be identified.

3–41. Show that $\qquad \left[\mathcal{A}\,,\mathcal{B}\right] \;\neq\; 0 \qquad \Rightarrow \qquad \left[\mathcal{B}\,,\mathcal{A}\right] \;\neq\; 0\,.$

This is a short exercise in operator algebra which some may consider intuitively true, though many quantum mechanical results are non-intuitive as are some results of operator algebra.

Remember that a commutator is an operator. Thus,

$$\left[\mathcal{A}\,,\mathcal{B}\right] \;\neq\; 0 \qquad \Rightarrow \qquad \left[\mathcal{A}\,,\mathcal{B}\right] \;=\; \mathcal{C} \qquad \text{is a good start.}$$

3–42. (a) Show that none of the conventional component orbital angular momentum operators

$$\mathcal{L}_x \;\rightarrow\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar\,, \qquad \mathcal{L}_y \;\rightarrow\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar\,, \qquad \mathcal{L}_z \;\rightarrow\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\hbar\,.$$

commute with other component orbital angular momentum operators.

(b) What is the implication for a complete set of commuting observables for orbital angular momentum that different components of orbital angular momentum do not commute?

Part (a) is mechanical. One of the implications of the previous exercise is that there are three commutators to consider rather than six. Calculate $\left[\mathcal{L}_x\,,\mathcal{L}_y\right]\,,\ \left[\mathcal{L}_x\,,\mathcal{L}_z\right]\,,\ \left[\mathcal{L}_y\,,\mathcal{L}_z\right]$ to show that $\left[\mathcal{L}_i\,,\mathcal{L}_j\right] \;\neq\; 0$ for $i \neq j\,.$ Part (b) may require more thought and is actually more to the point of this chapter.

3–43. A researcher is interested in a system with a total energy operator $\mathcal{H} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & i \\ 0 & -i & 2 \end{pmatrix}$, but is disappointed to find that $\mathcal{H}$ is degenerate. The system also has observable quantities $\mathcal{F} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & -i \\ 1 & i & 0 \end{pmatrix}$ and $\mathcal{M} = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 3 & -i \\ 0 & i & 3 \end{pmatrix}$. Design a measurement for the researcher, then find all appropriate values and functions given the state function $|\psi(0)> = \begin{pmatrix} -3i \\ 5 \\ 4i \end{pmatrix}$.

As problem 3–21 is the numerical culmination of the first three chapters, this exercise is the line beyond which all problems and exercises must first be considered in the generality of $\mathbb{C}^\infty$. That some systems can be addressed in smaller subspaces as addressed predominantly in the first three chapters is physically fortuitous. That the ideas and arguments of smaller subspaces can often be extended to $\mathbb{C}^\infty$ is frequently convenient.

Possibilities, probabilities, expectation values, uncertainties, and the time evolving wave function are appropriate values and functions that can be known. The characteristic polynomial of the appropriately chosen operator may be challenging to factor. One of the eigenvalues is 5, so dividing the appropriate characteristic polynomial by $\lambda - 5$ may make this exercise more straightforward.

Per problem 3–21, the first step is to find a complete set of commuting observables.

Chapter 4

Continuous Systems I

The extension from $\mathbb{C}^2$ and $\mathbb{C}^3$ to $\mathbb{C}^\infty$ is the primary subject of this chapter. Werner Heisenberg originated **matrix mechanics** in the mid 1920's. It relies on matrix and vector algebra. Erwin Schrodinger originated **wave mechanics**, relying on integral and differential calculus, about the same time. P. A. M. (Paul Adrian Maurice) Dirac showed the two distinctly different computational approaches are formally equivalent. Dirac created what he initially named **transformation theory**, in part to describe quantum mechanical phenomenon free of the limitations of either Heisenberg's or Schrodinger's approach. **Dirac notation** is independent of basis, which is a significant advantage. The idea is to frame the problem in abstract Hilbert space relying only on the postulates of quantum mechanics, then complete the specifics of the calculation using the more expedient method.

Heisenberg was awarded the Nobel Prize in Physics in 1932 for the creation of matrix mechanics. Schrodinger and Dirac shared the award in 1933 for their contributions to quantum mechanics. Dirac revealed the expediency of his working notes only in 1939 in the third edition of *The Principles of Quantum Mechanics*. Dirac notation has since become an essentially necessary part of the language of modern quantum mechanics. Dirac created other expediencies, one of which is the **Dirac delta function**, or just the **delta function**.

The first three chapters have been primarily a blend of Heisenberg and Dirac. The operators used to this point have all been matrix operators. Schrodinger's approach is calculus based featuring differential operators. The general strategy of this chapter is to further develop Dirac's methods and then use them to transition to Schrodinger's. Schrodinger's method will then be more completely developed in the later part of this chapter and future chapters.

4–1. Explain the concept that an infinite dimensional vector can model a continuous function.

What follows is a plausibility argument rather than a proof. The proof depends on the phenomenon of convergence which is beyond our scope. You should, nevertheless, appreciate the ideas of the argument that are behind an actual proof as well as the basic point that an infinite dimensional vector can model a continuous function.

Consider the continuous function

$$f(x) \;=\; x^3 - 13x^2 + 48x - 49$$

on the closed interval $\left[\,1\,,\;8\,\right]$. There is nothing remarkable about this polynomial function other than it has some variation and convenient y values within the interval of interest. Since the rule defining $f(x)$ is known, it is straightforward to find y values for integral x values,

x	$f(x)$
1	-13
2	3
3	5
4	-1
5	-9
6	-13
7	-7
8	15

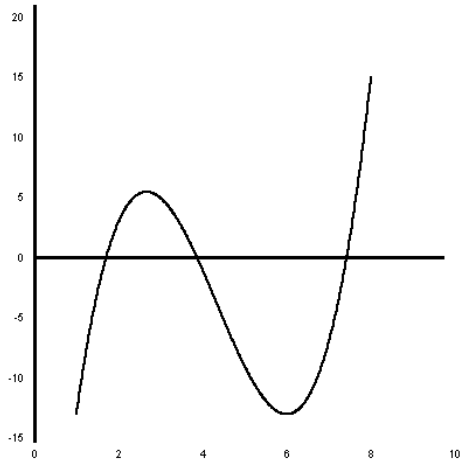

Fig. 4–1a. $f(x) = x^3 - 13x^2 + 48x - 49$.

Now suppose that we did not have the rule $x^3 - 13x^2 + 48x - 49$, but had only the information in the table. We could create a graph that would be a reasonable approximation to the continuous graph in figure 4–1a. The table, however, is equivalent to defining

$$|\, f(x) > \;=\; \begin{pmatrix} -13 \\ 3 \\ 5 \\ -1 \\ -9 \\ -13 \\ -7 \\ 15 \end{pmatrix}$$

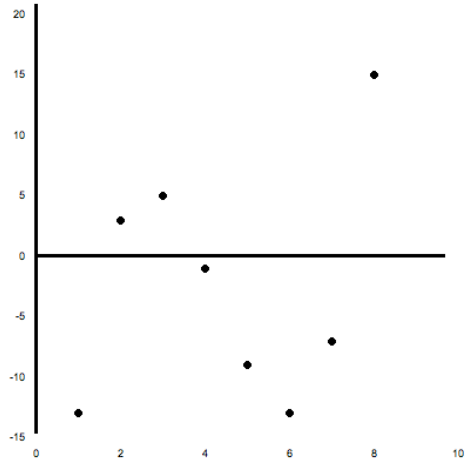

Fig. 4–1b. Integral values of x.

and should we want any functional value, simply form an inner product $< i \,|\, f(x) >$, where $< i \,|$ is the unit vector corresponding to the ith position. This means, for example,

$$< 1 \,|\, f(x) > = \begin{pmatrix} 1, & 0, & 0, & 0, & 0, & 0, & 0, & 0 \end{pmatrix} \begin{pmatrix} -13 \\ 3 \\ 5 \\ -1 \\ -9 \\ -13 \\ -7 \\ 15 \end{pmatrix} = -13$$

$$<2\,|\,f(x)> \;=\; \begin{pmatrix}0,\,1,\,0,\,0,\,0,\,0,\,0,\,0\end{pmatrix}\begin{pmatrix}-13\\3\\5\\-1\\-9\\-13\\-7\\15\end{pmatrix} \;=\; 3$$

$$<3\,|\,f(x)> \;=\; \begin{pmatrix}0,\,0,\,1,\,0,\,0,\,0,\,0,\,0\end{pmatrix}\begin{pmatrix}-13\\3\\5\\-1\\-9\\-13\\-7\\15\end{pmatrix} \;=\; 5$$

and so on. Now imagine that we had integral and half-integral values of x in the ket vector $|\,f(x)>$, which would contain 15 components. A new definition of the units vectors $|\,i>$ or $<i\,|$ to be 15 unit vectors is required to extend this mechanism. This refinement would provide a better approximation. If we had integral, half-integral, and quarter integral values of x in the ket vector $|\,f(x)>$, it would contain 29 components. Another new definition of the units vectors $|\,i>$ or $<i\,|$ to be 29 unit vectors would be required. Portions of this approximation are becoming close to a graph of a continuous function in a practical sense, depending on the size of the points used to make the graph. This extension could ostensibly be continued to an arbitrarily large number of points, or even an infinite number of points. That is

$$|\,f(x)> \;=\; \begin{pmatrix}f(x_1)\\f(x_2)\\f(x_3)\\\vdots\end{pmatrix}$$

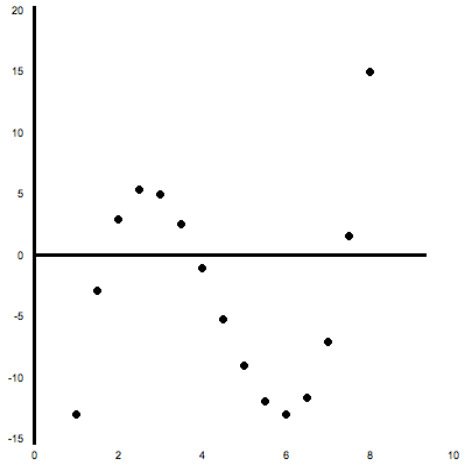

Fig. 4–1c. 15 points of $f(x)$.

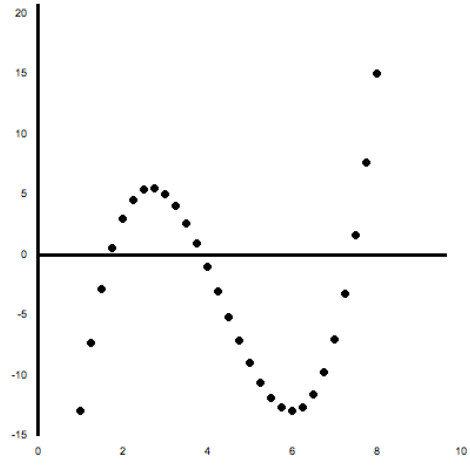

Fig. 4–1d. 29 points of $f(x)$.

where the units vectors $|\,i>$ or $<i\,|$ are of corresponding arbitrarily large or infinite extent. In fact, the "continuous" function of figure 4–1a is created in this manner with 600 points.

Postscript: Again, this is simply a plausibility argument. Questions involving convergence are beyond our scope. The intent of this problem is to provide a mental picture. The overall intent of this volume is to provide a modern context to the calculations of non-relativistic quantum mechanics which realistically cannot be obtained without extension to infinite dimensions.

The Dirac delta function is properly defined

$$\int_{-\infty}^{\infty} \delta(x)\,dx \;=\; \begin{cases} 1 & \text{if } x = 0\,, \\ 0 & \text{if } x \neq 0\,. \end{cases}$$

Notice that it appears as part of an integrand in our definition. It is only when a delta function is outside of an integral that debate ensues. The incomplete definition

$$\delta(x)\,dx \;=\; \begin{cases} 1 & \text{if } x = 0, \\ 0 & \text{if } x \neq 0 \end{cases}$$

is what seems to create much of the discussion.

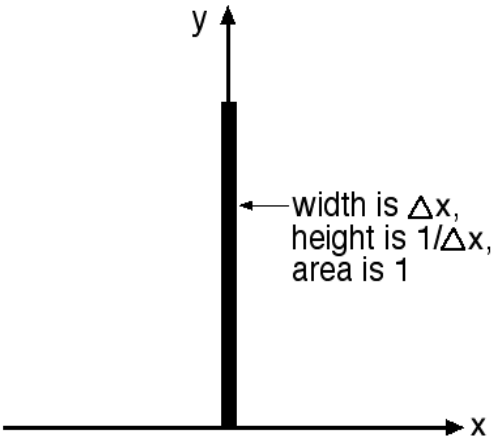

Figure 4–2. Delta function at $x = 0$.

The Dirac delta function should only appear as a factor in an integrand. Dirac wrote "...it will be something which is to be used ultimately in an integrand." Nevertheless, delta functions commonly appear apart from an integral symbol in modern literature. Dirac commonly wrote his delta functions without an integral symbol. The Dirac delta function is an idealization, much the same way as a mathematical point will model the location of a classical particle. Dirac indicates it is "...merely a convenient notation, enabling us to express in a concise form certain relations which we could, if necessary, rewrite in a form not involving improper functions, but only in a cumbersome way which would tend to obscure the argument[1]." If the system is discrete, a Kronecker delta is appropriate to model an "all or none" quantity. If the system is continuous, a Dirac delta function is appropriate to model an "all or none" situation.

Likely the most straightforward graph of a delta function is zero everywhere except for a tall, thin rectangle inside a domain of length Δx. The area of the rectangle is length $\times$ width, or

$$\Delta x\,\frac{1}{\Delta x} \;=\; 1$$

If the domain is diminished, the function must become "taller" to preserve the area at 1. In the limit of $\Delta x \to 0$, the functional value goes to ∞, but the area is still 1. The delta function is an idealization of an infinitely high, infinitely thin spike with an area of 1.

The mathematical interpretation of the Dirac delta function is varied. Some view it as an actual function, others view it as a generalized function[2], others classify it as a distribution. Some consider it nothing more than a pathological mathematical object, devoid of recognition. Dirac considered it an improper function. The delta function is an extension of the Kronecker delta to continuous systems. All continuous systems involve infinities which present problems that do not exist in finite systems. All calculus problems involve infinities. That calculus is useful is evidence that the sum (or difference or quotient or...) of some infinities converge. The problem of convergence remains a research topic within multiple realms of mathematics. We do not address the

[1] Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, England, 1958), 4th ed., pp. 58-59.

[2] Lighthill, *An Introduction to Fourier Analysis and Generalised Functions* (Cambridge University Press, Cambridge, England, 1958).

problem of convergence here, rather, we do attempt to demonstrate how the Dirac delta function is useful and use it to develop other tools appropriate to introductory quantum mechanics. See Boas[3], Arfken[4], or your favorite text on mathematical physics for greater depth.

Finally, imagine integrating over a delta function. The area under the curve is 1, given that the delta function is within the limits of integration. If the delta function is not within the limits of integration, the value of the integral is zero.

For instance, $\int_{-\infty}^{\infty} \delta(x)\,dx = 1$ and $\int_{-1}^{1} \delta(x)\,dx = 1$ where the delta function is at $x = 0$ and is within the limits of integration, but $\int_{1}^{\infty} \delta(x)\,dx = 0$ and $\int_{-\infty}^{-1} \delta(x)\,dx = 0$, because 0 is not within the limits of integration.

4–3. Evaluate $\int_{-\infty}^{\infty} (x+3)\,\delta(x)\,dx$.

A delta function will generally appear as a factor in an integrand, rather than as the complete integrand. The factor $(x+3)$ will range from $-\infty$ to ∞ given the limits of integration, but the delta function is zero everywhere except at $x = 0$, and

$$0 \times \text{anything} = 0,$$

to include $-\infty \cdot 0 = 0$, and $\infty \cdot 0 = 0$. Thus, the entire integrand, $(x+3)\,\delta(x)$, is zero everywhere except at $x = 0$. At $x = 0$, the delta function has area 1, so the integral there is the functional value at zero which is $f(0) = 3$, times the 1 of the delta function, so the integral of the product is 3.

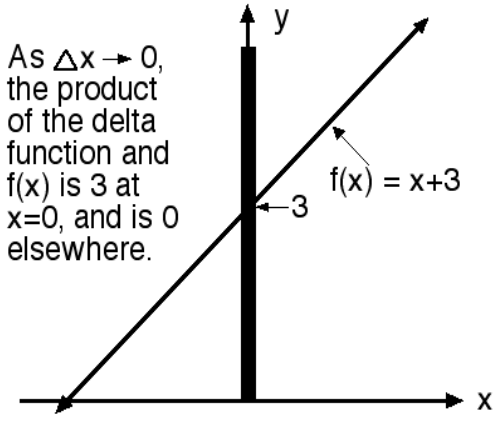

Figure 4–3. The infinitely tall, infinitely thin spike of area 1 times $f(0) = 3$, thus, the integral of the product is 3.

$$\int_{-\infty}^{\infty} (x+3)\,\delta(x)\,dx = (x+3)\Big|_{x=0} = 0+3 = 3.$$

Postscript: Notice that an anti-derivative of $f(x) = x+3$ is unnecessary for an integrand containing a delta function.

The symbol $\Big|_{x=0}$ means "evaluated at $x =$ zero." Other examples of this symbology are $\Big|_{x=2}$ meaning "evaluated at $x = 2$," and $\Big|_{\theta=-\pi}$ meaning "evaluated at $\theta = -\pi$."

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[3] Boas, *Mathematical Methods in the Physical Sciences* (John Wiley & Sons, New York, 1983), 2nd ed., pp. 665-670.

[4] Arfken, *Mathematical Methods for Physicists* (Academic Press, New York, 1970), 2nd ed., pp. 413-415.

4–4. Evaluate $\displaystyle\int_{-\infty}^{\infty} \big(\,x+3\,\big)\,\delta\,(x-2)\,dx$ and $\displaystyle\int_{-\infty}^{0} \big(\,x+3\,\big)\,\delta\,(x-2)\,dx\,.$

What is the meaning of $\delta\,(x-2)\,?$ Where the argument of the delta function is zero, there is a tall, thin spike of area 1, so that tall, thin spike is now at

$$x-2 \;=\; 0 \qquad \Leftrightarrow \qquad x \;=\; 2\,.$$

The tall, thin spike is shifted two units to the right. Similarly, $\delta\,(x+5)$ means the tall, thin spike is at $x+5 \;=\; 0 \;\Leftrightarrow\; x \;=\; -5\,,$ and $\delta\,(\theta-\pi)$ means the tall, thin spike is at $\theta-\pi \;=\; 0 \;\Leftrightarrow\; \theta \;=\; \pi\,.$

If the value that makes the argument of the delta function zero is not within the limits of integration, the entire integral is zero.

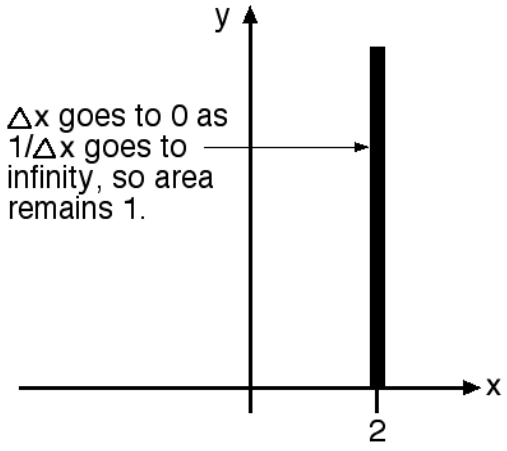

Figure 4–4. Delta function at $x = 2\,.$

$$\int_{-\infty}^{\infty} \big(\,x+3\,\big)\,\delta\,(x-2)\,dx \;=\; \big(\,x+3\,\big)\Big|_{x\,=\,2} \;=\; 2+3 \;=\; 5\,.$$

$$\int_{-\infty}^{0} \big(\,x+3\,\big)\,\delta\,(x-2)\,dx \;=\; 0 \quad \text{because } 2 \text{ is not within the limits of integration.}$$

Postscript: The practice of "shifting" the tall, thin spike that is the delta function to the left or right is encountered frequently. In general, "shifting" the delta function to $x-a \;=\; 0 \;\Leftrightarrow\; x \;=\; a\,,$

$$\text{and} \qquad \int_{-\infty}^{\infty} f\,(x)\,\delta\,(x-a)\,dx \;=\; f\,(x)\Big|_{x\,=\,a} \;=\; f\,(a)\,.$$

Continue to pay attention to the limits of integration. Should the value that makes the argument of the delta function zero be outside of the limits of integration, the value of entire integral is zero.

4–5. Evaluate (a) $\displaystyle\int_{-1}^{1} \big(\,x+3\,\big)\,\delta(x)\,dx$ (b) $\displaystyle\int_{-\infty}^{\infty} \big(\,x+3\,\big)\,\delta(x+9)\,dx$

(c) $\displaystyle\int_{0}^{\infty} \big(\,x+3\,\big)\,\delta(x+9)\,dx$ (d) $\displaystyle\int_{0}^{\infty} \big(\,3x^2+x+3\,\big)\,\delta(x-2)\,dx$

(e) $\displaystyle\int_{-\infty}^{0} \big(\,3x^2+x+3\,\big)\,\delta(x-2)\,dx$ (f) $\displaystyle\int_{-\pi}^{\pi} \big(\,\cos\theta\,\big)\,\delta(\theta)\,d\theta$

(g) $\displaystyle\int_{0}^{\infty} \big(\,3x^2+x+3\,\big)\,\delta(x-4)\,dx$ (h) $\displaystyle\int_{-\pi}^{\pi} \big(\,\cos\theta\,\big)\,\delta(\theta-2\pi)\,d\theta$

$$\int_a^c f(x)\,\delta(x-b)\,dx \;=\; f(x)\Big|_{x=b} \;=\; f(b) \quad \text{given that } \; a<b<c\,, \text{ and is zero otherwise.}$$

(a) $\displaystyle\int_{-1}^{1} \big(x+3\big)\,\delta(x)\,dx \;=\; \big(x+3\big)\Big|_{x=0} \;=\; 0+3 \;=\; 3$

(b) $\displaystyle\int_{-\infty}^{\infty} \big(x+3\big)\,\delta(x+9)\,dx \;=\; \big(x+3\big)\Big|_{x=-9} \;=\; -9+3 \;=\; -6$

(c) $\displaystyle\int_{0}^{\infty} \big(x+3\big)\,\delta(x+9)\,dx \;=\; 0$ because $x=-9$ is not between 0 and ∞

(d) $\displaystyle\int_{0}^{\infty} \big(3x^2+x+3\big)\,\delta(x-2)\,dx \;=\; \big(3x^2+x+3\big)\Big|_{x=2} \;=\; 3\cdot 2^2+2+3 \;=\; 17$

(e) $\displaystyle\int_{-\infty}^{0} \big(3x^2+x+3\big)\,\delta(x-2)\,dx \;=\; 0$ because $x=2$ is not between $-\infty$ and 0

(f) $\displaystyle\int_{-\pi}^{\pi} \big(\cos\theta\big)\,\delta(\theta)\,d\theta \;=\; \big(\cos\theta\big)\Big|_{\theta=0} \;=\; \cos 0 \;=\; 1$

(g) $\displaystyle\int_{0}^{\infty} \big(3x^2+x+3\big)\,\delta(x-4)\,dx \;=\; \big(3x^2+x+3\big)\Big|_{x=4} \;=\; 3\cdot 4^2+4+3 \;=\; 55$

(h) $\displaystyle\int_{-\pi}^{\pi} \big(\cos\theta\big)\,\delta(\theta-2\pi)\,d\theta \;=\; 0$ because $\theta=2\pi$ is not between $-\pi$ and π

4–6. Evaluate (a) $\displaystyle 2\int_{-\pi}^{\pi} \cos(2\theta)\,\delta(\theta)\,d\theta$ (b) $\displaystyle 2\pi\int_{-\pi}^{\pi} \cos(2\theta)\,\delta\left(\theta-\frac{\pi}{3}\right)\,d\theta$

(c) $\displaystyle\int_{0}^{\infty} A\cos(x)\,e^{-x^2}\,\delta(x+1)\,dx$ (d) $\displaystyle\int_{-\pi}^{\pi} A\cos(x)\,e^{-x^2}\,\delta(x+1)\,dx$

(e) $\displaystyle\int \cos\left(\frac{n\pi x}{l}\right)\sin\left(\frac{n\pi x}{l}\right)\,\delta(x-l)\,dx, \quad n=1,2,3,\ldots$

(f) $\displaystyle\int \big(16\xi^4-48\xi^2+12\big)\,\delta(\xi-2)\,d\xi$

(g) $\displaystyle\int \frac{2}{\sqrt{27}}\,a_0^{-3/2}\left(1-\frac{2r}{3a_0}+\frac{2r^2}{27a_0^2}\right)e^{-r/3a_0}\,\delta(r-a_0)\,dr$

(h) $\displaystyle\int_0^{\pi} d\theta\int_0^{2\pi} d\phi\,\sqrt{\frac{105}{32\pi}}\,\sin^2\theta\,\cos\theta\,e^{2i\phi}\,\delta\left(\theta-\frac{\pi}{4}\right)\,\delta\left(\phi-\frac{\pi}{2}\right)$

(i) $\displaystyle\int_0^{1} dr\int_{-\infty}^{\infty} d\theta\,\frac{1}{r^2}\,\sin(\theta)\,\delta(r-a)\,\delta\left(\theta-\frac{\pi}{3}\right), \quad 0<a<1\,.$

This is a continuation of the last problem with integrands that are slightly more challenging. It is intended to amplify and extend your abilities in evaluating integrals containing delta functions.

Pay attention to the limits of integration. The integral is zero if the value that makes the argument of the delta function zero is not within the limits of integration. If the value that makes the argument of the delta function zero is within the limits of integration, the value of the integral is the functional value of the integrand evaluated at that point. Again,

$$\int_a^b f(x)\,\delta(x-c)\,dx \;=\; f(x)\Big|_{x=c} \;=\; f(c) \quad \text{if} \quad a < c < b\,, \quad 0 \;\text{ otherwise.}$$

Notice parts (e), (f), and (g) do not have limits of integration. An integral with a delta function without explicit limits means that "all space" is implied. Thus, the limits $-\infty$ and ∞ are implied in parts (e) and (f). Part (g) concerns only the radial component in spherical coordinates, so "all space" means from 0 to ∞ for the radial parameter r.

Address each variable of integration independently for the double integrals of part (h) and (i).

(a) The argument of the delta function is zero at $\theta = 0$, so

$$2\int_{-\pi}^{\pi} \cos(2\theta)\,\delta(\theta)\,d\theta \;=\; 2\cos(2\theta)\Big|_{\theta=0} \;=\; 2\cos(0) \;=\; 2\cdot 1 \;=\; 2\,.$$

(b) $\theta - \dfrac{\pi}{3} = 0 \quad\Leftrightarrow\quad \theta = \dfrac{\pi}{3}\,, \quad$ and $\quad -\pi < \dfrac{\pi}{3} < \pi \quad$ therefore

$$2\pi\int_{-\pi}^{\pi} \cos(2\theta)\,\delta\left(\theta - \frac{\pi}{3}\right)\,d\theta \;=\; 2\pi\cos\frac{2\pi}{3} \;=\; 2\pi\left(-\frac{1}{2}\right) \;=\; -\pi$$

(c) $x+1 = 0 \quad\Leftrightarrow\quad x = -1\,,$ and -1 is not between 0 and ∞, so the integral is zero.

(d) $x+1 = 0 \quad\Leftrightarrow\quad x = -1\,,$ and $-\pi < -1 < \pi\,,$ so

$$\int_{-\pi}^{\pi} A\cos(x)\,e^{-x^2}\,\delta(x+1)\,dx \;=\; A\cos(-1)\,e^{-(-1)^2} \;=\; \frac{0.5403\,A}{e} \;=\; 0.1988\,A$$

(e) The argument of the delta function is zero at $x - l = 0 \quad\Leftrightarrow\quad x = l\,,$ so

$$\int_{-\infty}^{\infty} \cos\left(\frac{n\pi x}{l}\right)\sin\left(\frac{n\pi x}{l}\right)\delta(x-l)\,dx \;=\; \cos\left(\frac{n\pi x}{l}\right)\sin\left(\frac{n\pi x}{l}\right)\Big|_{x=l}$$

$$=\; \cos(n\pi)\,\sin(n\pi) \;=\; \cos(n\pi)\,(0) \;=\; 0 \quad \text{for all} \quad n\,.$$

(f) $-\infty < 2 < \infty\,,$ therefore

$$\int \left(16\xi^4 - 48\xi^2 + 12\right)\delta(\xi - 2)\,d\xi \;=\; 16\cdot 2^4 - 48\cdot 2^2 + 12 \;=\; 256 - 192 + 12 \;=\; 76$$

(g) $0 < a_0 < \infty\,,$ thus

$$\int \frac{2}{\sqrt{27}}\,a_0^{-3/2}\left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right)e^{-r/3a_0}\,\delta(r-a_0)\,dr \;=\; \frac{2}{\sqrt{27}}\,a_0^{-3/2}\left(1 - \frac{2a_0}{3a_0} + \frac{2a_0^2}{27a_0^2}\right)e^{-a_0/3a_0}$$

$$= \frac{2}{\sqrt{27}}\, a_0^{-3/2} \left(1 - \frac{2}{3} + \frac{2}{27}\right) e^{-1/3} = \frac{22}{81\sqrt{3}}\, a_0^{-3/2}\, e^{-1/3}$$

(h) Both angular parameters are between their respective limits of integration, thus

$$\int_0^{\pi} d\theta \int_0^{2\pi} d\phi \sqrt{\frac{105}{32\pi}}\, \sin^2\theta\, \cos\theta\, e^{2i\phi}\, \delta\left(\theta - \frac{\pi}{4}\right)\, \delta\left(\phi - \frac{\pi}{2}\right)$$

$$= \sqrt{\frac{105}{32\pi}}\, \sin^2\frac{\pi}{4}\, \cos\frac{\pi}{4}\, e^{2i\pi/2} = \sqrt{\frac{105}{32\pi}}\, \frac{1}{2}\, \frac{1}{\sqrt{2}}\, e^{i\pi} = -\sqrt{\frac{105}{256\pi}} \qquad \text{using Euler's equation.}$$

(i) Both parameters are between their respective limits of integration given $0 < a < 1$,

$$\int_0^1 dr \int_{-\infty}^{\infty} d\theta\, \frac{1}{r^2}\, \sin(\theta)\, \delta(r-a)\, \delta\left(\theta - \frac{\pi}{4}\right) = \int_0^1 dr\, \frac{1}{r^2} \left(\Big[\sin(\theta)\Big]_{\theta=\pi/4}\right) \delta(r-a)$$

$$= \int_0^1 dr\, \frac{1}{r^2}\, \frac{\sqrt{2}}{2}\, \delta(r-a) = \frac{\sqrt{2}}{2} \int_0^1 dr\, \frac{1}{r^2}\, \delta(r-a) = \frac{\sqrt{2}}{2}\, \frac{1}{r^2}\Big|_{r=a} = \frac{\sqrt{2}}{2a^2}$$

Postscript: Many of the functions composing portions of the integrands are realistic functions of quantum mechanics that will be encountered in later chapters. Sines and cosines will repeatedly be encountered in discussions of square wells, orbital angular momentum, and elsewhere. The function in part (h) is the spherical harmonic $Y_{3,2}(\theta, \phi)$ describing orbital angular momentum quantum number $l = 3$ and magnetic quantum number $m = 2$. Spherical harmonics are also used as a portion of the solutions to the hydrogen atom. Any factor of the form k^{-x^2}, where k is any constant, is a "bell-shaped" curve that we will call a "Gaussian" function. The form $e^{-\alpha x^2}$ will be seen frequently using varied values of a constant α. Part (f) uses a Hermite polynomial describing the fourth excited state of the quantized simple harmonic oscillator. Part (g) includes the radial component of the hydrogen atom for principal quantum number $n = 3$ and orbital angular momentum quantum number $l = 0$, and a_0 is the Bohr radius $= 5.29 \times 10^{-11}$ meters.

In the interest of reading notation, the double integral of part (h) concerns only the angular components of spherical coordinates. The normal conventions for spherical coordinates are that the polar angle θ is the angle of depression from the z-axis so ranges from 0 to π, and the azimuthal angle ϕ ranges from 0 to 2π. The limits of integration for the double integral for part (h) cover "all space" for the angular components of this double integral, and it could be written

$$\int d\theta \int d\phi \sqrt{\frac{105}{32\pi}} \sin^2\theta\, \cos\theta\, e^{2i\phi}\, \delta\left(\theta - \frac{\pi}{4}\right)\, \delta\left(\phi - \frac{\pi}{2}\right)$$

without limits of integration and with the same meaning as the integral posed in part (h).

Remember that an anti-derivative <u>is not required</u> for an integrand containing a delta function. An integrand with a delta function <u>is not</u> a Riemann integral.

4–7. Evaluate (a) $\int f(x)\,\delta(ax-b)\,dx\,, \quad a\,,\ b\,>\,0\,;$ and (b) $\int \left(x^2-2x+3\right)\delta(2x-6)\,dx\,.$

Part (a) of this problem introduces a more general displacement for a delta function. A coefficient other than 1 on an independent variable as part of the argument of a delta function complicates the situation. The key is to change variables to y = argument of the delta function so that the contribution of the differential element is properly considered.

(a) Let $y = ax - b \quad \Rightarrow \quad x = \dfrac{y+b}{a}$ and $dy = a\,dx \quad \Rightarrow \quad dx = \dfrac{dy}{a}\,.$
The implied limits of integration remain $-\infty$ and $\infty\,,$

$$\Rightarrow \quad \int f(x)\,\delta(ax-b)\,dx = \int f\left(\frac{y+b}{a}\right)\delta(y)\,\frac{dy}{a} = \frac{1}{a}\,f\left(\frac{y+b}{a}\right)\Big|_{y=0} = \frac{1}{a}\,f\left(\frac{b}{a}\right).$$

(b) $a = 2\,, \quad \dfrac{b}{a} = \dfrac{6}{2} = 3 \quad \Rightarrow \quad \int \left(x^2-2x+3\right)\delta(2x-6)\,dx = \dfrac{1}{2}\left(3^2-2\,(3)+3\right) = 3\,.$

Postscript: Notice that should the argument of the delta function simply be set equal to zero without the change of variables, the evaluation of the integral in part (b) is off by a factor of 2.

4–8. (a) What are even and odd functions?

(b) What is the origin of the terms even and odd function?

(c) Is the Dirac delta function, even, odd, or neither?

(d) How are even and odd functions used?

Most functions are neither even nor odd, but symmetry can occasionally make life simpler.

(a) A function is even if $f(-x) = f(x)\,,$ like a cosine, and a function is odd if $f(-x) = -f(x)\,,$ like a sine. The graph of an even function is symmetric about the vertical axis. If the graph of an even function is folded on the vertical axis, the two half curves overlap. The graph of an odd function is symmetric about the origin. If the graph of an odd function is cut on the vertical axis and rotated 180 degrees around the origin, the two half curves overlap. Most functions do not have central symmetry so are neither even nor odd. For example, $f(x) = x+1$ is neither even nor odd.

(b) Polynomial functions with even powers, for instance, $f(x) = x^4 - x^2$ are even because

$$f(-x) = (-x)^4 - (-x)^2 = x^4 - x^2 = f(x)$$

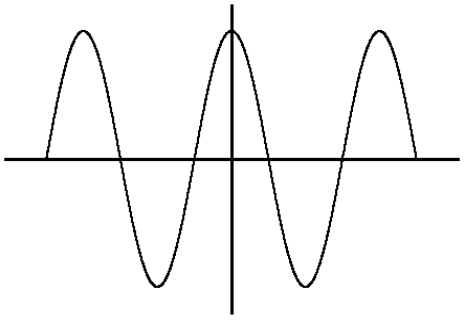

Fig. 4–5a. Symmetric about y-axis.

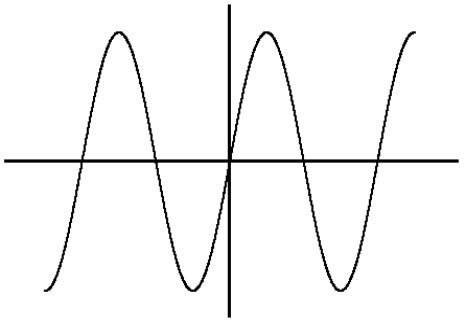

Fig. 4–5b. Symmetric about origin.

Polynomial functions with odd powers, for instance, $f(x) = x^3 + x$ are odd because

$$f(-x) = (-x)^3 + (-x) = -x^3 - x = -(x^3 + x) = -f(x)$$

and the designations even/odd functions originate in these even/odd powers of polynomial functions. Regardless of origin, an even function is symmetric about the vertical axis, and an odd function is symmetric about the origin.

Most functions are neither even nor odd. For $f(x) = x + 1$, for instance,

$$f(-x) = -x + 1 \neq f(x), \qquad \text{and} \qquad f(-x) = -x + 1 \neq -(x + 1) = -f(x).$$

(c) The Dirac delta function is an even function. This fact is often expressed

$$\delta(-x) = \delta(x) \qquad \text{and} \qquad \delta(x - x') = \delta(x' - x).$$

This notation is incomplete because a delta function is "something which is to be used ultimately in an integrand." A function and integral with the limits indicating "all space" are implicit, *i.e.*,

$$\delta(x - x') = \delta(x' - x) \quad \Rightarrow \quad \int_{-\infty}^{\infty} f(x)\,\delta(x - x')\,dx = \int_{-\infty}^{\infty} f(x)\,\delta(x' - x)\,dx.$$

The function, integral, and limits are often omitted in the interest of brevity and to avoid "clutter." These can be attached to complete the meaning of relationships involving "naked" delta functions.

(d) The process of evaluating some integrals can be simplified should the integrand be an even or odd function when the integral has symmetric limits. The integral of an odd function between symmetric limits is zero, and what may initially appear as a difficult calculation may be completed by inspection. The integral of an even function between symmetric limits is twice the integral from a lower limit of zero to the upper limit of the original integral. Many tables publish solutions to some integrals with even integrands from 0 to an upper limit rather than between symmetric limits; from 0 to ∞, or from 0 to π, rather than from $-\infty$ to ∞, or from $-\pi$ to π.

4–9. Identify the following functions as even, odd, or neither.

(a) $A\cos(x)\,e^{-x^2}$

(b) $\cos\left(\frac{n\pi x}{l}\right)\sin\left(\frac{n\pi x}{l}\right), \quad n = 1, 2, 3, \ldots$

(c) $16\xi^4 - 48\xi^2 + 12$

(d) $\frac{2}{\sqrt{27}}\,a_0^{-3/2}\left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right)$

(e) $\sqrt{\frac{105}{32\pi}}\sin^2\theta\cos\theta$

(f) $x^2\sin(x)\,e^{-x^2}$

Practice recognizing even and odd functions is appropriate. You should know that the product of an even function and a second even function is an even function. The product of an odd function and a second odd function is an even function. The product of an even function and an odd function is an odd function. Proofs of these statements are straightforward and are left as exercises.

(a) A cosine is even, the Gaussian e^{-x^2} is even, the constant A amplifies or contracts the vertical magnitude without affecting symmetry, therefore, this is an even function. Normalization constants cannot affect symmetry in general.

(b) A cosine is even, a sine is odd, therefore, this function is odd.

(c) This function is even. The constant term "$+12$" is equivalent to "$+12x^0$" where the power "0" is an even number, so all exponents of this polynomial function are even. Notice also that this function satisfies the definition $f(-\xi) = f(\xi)$.

(d) Neither even nor odd. Quadratic, linear, and constant terms cannot have central symmetry.

(e) A sine is odd, but a sine squared is even, times an even cosine; this function is even.

(f) Even x^2, times odd $\sin(x)$, times even e^{-x^2}, is odd.

4–10. Show that $\int \delta(x)\,dx = \Theta(x)$.

This problem introduces the **theta function**. The delta function is the derivative of the theta function, as this problem demonstrates in integral form. The theta function is useful in establishing some of the properties of the delta function and in some problems involving discontinuities.

The theta function, also known as the step function or the Heaviside step function, is defined

$$\Theta(x) = \begin{cases} 1, & \text{if } x > 0, \\ 0, & \text{if } x < 0. \end{cases}$$

If we "shift" the origin to $x = x'$,

$$\Theta(x - x') = \begin{cases} 1, & \text{if } x > x', \\ 0, & \text{if } x < x'. \end{cases}$$

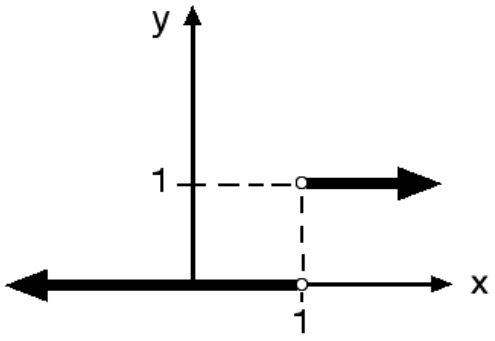

Figure 4–6. Theta function $\Theta(x-1)$.

The last equation is illustrated in the figure for $x' = 1$. Notice that $\Theta(x)$ is not defined at $x = 0$ (or $\Theta(x - x')$ at $x - x' = 0$), and $\Theta(x)$ is not continuous at $x = 0$ (or $\Theta(x - x')$ at $x - x' = 0$). Like the delta function, the theta function is another "improper" function. It does not possess the property of continuity at the location where the argument is equal to zero.

Again, the limits of integration are $-\infty$ and ∞ (or all space) when a proper integral is anticipated and limits are not stated. Limits are the key to the meaning of the premise. Break the integral into two integrals at an arbitrarily small $\epsilon < 0$. This means the limits on the first integral are $-\infty$ to $-\epsilon$ and the limits on the second integral are $-\epsilon$ to ∞. Examine the behavior of both integrals in the limit $\epsilon \to 0$.

$$\int_{-\infty}^{\infty} \delta(x)\,dx \;=\; \int_{-\infty}^{-\epsilon} \delta(x)\,dx \;+\; \int_{-\epsilon}^{\infty} \delta(x)\,dx,$$

where ϵ is an arbitrarily small number. There are two cases, either $x > 0$ or $x < 0$. If $x > 0$,

$$\int_{-\infty}^{-\epsilon} \delta(x)\,dx \;+\; \int_{-\epsilon}^{\infty} \delta(x)\,dx \;=\; 0 + 1 \;=\; 1\,,$$

where the first integral is zero because values of $x > 0$ are not within the limits of the integral, and the second integral is 1 per the definition of the Dirac delta function. If $x < 0$, then

$$\int_{-\infty}^{-\epsilon} \delta(x)\,dx \;+\; \int_{-\epsilon}^{\infty} \delta(x)\,dx \;=\; 0 + 0 \;=\; 0\,,$$

where the first integral is zero because the argument of the delta function cannot assume the value of $x = 0$ within limits that are both less than zero. The second integral is zero because the values $x < 0$ are not within the limits of the integral. If the circumstance $-\epsilon < x < 0$ were to occur, the second integral would be 1, but picking another ϵ such that $x < -\epsilon$ restores the situation in which both integrals vanish. Therefore, in the limit that $\epsilon \to 0$,

$$\int \delta(x)\,dx \;=\; \begin{cases} 1\,, & \text{if} \quad x > 0 \\ 0\,, & \text{if} \quad x < 0 \end{cases} \;=\; \Theta(x)\,.$$

Postscript: The differential form of the theta/delta relationship is $\dfrac{d\,\Theta(x)}{dx} \;=\; \delta(x)\,.$

Remember that the delta function has an area of 1. A practical way to understand the theta function as the integral of a delta function is to start at negative infinity, the value of the integral is the area under the curve which is zero until reaching the argument of the delta function, the area under the curve becomes 1 at that point, and the rest of the journey to positive infinity adds zero more area.

Oliver Heaviside was a largely self taught electrical engineer and physicist, and being self taught, originated his own notation to extend James Clerk Maxwell's work on electromagnetic theory well before Dirac. Heaviside used an all-or-nothing "function" where it was "all" <u>after</u> a certain point. Dirac wanted an all-or-nothing "function" <u>at</u> a certain point.

4–11. Evaluate (a) $\displaystyle\int \delta'(x-3)\,x^2\,dx$ (b) $\displaystyle\int \delta'(x-1)\,e^{-x^2}\,dx$

(c) $\displaystyle\int (3x^3 - 5x^2)\,\delta'(x+2)\,dx$ (d) $\displaystyle\int \cos\theta\,\delta'\left(\theta - \frac{\pi}{4}\right)\,d\theta$

(e) $\displaystyle\int \sin^2\theta\,\delta'\left(\theta - \frac{\pi}{3}\right)\,d\theta$ (f) $\displaystyle\int x^2\,e^{-x^2}\,\delta'(x-a)\,dx$

This problem introduces derivatives of delta functions. Shankar[5] introduces his version of the postulates of quantum mechanics using a delta function and the derivative of a delta function, and they are encountered elsewhere in the literature. Thus, at least minimal familiarity is appropriate.

Derivatives of delta functions are also always intended to be used as a portion of an integrand though they will frequently appear without an integral or companion function for reasons of notational economy. The derivative of the Dirac delta function is the negative of the derivative of the companion function evaluated at the point that makes the argument of δ' zero. Symbolically,

$$\int \delta'(x-a)\, f(x)\, dx \;=\; -f'(a)\,.$$

(a) For $f(x) = x^2$, $f'(x) = 2x$, so $\displaystyle\int \delta'(x-3)\, x^2\, dx \;=\; -2x\Big|_{x=3} \;=\; -2(3) \;=\; -6$

(b) $f(x) = e^{-x^2} \;\Rightarrow\; f'(x) = -2x\, e^{-x^2}$, so $\displaystyle\int \delta'(x-1)\, e^{-x^2}\, dx \;=\; 2(1)\, e^{-1^2} \;=\; \frac{2}{e}$

(c) $f(x) = 3x^3 - 5x^2 \;\Rightarrow\; f'(x) = 9x^2 - 10x$, so

$$\int (3x^3 - 5x^2)\, \delta'(x+2)\, dx \;=\; -\big(9x^2 - 10x\big)\Big|_{x=-2} \;=\; -9(-2)^2 + 10(-2) \;=\; -36 - 20 \;=\; -56$$

(d) $f(\theta) = \cos\theta \;\Rightarrow\; f'(\theta) = -\sin\theta \;\Rightarrow\; \displaystyle\int \cos\theta\, \delta'\left(\theta - \frac{\pi}{4}\right) d\theta \;=\; \sin\frac{\pi}{4} \;=\; \frac{\sqrt{2}}{2}$

(e) $f(\theta) = \sin^2\theta \;\Rightarrow\; f'(\theta) = 2\sin\theta\,\cos\theta$

$$\Rightarrow \quad \int \sin^2\theta\, \delta'\left(\theta - \frac{\pi}{3}\right) d\theta \;=\; -2\sin\frac{\pi}{3}\cos\frac{\pi}{3} \;=\; -2\,\frac{\sqrt{3}}{2}\,\frac{1}{2} \;=\; -\frac{\sqrt{3}}{2}$$

(f) $f(x) = x^2\, e^{-x^2} \;\Rightarrow\; f'(x) = 2x\, e^{-x^2} + x^2\, e^{-x^2}(-2x) = 2x\, e^{-x^2} - 2x^3\, e^{-x^2}$, so

$$\int x^2\, e^{-x^2}\, \delta'(x-a)\, dx \;=\; -2a\, e^{-a^2} + 2a^3\, e^{-a^2}$$

Postscript: Limits indicating all space are implied for all six examples, meaning from 0 to π for parts (d) and (e), and $-\infty$ to $+\infty$ for the other four parts. The delta function is the most useful of the three improper functions discussed in our development.

4–12. Evaluate

(a) $\displaystyle\int V_0 \left(\frac{a}{x} - \frac{x}{a}\right)^2 \delta'(x-a)\, dx\,,$ and

(b) $\displaystyle\int V_0 \left(\frac{a}{x} - \frac{x}{a}\right)^2 \delta'(x-b)\, dx\,.$

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[5] Shankar, *Principles of Quantum Mechanics* (Plenum Press, New York, 1994), 2nd ed., chap. 4.

The potential given in this problem is realistic and is sometimes used to model an asymmetric potential well in radial coordinates (*i.e.*, $x \to r$ and $r > 0$).

(a) The derivative of the function is

$$V_0 \frac{d}{dx}\left(ax^{-1} - \frac{x}{a}\right)^2 = V_0\, 2\left(\frac{a}{x} - \frac{x}{a}\right)\left(-ax^{-2} - \frac{1}{a}\right) = -2\,V_0\left(\frac{a}{x} - \frac{x}{a}\right)\left(\frac{a}{x^2} + \frac{1}{a}\right)$$

$$\Rightarrow \quad \int V_0\left(\frac{a}{x} - \frac{x}{a}\right)^2 \delta'(x-a)\,dx = -\left[-2\,V_0\left(\frac{a}{x} - \frac{x}{a}\right)\left(\frac{a}{x^2} + \frac{1}{a}\right)\right]_{x=a}$$

$$= 2\,V_0\left(\frac{a}{a} - \frac{a}{a}\right)\left(\frac{a}{a^2} + \frac{1}{a}\right) = 2\,V_0\,(0)\left(\frac{2}{a}\right) = 0\,.$$

(b) Having calculated the derivative for part (a),

$$\int V_0\left(\frac{a}{x} - \frac{x}{a}\right)^2 \delta'(x-b)\,dx = -\left[-2\,V_0\left(\frac{a}{x} - \frac{x}{a}\right)\left(\frac{a}{x^2} + \frac{1}{a}\right)\right]_{x=b}$$

$$= 2\,V_0\left(\frac{a}{b} - \frac{b}{a}\right)\left(\frac{a}{b^2} + \frac{1}{a}\right) = 2\,V_0\left(\frac{a^2}{b^3} + \frac{1}{b} - \frac{1}{b} - \frac{b}{a^2}\right) = 2\,V_0\left(\frac{a^2}{b^3} - \frac{b}{a^2}\right).$$

4–13. Establish relations applicable to continuous systems in position space, momentum space, and energy space, for (a) the orthonormality condition and (b) the completeness relation.

Infinities are inherent in descriptions of systems that are continuous. Physicists frequently reason using finite dimensional analogs treating the infinite as a generalization[6]. This seems a practical, if not mathematically rigorous, necessity.

There is enough new notation in this problem that you should simply read the discussion carefully. If you prefer to venture an effort on your own, realize that in position space, for instance,

$$i \text{ or } x_i \longrightarrow x\,, \qquad \delta_{ij} \longrightarrow \delta(x - x')\,, \qquad \text{and} \qquad \sum_i \longrightarrow \int dx\,,$$

when generalizing from the discrete to the continuous.

(a) The orthonormality condition is denoted $< i \,|\, j > = \delta_{ij}$ in general. If specifically in position space, it can be written $< x_i \,|\, x_j > = \delta_{ij}$ where x_i and x_j denote unit vectors that corresponded to the i^{th} and j^{th} positions on the x-axis. If $i = j$, then $< x_i \,|\, x_j > = 1$. Let the distance between unit vectors approach zero, modeling a continuous system. The discrete x_i and x_j become indistinguishable as the distance between them approaches zero, so are superseded by x and x' for continuous systems. Symbology that describes coincidence or non-coincidence is then,

$$< x_i \,|\, x_j > = \delta_{ij} \quad \longrightarrow \quad < x \,|\, x' > = \delta(x - x') \quad \text{for a continuous system in position space.}$$

[6] Cohen-Tannoudji, Diu, & Laloe, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), 4th ed., pp. 94.

If the argument is made in momentum space, $<p_i\,|\,p_j> \;=\; \delta_{ij} \;\longrightarrow\; <p\,|\,p'> \;=\; \delta\,(p-p')$.

If the argument is made in energy space, $<E_i\,|\,E_j> \;=\; \delta_{ij} \;\longrightarrow\; <E\,|\,E'> \;=\; \delta\,(E-E')$.

(b) The completeness relation is $\displaystyle\sum_{i=1}^{n} |\,i><i\,| \;=\; \mathcal{I}$ or $\displaystyle\sum_{i=1}^{n} |\,x_i><x_i\,| \;=\; \mathcal{I}$ for position space. In the limit as $n \to \infty$, $|\,x_i> \to |\,x>$ and $\displaystyle\sum_i \;\to\; \int dx$, so

$$\sum_{i=1}^{n} |\,x_i><x_i\,| \;=\; \mathcal{I} \;\longrightarrow\; \int |\,x><x\,|\,dx \;=\; \mathcal{I} \quad \text{for position space,}$$

$$\sum_{i=1}^{n} |\,p_i><p_i\,| \;=\; \mathcal{I} \;\longrightarrow\; \int |\,p><p\,|\,dp \;=\; \mathcal{I} \quad \text{for momentum space, and}$$

$$\sum_{i=1}^{n} |\,E_i><E_i\,| \;=\; \mathcal{I} \;\longrightarrow\; \int |\,E><E\,|\,dE \;=\; \mathcal{I} \quad \text{for energy space.}$$

Postscript: A Riemann integral often concerns the area under a curve where the area is approximated by $\displaystyle\sum_i^n f\,(x_i)\,\Delta\,x$. Then as $n \to \infty$, $\Delta\,x \to 0$, and $\displaystyle\sum_i f\,(x_i)\,\Delta\,x \;\to\; \int f\,(x)\,dx$, but is subject to conditions for convergence. The relations established in this problem should be viewed as definitions because of questions of convergence.

4–14. In position space, generalize the statements for (a) probability $\displaystyle\sum_{i=1}^{n} P_i \;=\; 1$,

(b) expectation value $<x> \;=\; \displaystyle\sum_{i=1}^{n} x_i P_i$, and

(c) a ket vector $|\,\psi> \;=\; \displaystyle\sum_{i=1}^{n} \psi_i\,|\,i>$ for discrete systems to continuous systems.

Continuous systems all involve infinities. Everyone who has taken the first course in calculus knows $f\,(x) \;=\; x^2 \;\;\Rightarrow\;\; f\,'(x) \;=\; 2x$, but explaining why is somewhat more difficult. At least one infinity is present in every calculus problem, including the simple differentiation of $f\,(x) \;=\; x^2$. Infinities cannot be treated as regular numbers. For instance, $\infty - \infty$ is probably not zero. It may be zero, or it may be infinity, negative infinity, or anything in between. Questions of convergence are generally formidable, nevertheless, use the conventions

$$i \;\text{ or }\; x_i \;\longrightarrow\; x\,, \qquad \delta_{ij} \;\longrightarrow\; \delta\,(x-x')\,, \qquad \text{and} \qquad \sum_i \;\longrightarrow\; \int dx\,,$$

when generalizing from the discrete to the continuous.

(a) Probability $\sum_{i=1}^{n} P_i = 1 \longrightarrow \int_{-\infty}^{\infty} P(x)\,dx = 1$ as $n \to \infty$.

(b) Expectation value $< x > = \sum_{i=1}^{n} x_i P_i \longrightarrow < x > = \int_{-\infty}^{\infty} x\,P(x)\,dx$ as $n \to \infty$.

(c) A ket vector $|\psi> = \sum_{i=1}^{n} \psi_i\,|i> \longrightarrow |\psi> = \int_{-\infty}^{\infty} \psi(x)\,|x>\,dx$ as $n \to \infty$.

Postscript: These should be considered as definitions because of questions of convergence.

4–15. Show that $< x\,|\,g > \;\to\; g(x)$ in continuous position space.

The bra $< x\,| \;\to\; (x_1,\, x_2,\, x_3,\, \ldots\, x_n)$ where $n \to \infty$ in continuous space. Using the last result of the previous problem and noting that x' is a dummy variable of position space,

$$< x\,|\,g > \;\to\; < x\,| \int g(x')\,|\,x' > \,dx' \;=\; \int g(x')\,< x\,|\,x' > \,dx'$$
$$= \int g(x')\,\delta(x - x')\,dx' \;=\; \int g(x')\,\delta(x' - x)\,dx' \;=\; g(x)$$

when the delta function is evaluated at $x' = x$.

Postscript: The solution uses $< x\,|\,x' > \;=\; \delta(x - x')$ to show $< x\,|\,g > \;\to\; g(x)$. Let's see... $< x\,|$ looks like $< x\,|$ in both relations, thus, there must be something different between $|\,x' >$ and $|\,g >$, and there is. $< x\,|$ and $|\,x' >$ are all possible positions in Hilbert space. $|\,g >$ is a functional form in Hilbert space. The relation $< x\,|\,g > \;\to\; g(x)$ says only that the abstract function g picks the appropriate position from Hilbert space to represent a conventional function of position. Again, this should be considered a plausibility argument rather than a "proof." As notation continues to evolve, it is actually rather ordinary to see $< x\,|\,\psi > \;=\; \psi(x)$ in any modern discussion of quantum mechanics.

While not developed explicitly here, $< p\,|\,\psi > \;\to\; \widehat{\psi}(p)$ and $< E\,|\,\psi > \;\to\; \widetilde{\psi}(E)$ are useful statements of the same basic phenomena. The use of a hat over a function in momentum space and the use of a tilde over a function in energy space are not essential. This notation is, nevertheless, conventional and we will employ these conventions throughout this text.

Just as $< v\,|\,w > \;=\; < w\,|\,v >^*$ in a discrete space, $< f\,|\,x > \;\to\; f^*(x)$ in continuous position space. Reversing the order of the infinite dimensional bras and kets results in a conjugate or adjoint relationship. Similarly, $< \psi\,|\,p > \;\to\; \widehat{\psi}^*(p)$ and $< \psi\,|\,E > \;\to\; \widetilde{\psi}^*(E)$ in continuous momentum space and energy space respectively.

4–16. Use the technique of insertion of the identity to establish expressions applicable to continuous systems in position space, momentum space, and energy space, for an inner product.

This problem establishes fundamental tenets within each of the three fundamental representations.

Use an inner product of two abstract vectors, say $< f \,|\, g >$. Insert the identity to get $< f \,|\, \mathcal{I} \,|\, g >$. Use the completeness relation for a continuous system for each space, then find the representations. You should find $< f \,|\, g > \;=\; \int f^*(x)\, g(x)\, dx$ for position space, for instance.

$$< f \,|\, g > = < f \,|\, \mathcal{I} \,|\, g > = < f \,|\, \left(\int |\, x >< x \,|\, dx \right) |\, g > = \int < f \,|\, x >< x \,|\, g >\, dx \rightarrow \int f^*(x)\, g(x)\, dx$$

$$< f \,|\, g > = < f \,|\, \mathcal{I} \,|\, g > = < f \,|\, \left(\int |\, p >< p \,|\, dp \right) |\, g > = \int < f \,|\, p >< p \,|\, g >\, dp \;\rightarrow\; \int \widehat{f}^*(p)\, \widehat{g}(p)\, dp$$

$$< f \,|\, g > \;=\; < f \,|\, \mathcal{I} \,|\, g > \;=\; < f \,|\, \left(\int |\, E >< E \,|\, dE \right) |\, g >$$

$$= \int < f \,|\, E >< E \,|\, g >\, dE \;\rightarrow\; \int \widetilde{f}^*(E)\, \widetilde{g}(E)\, dE\,.$$

4–17. Show that $< \mathcal{A} > \;=\; \int \psi^*(x)\, \mathcal{A}\, \psi(x)\, dx$ in position space.

Recall that in position space $|\, \psi > \;=\; \int_{-\infty}^{\infty} \psi(x)\; |\, x >\, dx\,.$

$$< \mathcal{A} > \;=\; < \psi \,|\, \mathcal{A} \,|\, \psi > \;=\; \int_{-\infty}^{\infty} < x \,|\, \psi^*(x)\, dx\; \mathcal{A} \int_{-\infty}^{\infty} \psi(x')\; |\, x' >\, dx'$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^*(x)\, \mathcal{A}\, \psi(x')\; < x \,|\, x' >\, dx\, dx'$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^*(x)\, \mathcal{A}\, \psi(x')\, \delta(x - x')\, dx\, dx'$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^*(x)\, \mathcal{A}\, \psi(x')\, \delta(x' - x)\, dx\, dx' \;=\; \int \psi^*(x)\, \mathcal{A}\, \psi(x)\, dx$$

where limits indicating all space are implied.

Postscript: Extensions to momentum and energy space are

$$< \mathcal{A} > \;=\; \int \widehat{\psi}^*(p)\, \mathcal{A}\, \widehat{\psi}(p)\, dp \qquad \text{and} \qquad < \mathcal{A} > \;=\; \int \widetilde{\psi}^*(E)\, \mathcal{A}\, \widetilde{\psi}(E)\, dE\,.$$

The result is applicable to all abstract operators, for instance $< \mathcal{A}^2 > \;=\; \int \psi^*(x)\, \mathcal{A}^2\, \psi(x)\, dx$ will be needed for uncertainty calculations.

4–18. Establish an expression for the normalization condition in position space.

This problem establishes the meaning of the phrases "square integrable" and "probability density."

The normalization condition is $< f \mid f > \; = \; 1 \quad \Rightarrow \quad \int f^{*}(x)\, f(x)\, dx \; = \; 1$ in position space.

Postscript: Similarly $< f \mid f > \; = \; 1 \quad \Rightarrow \quad \int \widehat{f}^{*}(p)\, \widehat{f}(p)\, dp \; = \; 1$ in momentum space, and

$$< f \mid f > \; = \; 1 \quad \Rightarrow \quad \int \widetilde{f}^{*}(E)\, \widetilde{f}(E)\, dE \; = \; 1 \quad \text{in energy space.}$$

That $< f \mid f > \; = \; 1 \quad \Rightarrow \quad \int f^{*}(x)\, f(x)\, dx \; = \; 1$ are consequences of the probability postulate, though the equation $\int f^{*}(x)\, f(x)\, dx \; = \; 1$ makes it apparent that the integral must converge. The means that not all functions are acceptable as quantum mechanical wave functions. For instance, $f(x) = x$ and $f(x) = \cos(x)$ cannot be normalized when considered over all space. The normalization condition in continuous position space is often written

$$\int \Big| f(x) \Big|^{2} dx \; = \; 1 \qquad \text{or} \qquad \int \Big| \psi(x) \Big|^{2} dx \; = \; 1$$

thus, it is said that an acceptable quantum mechanical wave function must be **square integrable**. Another way to say the same thing in the language of linear algebra is an acceptable quantum mechanical wave function must belong to the **vector space** $\boldsymbol{L_2}$, denoted $\boldsymbol{L^2}$ in some texts.

The quantity $\big| \psi(x) \big|^{2}$ is probability per unit length known as **probability density**.

4–19. Given the wave function $\psi(x) = x$ on the interval $0 < x < 3$,

(a) normalize $\psi(x)$.

(b) What are possible results of a measurement of position?

(c) What is the probability of measuring a position between 0 and 1?

(d) What is the probability of measuring a position between 1 and 2?

(e) What is the probability of measuring a position between 2 and 3?

(f) What is the sum of the probabilities in parts (c) through (e)? Explain your result.

(g) What is the expectation value of position?

(h) What is the uncertainty of position?

The postulates indicate we can know the possibilities, the probabilities, the expectation values, and uncertainties whether the system is discrete or continuous. Thus, this problem asks the same questions as those in chapters 2 and 3.

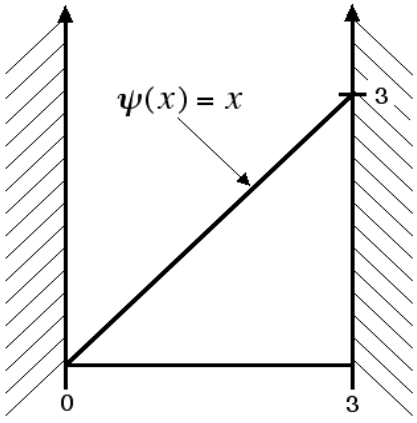

Figure 4–7a. Wave function sketch.

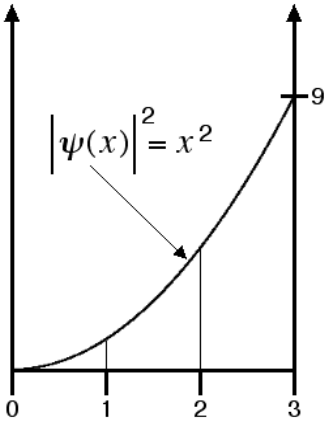

Figure 4–7b. Probability density sketch.

A function not square integrable over all space generally is square integrable on an interval. The interval represents an impenetrable potential energy function with infinitely thick, infinitely high walls. The wave function represents a particle in an inescapable one-dimensional box. These are pedagogical conditions. The interval/idealized potential energy function is used to obtain mathematically favorable conditions to demonstrate how the questions of quantum mechanics are addressed for a continuous system. The given wave function cannot be normalized over all space but it is square integrable on the interval $0 < x < 3$ for part (a). The probability that the particle exists is $\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 1$, however, all available space for the perfectly confined particle is between 0 and 3 so this becomes $\int_0^3 \psi^*(x)\,\psi(x)\,dx = 1$.

The answer to part (b) is any position between 0 and 3. Any value between 0 and 3 is an eigenvalue of a continuous system.

Notice that parts (c) through (e) ask for probabilities on sub-intervals. The probability of the particle being located between a and b is $\int_a^b \psi^*(x)\,\psi(x)\,dx$. Notice also that the intervals of parts (c) through (e) cover all available space, or "all space" for the perfectly confined system, without overlap so must sum to 1 in part (f).

Since $<\mathcal{A}> = \int \psi^*(x)\,\mathcal{A}\,\psi(x)\,dx$ and $\mathcal{X} \rightarrow x$ in position space, the expectation value of position is $<x> = \int \psi^*(x)\,x\,\psi(x)\,dx$ for part (g). $\triangle x = \left(<x^2> - <x>^2 \right)^{1/2}$ is uncertainty where $<x>^2$ is the square of $<x>$, and $<x^2> = \int \psi^*(x)\,x^2\,\psi(x)\,dx$.

The sketch of the probability density (figure 4–7b) can be visualized by squaring magnitudes from the sketch of the wave function. Notice that the vertical scales on the two sketches are different. The probability calculations are $\int_a^b \left|\psi(x)\right|^2 dx$ which is the area under the probability

density curve between a and b. It should be apparent from figure 4–7b that

$$\int_0^1 \left|\psi(x)\right|^2 dx \quad < \quad \int_1^2 \left|\psi(x)\right|^2 dx \quad < \quad \int_2^3 \left|\psi(x)\right|^2 dx\,.$$

(a) $\displaystyle\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx \;=\; 1 \;\rightarrow\; \int_0^3 (x\,N)^*\,(N\,x)\,dx \;=\; 1 \quad\Rightarrow\quad |\,N\,|^2 \int_0^3 x^2\,dx \;=\; 1 \quad\Rightarrow$

$$|\,N\,|^2 \frac{1}{3}\,x^3\Big|_0^3 \;=\; 1 \;\Rightarrow\; |\,N\,|^2 \frac{1}{3}\left(3^3 - 0^3\right) \;=\; 1 \;\Rightarrow\; |\,N\,|^2 9 \;=\; 1 \;\Rightarrow\; N \;=\; \frac{1}{3} \;\Rightarrow\; \psi(x) \;=\; \frac{1}{3}\,x\,.$$

(b) Any value between 0 and 3 is a possible result of a measurement.

(c) $\displaystyle P(0<x<1) \;=\; \int_0^1 \left(x\,\frac{1}{3}\right)^* \left(\frac{1}{3}\,x\right) dx \;=\; \frac{1}{9}\int_0^1 x^2\,dx \;=\; \frac{1}{9}\,\frac{1}{3}\,x^3\Big|_0^1 \;=\; \frac{1}{27}\left(1^3 - 0^3\right) \;=\; \frac{1}{27}\,.$

(d) $\displaystyle P(1<x<2) \;=\; \int_1^2 \left(x\,\frac{1}{3}\right)^* \left(\frac{1}{3}\,x\right) dx \;=\; \frac{1}{9}\int_1^2 x^2\,dx \;=\; \frac{1}{9}\,\frac{1}{3}\,x^3\Big|_1^2 \;=\; \frac{1}{27}\left(2^3 - 1^3\right) \;=\; \frac{7}{27}\,.$

(e) $\displaystyle P(2<x<3) \;=\; \int_2^3 \left(x\,\frac{1}{3}\right)^* \left(\frac{1}{3}\,x\right) dx \;=\; \frac{1}{9}\int_2^3 x^2\,dx \;=\; \frac{1}{9}\,\frac{1}{3}\,x^3\Big|_2^3 \;=\; \frac{1}{27}\left(3^3 - 2^3\right) \;=\; \frac{19}{27}\,.$

(f) $\displaystyle \sum P \;=\; \frac{1}{27} \;+\; \frac{7}{27} \;+\; \frac{19}{27} \;=\; \frac{27}{27} \;=\; 1\,.$ The three probabilities requested cover "all space" for this system without overlap so must sum to 1.

(g) $\displaystyle <\mathcal{X}> \;\rightarrow\; <x> \;=\; \int_{-\infty}^{\infty} \psi^*(x)\;x\;\psi(x)\,dx \;=\; \int_0^3 \left(x\,\frac{1}{3}\right)^* x\,\left(\frac{1}{3}\,x\right) dx \;=\; \frac{1}{9}\int_0^3 x^3\,dx$

$$= \;\frac{1}{9}\,\frac{1}{4}x^4\Big|_0^3 \;=\; \frac{1}{36}\left(3^4 - 0^4\right) \;=\; \frac{81}{36} \;=\; \frac{9}{4}\,.$$

(h) $\displaystyle <\mathcal{X}^2> \;\rightarrow\; <x^2> \;=\; \int_{-\infty}^{\infty} \psi^*(x)\;x^2\;\psi(x)\,dx \;=\; \int_0^3 \left(x\,\frac{1}{3}\right)^* x^2\,\left(\frac{1}{3}\,x\right) dx \;=\; \frac{1}{9}\int_0^3 x^4\,dx$

$$= \;\frac{1}{9}\,\frac{1}{5}x^5\Big|_0^3 \;=\; \frac{1}{45}\left(3^5 - 0^5\right) \;=\; \frac{243}{45} \;=\; \frac{27}{5}$$

$$\Rightarrow \quad \triangle x \;=\; \left(<x^2> - <x>^2\right)^{1/2} \;=\; \left(\frac{27}{5} - \frac{81}{16}\right)^{1/2} \;=\; \left(\frac{432 - 405}{80}\right)^{1/2} \;=\; \left(\frac{27}{80}\right)^{1/2} \;\approx\; 0.5809\,.$$

Postscript: $\displaystyle\int_a^a f(x)\,dx \;=\; 0$ for any $f(x)$ and for any a. Probability for a continuous system makes sense only for an interval $a < x < b$ where $a \neq b$ (though $a = -\infty$ and/or $b = \infty$ are common) because the probability of the result of a measurement being one number is zero.

Sketches of the wave function and probability density showing the expectation value and uncertainty centered on the expectation value follow.

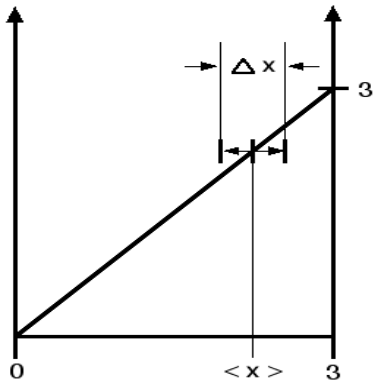

Figure 4–7c. Wave function sketch.

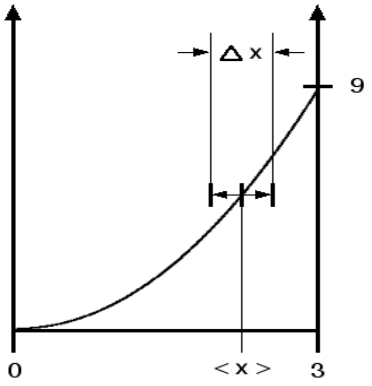

Figure 4–7d. Probability density sketch.

This problem has introduced calculations for possibilities, probabilities, expectation values, and uncertainties for a continuous system.

4–20. Given the wave function $\psi(x) = \cos(x)$ on the interval $-\frac{3\pi}{2} < x < \frac{3\pi}{2}$,

(a) sketch $\psi(x)$ and $\left|\psi(x)\right|^2$.

(b) Normalize $\psi(x)$.

(c) What are possible results of a measurement of position?

(d) What is the probability of measuring a position between $-3\pi/2$ and 0,?

(e) What is the probability of measuring a position between 0 and $\pi/2$?

(f) What is the probability of measuring a position between $\pi/2$ and $3\pi/2$?

(g) What is the expectation value of position?

(h) What is the uncertainty of position?

(i) Annotate the expectation value and uncertainty of position on your part (a) sketches.

This is a second infinite square well with a slightly more complicated wave function. Sketches or graphs of $\psi(x)$ and $\left|\psi(x)\right|^2$ are often created to illustrate a wave function and are seen below.

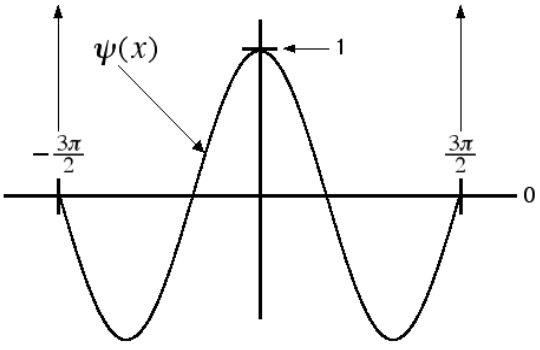

Figure 4–8a. Wave function sketch.

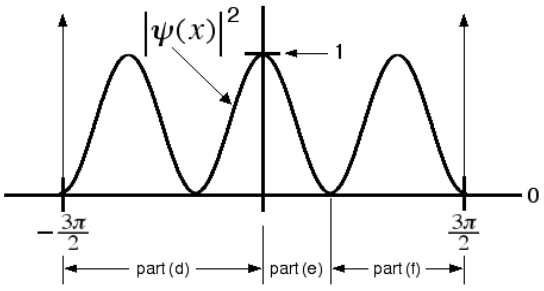

Figure 4–8b. Probability density sketch.

Part (a) (unnormalized) is completed in the prescript to discuss salient features and how sketches may be used. First, the wave function $\psi(x) = \cos(x)$ also cannot be normalized over all space but it is square integrable on an interval. The interval defines an infinite square well in one dimension. A significant degree of symmetry about the vertical axis should be apparent. Notice that though negative values of the wave function are possible, negative values of the probability density are not possible. The part (b) normalization ensures that the area under the probability density curve is 1. By just examining the probability density curve and its symmetry, the answer to part (d) should be 1/2, the answer to part (e) should be 1/6, and the answer to part (f) should be 1/3. The symmetry of the wave function should indicate $<x> = 0$. The calculations follow to illuminate the procedures, and the part (h) calculation of uncertainty is more challenging. Nevertheless, many of the parts of this problem can be done without a calculation.

Notice also that the limits of integration are symmetric, thus the even/odd function arguments discussed earlier in this chapter are useful. The integral of an odd function (expectation value) between symmetric limits is zero, and the integral of an even function (normalization, all probabilities, and $<x^2>$) is twice the integral between zero and the upper limit.

(b) $$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx \;\rightarrow\; \int_{-3\pi/2}^{3\pi/2} \cos^*(x)\,N^*\,N\,\cos(x)\,dx \;=\; |N|^2\,2\int_0^{3\pi/2}\cos^2(x)\,dx$$

$$= |N|^2\,2\left[\frac{1}{2}x + \frac{1}{4}\sin(2x)\right]_0^{3\pi/2} = |N|^2\left(x\Big|_0^{3\pi/2} + \frac{1}{2}\sin(2x)\Big|_0^{3\pi/2}\right)$$

$$= |N|^2\left(\frac{3\pi}{2} - 0 + \frac{1}{2}(0-0)\right) = 1 \quad\Rightarrow\quad N = \sqrt{\frac{2}{3\pi}} \quad\Rightarrow\quad \psi(x) = \sqrt{\frac{2}{3\pi}}\,\cos(x).$$

(c) The possibilities are any x between $-3\pi/2$ and $3\pi/2$.

(d) $$P\left(-\frac{3\pi}{2} < x < 0\right) = \int_{-3\pi/2}^{0}\left(\cos(x)\sqrt{\frac{2}{3\pi}}\right)^*\left(\sqrt{\frac{2}{3\pi}}\,\cos(x)\right)dx = \frac{2}{3\pi}\int_{-3\pi/2}^{0}\cos^2(x)\,dx$$

$$= \frac{2}{3\pi}\left[\frac{1}{2}x + \frac{1}{4}\sin(2x)\right]_{-3\pi/2}^{0} = \frac{2}{3\pi}\left[\frac{1}{2}\left(0 - -\frac{3\pi}{2}\right) + \frac{1}{4}(0-0)\right] = \frac{2}{3\pi}\left(\frac{3\pi}{4}\right) = \frac{1}{2}.$$

(e) The only changes from parts (b) and (d) are the limits of integration, thus

$$P\left(0 < x < \frac{\pi}{2}\right) = \frac{2}{3\pi}\left[\frac{1}{2}x + \frac{1}{4}\sin(2x)\right]_0^{\pi/2} = \frac{2}{3\pi}\left[\frac{1}{2}\left(\frac{\pi}{2} - 0\right) + \frac{1}{4}(0-0)\right] = \frac{2}{3\pi}\left(\frac{\pi}{4}\right) = \frac{1}{6},$$

(f) $$P\left(\frac{\pi}{2} < x < \frac{3\pi}{2}\right) = \frac{2}{3\pi}\left[\frac{1}{2}x + \frac{1}{4}\sin(2x)\right]_{\pi/2}^{3\pi/2} = \frac{2}{3\pi}\left[\frac{1}{2}\left(\frac{3\pi}{2} - \frac{\pi}{2}\right) + \frac{1}{4}(0-0)\right] = \frac{2}{3\pi}\left(\frac{\pi}{2}\right) = \frac{1}{3}.$$

(g) $$<x> \;=\; \int_{-3\pi/2}^{3\pi/2}\left(\cos(x)\sqrt{\frac{2}{3\pi}}\right)^* x\left(\sqrt{\frac{2}{3\pi}}\,\cos(x)\right)dx \;=\; \frac{2}{3\pi}\int_{-3\pi/2}^{3\pi/2} x\,\cos^2(x)\,dx.$$

The cosine is an even function, the square of the cosine is an even function, times x which is odd so the integrand is an overall odd function, which between symmetric limits is zero. Nevertheless,

$$<x> \;=\; \frac{2}{3\pi}\int_{-3\pi/2}^{3\pi/2} x\,\cos^2(x)\,dx \;=\; \frac{2}{3\pi}\left[\frac{x^2}{4} \;+\; \frac{x}{4}\sin(2x) \;+\; \frac{1}{8}\cos(2x)\right]_{-3\pi/2}^{3\pi/2}$$

$$= \frac{2}{3\pi}\left[\frac{1}{4}\left(\left(\frac{3\pi}{2}\right)^2 - \left(-\frac{3\pi}{2}\right)^2\right) \;+\; \frac{1}{4}\left(\left(\frac{3\pi}{2}\right) - \left(-\frac{3\pi}{2}\right)\right)(0-0) \;+\; \frac{1}{8}\Big(\cos(3\pi) - \cos(-3\pi)\Big)\right]$$

$$= \frac{2}{3\pi}\left[0+0+\frac{1}{8}\Big(-1--1\Big)\right] \;=\; 0\,, \quad \text{which serves only to illustrate previous comments.}$$

(h) $$<x^2> \;=\; \int_{-3\pi/2}^{3\pi/2}\left(\cos(x)\sqrt{\frac{2}{3\pi}}\right)^{*} x^2\left(\sqrt{\frac{2}{3\pi}}\;\cos(x)\right)dx \;=\; \frac{2}{3\pi}\int_{-3\pi/2}^{3\pi/2} x^2\,\cos^2(x)\,dx$$

$$= \frac{4}{3\pi}\int_{0}^{3\pi/2} x^2\,\cos^2(x)\,dx \;=\; \frac{4}{3\pi}\left[\frac{x^3}{6} \;+\; \left(\frac{x^2}{4}-\frac{1}{8}\right)\sin(2x) \;+\; \frac{x}{4}\cos(2x)\right]_{0}^{3\pi/2}$$

where the $\sin(3\pi) \;=\; \sin(0) \;=\; 0\,,$ so the middle term does not contribute. Then

$$<x^2> \;=\; \frac{4}{3\pi}\left[\frac{1}{6}\left(\frac{3\pi}{2}\right)^3 \;-\; 0 \;+\; \frac{3\pi}{8}(-1) - 0\right] \;=\; \frac{4}{3\pi}\left[\frac{27\pi^3}{48} - \frac{3\pi}{8}\right] \;=\; \frac{3\pi^2}{4} - \frac{1}{2}\,, \text{ and}$$

$$\triangle x \;=\; \big(\,<x^2> - <x>^2\,\big)^{1/2} \;=\; \left(\frac{3\pi^2}{4} - \frac{1}{2} - 0^2\right)^{1/2} \;=\; 2.627\,.$$

(i) Normalized sketches annotating expectation value and uncertainty are seen below.

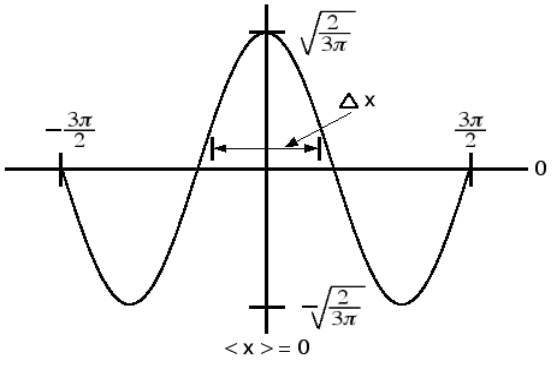

Figure 4–8c. Wave function sketch.

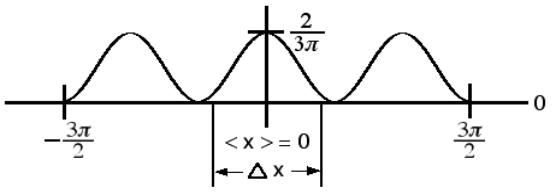

Figure 4–8d. Probability density sketch.

Postscript: Realize that a measurement of position is actually an interval limited by the quality of the equipment used to measure. A measurement cannot be precisely $1.7\ \mu m$ or -0.49 Å for instance, it will be $1.7\,\mu m \pm 0.00005\ \mu m$ or -0.49 Å $\pm\, 0.000001$ Å, or the like.

The calculations in the first two problems addressing continuous wave functions are deliberately detailed. Techniques that can make calculation more direct are applied in the next and future problems. For instance, recognizing the integrands of even and odd function between symmetric limits can be helpful. The normalization and probability integrals will have the same integrand, thus differing limits can be applied to the same anti-derivative.

4–21. Given the wave function $\psi(x) = e^{-\alpha x^2}$,

(a) sketch $\psi(x)$ and $\left|\psi(x)\right|^2$.

(b) Normalize $\psi(x)$.

(c) What are possible results of a measurement of position?

Use $\alpha = 1/8$ for parts (d) through (h).

(d) What is the probability of measuring a position between $-\infty$ and 0,?

(e) What is the probability of measuring a position between 0 and 2?

(f) What is the probability of measuring a position between 2 and ∞?

(g) What is the expectation value of position?

(h) What is the uncertainty of position?

(i) Annotate the expectation value and uncertainty of position on your part (a) sketches.

A function of the form $f(x) = k^{-\alpha x^2}$ where k and α are real constants is a bell-shaped curve, generally known in the field of statistics as a **normal** curve, and generally known within most fields of physics as a **Gaussian** curve. The part (a) sketches (unnormalized) are seen below. Both curves are Gaussian, though the probability density curve is thinner than the wave function curve. Both curves have a maximum of 1 at $x = 0$ before normalization.

The curve $f(x) = k^{-x^2}$ will only be useful if the independent variable x is dimensionless. Since x will nearly invariably carry units, the form $f(x) = k^{-\alpha x^2}$ is more commonly encountered in physics applications. The constant α will have units that are the inverse of the square of

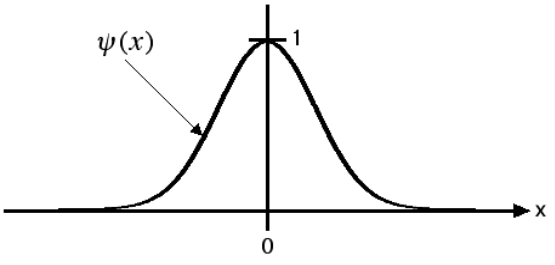

Figure 4–9a. Wave function sketch.

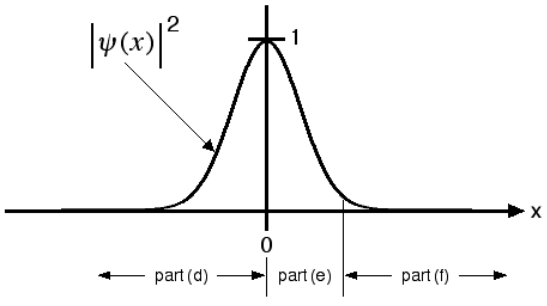

Figure 4–9b. Probability density sketch.

the units of x making the exponent dimensionless. Since x is position in one dimension, that is length in this problem, α will have dimensions of the inverse of the square of length. The direction to use $\alpha = 1/8$ in parts (d) through (h) means $\alpha = \dfrac{1}{8 \text{ units of (length)}^2}$. If x is in nanometers, $\alpha = \dfrac{1}{8\ nm^2}$, and if x is in picometers, $\alpha = \dfrac{1}{8\ pm^2}$, for instance. Units are not carried in the calculations to reduce clutter.

The wave function $\psi(x) = e^{-\alpha x^2}$ is square integrable between $-\infty$ and ∞. Form 3.323.2 from Gradshteyn and Ryzhik for the normalization process is

$$\int_{-\infty}^{\infty} \exp\left(-p^2x^2 \pm qx\right) dx \;=\; \exp\left(\frac{q^2}{4p^2}\right) \frac{\sqrt{\pi}}{p}\,, \qquad p > 0\,.$$

Gleaned from the symmetry of the probability density sketch is that the part (d) probability is 1/2 (and part (d) is done), that the sum of parts (e) and (f) also must be 1/2 (a fact used in the solution to part (f)), and that the expectation value is zero (and part (g) is done).

For the part (e) probability calculation, form 3.321.2 from Gradshteyn and Ryzhik is

$$\int_0^u e^{-p^2x^2} dx \;=\; \frac{\sqrt{\pi}}{2p} \operatorname{erf}(pu)\,, \qquad p > 0\,.$$

The $\operatorname{erf}(x)$ is the **error function** related to the Gaussian/normal curve. Values are readily available on line or in tables. The abbreviated table

x	0	0.5	0.7071	1.0	1.4142	1.5	2.0	2.1213
$\operatorname{erf}(x)$	0.0000	0.5205	0.6827	0.8427	0.9545	0.9661	0.9953	0.9973

is adequate for the moment.

The last integral required is form 3.461.2 from Gradshteyn and Ryzhik,

$$\int_0^{\infty} x^{2n}\, e^{-px^2} dx \;=\; \frac{(2n-1)!!}{2\,(2p)^n} \sqrt{\frac{\pi}{p}}\,, \qquad p > 0\,, \qquad n = 0\,,\ 1\,,\ 2\,,\ 3\,,\ \ldots$$

for the uncertainty calculation. The double factorial of 1 is 1.

Gaussian forms will be frequently encountered in future chapters.

(b) $\quad <\psi\,|\,\psi> \;=\; 1 \;\Rightarrow\; \displaystyle\int_{-\infty}^{\infty} \left(\mathrm{A}\, e^{-\alpha x^2}\right)^* \left(\mathrm{A}\, e^{-\alpha x^2}\right) dx \;=\; 1 \;\Rightarrow\; \left|\,\mathrm{A}\,\right|^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2}\, dx \;=\; 1\,.$

Using form 3.323.2 from Gradshteyn and Ryzhik, the integral has $p^2 = 2\alpha\,,\ \ q = 0\,,$ therefore

$$\left|\,\mathrm{A}\,\right|^2 e^0 \sqrt{\frac{\pi}{2\alpha}} \;=\; 1 \quad\Rightarrow\quad \left|\,\mathrm{A}\,\right|^2 \sqrt{\frac{\pi}{2\alpha}} \;=\; 1 \quad\Rightarrow\quad \mathrm{A} \;=\; \left(\frac{2\alpha}{\pi}\right)^{1/4} \quad\Rightarrow\quad \psi(x) \;=\; \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}\,.$$

(c) All positions in one spatial dimension are possible results of a measurement. All values of x such that $-\infty < x < \infty$ are eigenvalues.

(d) For $\alpha = \dfrac{1}{8}\,,$ the result of part (b) is $\psi(x) = \left(\dfrac{2}{8\pi}\right)^{1/4} e^{-x^2/8}$

$$\Rightarrow \quad P(-\infty < x < 0) \;=\; \int_{-\infty}^{0} \left(e^{-x^2/8} \left(\frac{1}{4\pi}\right)^{1/4}\right)^* \left(\frac{1}{4\pi}\right)^{1/4} e^{-x^2/8}\, dx \;=\; \sqrt{\frac{1}{4\pi}} \int_{-\infty}^{0} e^{-x^2/4}\, dx\,.$$

This is $\frac{1}{2}$ because the total area under figure 4–9b must be 1, and the interval corresponds to half of the symmetrical probability density domain. The integral is developed for pedagogical reasons, but is evaluated by inspection of the sketch.

(e) $P\,(0 < x < 2) \;=\; \sqrt{\frac{1}{4\pi}} \int_0^2 e^{-x^2/4}\,dx$ which is the same integral with different limits. Then using integral 3.321.2, $\quad p^2 = \frac{1}{4} \quad \Rightarrow \quad p = \frac{1}{2} \quad$ and

$$P\,(0 < x < 2) \;=\; \sqrt{\frac{1}{4\pi}}\,\frac{\sqrt{\pi}}{2\left(\frac{1}{2}\right)}\,\mathrm{erf}\left(\left(\frac{1}{2}\right)2\right) \;=\; \frac{1}{2}\,\mathrm{erf}\,(1) \;=\; \frac{1}{2}\,(0.8427) \;=\; 0.42135\,.$$

(f) The interval $2 < x < \infty$ completes the domain without overlap so

$$P\,(2 < x < \infty) \;=\; 1 - 0.5 - 0.42135 \;=\; 0.07865 \quad \text{or} \quad 0.5 - 0.42135 \;=\; 0.07865\,.$$

(g) The symmetry of figure 4–9b indicates $<x> \;=\; 0\,,$ or

$$\alpha = \frac{1}{8} \;\Rightarrow\; \psi\,(x) \;=\; \left(\frac{2}{8\pi}\right)^{1/4} e^{-x^2/8} \;\Rightarrow\; <x> = \int_{-\infty}^{\infty} \left(e^{-x^2/8}\left(\frac{1}{4\pi}\right)^{1/4}\right)^{*} x \left(\frac{1}{4\pi}\right)^{1/4} e^{-x^2/8}\,dx$$

$$= \sqrt{\frac{1}{4\pi}} \int_{-\infty}^{\infty} x\,e^{-x^2/4}\,dx$$ where the product of the odd function x and the even function $e^{-x^2/4}$ is an odd function, which when integrated between symmetric limits is zero, or $<x> \;=\; 0\,.$

(h) $<x^2> \;=\; \frac{1}{2}\sqrt{\frac{1}{\pi}} \int_{-\infty}^{\infty} x^2\,e^{-x^2/4}\,dx$ by extension from part (g), which is an even integrand between symmetric limits so $<x^2> \;=\; \sqrt{\frac{1}{\pi}} \int_0^{\infty} x^2\,e^{-x^2/4}\,dx$ where $n = 1$ and $p = \frac{1}{4}$ for integral 3.461.2,

$$\Rightarrow \quad <x^2> \;=\; \sqrt{\frac{1}{\pi}}\,\frac{(2\cdot 1 - 1)!!}{2\left(\frac{2}{4}\right)^1}\sqrt{\frac{\pi}{1/4}} \;=\; \frac{1!!}{\sqrt{\pi}}\sqrt{4\pi} \;=\; 2\,,$$

$$\Rightarrow \quad \triangle x \;=\; \left(<x^2> - <x>^2\right)^{1/2} \;=\; \left(2 - 0^2\right)^{1/2} \;=\; \sqrt{2}\,.$$

(i) Normalized sketches showing expectation value and uncertainty follow.

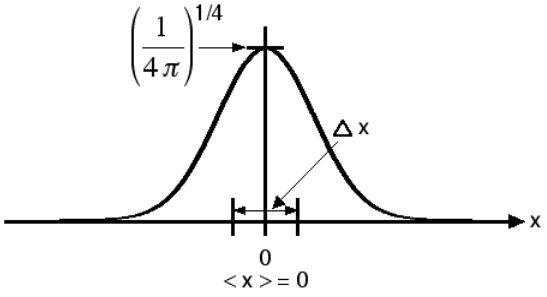

Figure 4–9c. Wave function sketch.

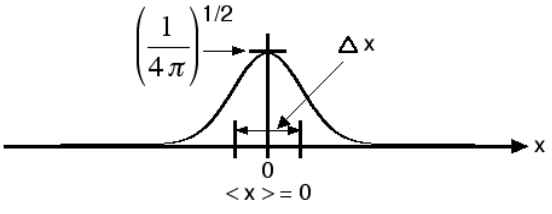

Figure 4–9d. Probability density sketch.

Postscript: The error function is defined

$$\text{erf}\,(x) \;=\; \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt\,.$$

It is often called the probability integral in the field of statistics. The error function is used to obtain a probability between zero and an upper limit for normally distributed (Gaussian) data.

4–22. Given that $\alpha = \dfrac{1}{(\text{length})^2}$, show that the wave function and probability density, and the probability, expectation value, and uncertainty calculations of the previous problem are dimensionally consistent.

The normalized wave function for $\psi(x) = e^{-\alpha x^2}$ is $\psi(x) = \left(\dfrac{2\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2}$. As is necessary, the exponential is dimensionless so all units are from the normalization constant in which $\alpha \;\rightarrow\; \dfrac{1}{(\text{length})^2}$ is the only factor with units. The dimensions of ψ are

$$\left(\frac{1}{(\text{length})^2}\right)^{1/4} \;\rightarrow\; \frac{1}{\sqrt{\text{length}}}\,.$$

The dimensions of probability density, the square of the norm of the wave function, are then $\dfrac{1}{\text{length}}$. The differential dx has units of length so the integral of probability density is dimensionless as is necessary for probability. The first moment is the expectation value for which x provides the units of length. The second moment for the uncertainty calculation is length squared, and uncertainty obtains units of length when the square root is applied.

Postscript: The Gaussian form $\psi(x) = e^{-\alpha x^2}$ is likely the simplest, however, it will be most frequently seen $\psi(x) = e^{-x^2/2\alpha^2}$ for reasons addressed in chapter 6.

Exercises

4–23. Evaluate (a) $\displaystyle\int_{-\infty}^{\infty} \big(x+7\big)\,\delta(x)\,dx$ (b) $\displaystyle\int_{-\infty}^{\infty} \big(k+4\big)\,\delta(k)\,dk$

(c) $\displaystyle\int_{-\infty}^{\infty} \big(x-5\big)\,\delta(x)\,dx$ (d) $\displaystyle\int_{-1}^{\infty} \big(t^2-5\big)\,\delta(t)\,dt$

(e) $\displaystyle\int_{1}^{\infty} \big(y+7\big)\,\delta(y)\,dy$ (f) $\displaystyle\int_{-1}^{1} \big(2x^2-x\big)\,\delta(x)\,dx$

(g) $\displaystyle\int_{-\infty}^{\infty} \big(x+7\big)\,\delta(x-6)\,dx$ (h) $\displaystyle\int_{0}^{\infty} \big(x+5\big)\,\delta(x-4)\,dx$

(i) $\displaystyle\int_{0}^{\infty} \big(x-5\big)\,\delta(x+4)\,dx$ (j) $\displaystyle\int_{-1}^{1} \big(x^3-4x^2+7x-3\big)\,\delta\left(x-\frac{1}{2}\right)\,dx$

Problems 4–2 through 4–6 discuss Dirac delta functions of this type, evaluated

$$\int_a^c f(x)\,\delta(x-b)\,dx \;=\; \begin{cases} f(b) & \text{if} \quad a<b<c\,, \\ 0 & \text{otherwise.} \end{cases}$$

Some who see delta functions for the first time are tempted to find an anti-derivative as some portion of their evaluation. An anti-derivative is not appropriate when the integrand contains a delta function; an integral with a delta function is not a Riemann integral. If the value that makes the argument of the delta function zero is between the limits of integration, the value of the integral is the functional value at that point. If the value that makes the argument of the delta function zero is not between the limits of integration, the value of the integral is zero.

4–24. Evaluate (a) $\displaystyle\int \sin^2\,\theta\,\delta(\theta)\,d\theta$ (b) $\displaystyle\int_{\pi}^{\infty} \sin^2\,\theta\,\delta(\theta)\,d\theta$

(c) $\displaystyle\int_{0}^{\pi} \sin^2\,\theta\,\cos\theta\,\delta\left(\theta+\frac{\pi}{3}\right)\,d\theta$ (d) $\displaystyle\int_{0}^{\pi} \sin^2\,\theta\,\cos\theta\,\delta\left(\theta-\frac{\pi}{3}\right)\,d\theta$

(e) $\displaystyle\int \cos^2(r)\,e^{-r}\,\delta(r-a)\,dr$ (f) $\displaystyle\int g(k)\,\left(Ae^{i(kx-\omega t)}\right)\,\delta(k)\,dk$

(g) $\displaystyle\int_{-a}^{a} \sqrt{\frac{1}{a}}\,\cos\left(\frac{\pi x}{2a}\right)\sqrt{\frac{3}{2a}}\,\left[1-\frac{x}{a}\right]\,\delta\left(x-\frac{a}{2}\right)\,dx$

(h) $\displaystyle\int_{-k}^{k} \big(32\xi^5-160\xi^3+120\xi\big)\,\delta\left(\xi+\frac{k}{2}\right)\,d\xi$

(i) $\displaystyle\int d\theta \int d\phi\,\sqrt{\frac{21}{64\pi}}\,\sin\theta\,\Big(5\cos^2\theta-1\Big)e^{-i\phi}\,\delta\left(\theta+\frac{\pi}{6}\right)\,\delta\left(\phi+\frac{\pi}{3}\right)$

(j) $\displaystyle\int d\phi \int d\theta \int dr\, \frac{8}{27\sqrt{6}} a_0^{-3/2} \left(1 - \frac{r}{6a_0}\right) \frac{r}{a_0} e^{-r/3a_0} \sin^2(\theta)\, e^{i\phi}\, \delta\left(r - \frac{a_0}{3}\right) \delta\left(\theta - \frac{\pi}{2}\right) \delta(\phi)$

Like the last exercise, except bigger, brighter, and shinier.

4–25. Evaluate (a) $\displaystyle\int_{-\pi}^{\pi} \sin(\theta)\, \delta\left(\theta - \frac{\pi}{6}\right) d\theta$ (b) $\displaystyle 2\int_0^{\infty} \cos(x)\, e^{-x^2}\, \delta\left(x - \frac{\pi}{2}\right) dx$

(c) $\displaystyle\int \frac{\mathrm{A}}{x^2 + b^2}\, \delta(x+1)\, dx$ (d) $\displaystyle\int \frac{\sin(p)\, \cos(p)}{p}\, \delta\left(p - \frac{\pi}{4}\right) dp$

Very much in the same vein as the last two exercises.

4–26. Show that $\displaystyle\int f(x)\, \delta\Big(ax + b(x-c)\Big)\, dx = \frac{1}{a+b}\, f\left(\frac{bc}{a+b}\right), \qquad a\,,\ b > 0\,.$

Procedurally similar to problem 4–7. Change variables to $y = ax + bx - bc$, the argument of the delta function. Solve this for x and that expression becomes the new argument for f. Then $dy = a\,dx + b\,dx \quad \Rightarrow \quad dx = \dfrac{dy}{a+b}$. The positive and negative infinite limits of integration remain unchanged under this change of variable. Since the delta function is now $\delta(y)$, evaluate the integrand as done with all delta functions for $y = 0$. That the multiplicative constants a and b are greater than zero means that you have only one case to consider.

4–27. Find (a) $\displaystyle\int f(x)\, \delta\Big(ax + b\Big)\, dx\,, \qquad a\,,\ b > 0\,;$ and

(b) $\displaystyle\int \big(x^2 - 2x + 3\big)\, \delta(2x+5)\, dx\,.$

This intends to reinforce the processes of the previous exercise and problem 4–7. Notice from problem 4–7 part (b), the delta function $\delta(2x-6)$ is not equivalent to a displacement of $+3$. The delta function $\delta(2x+5)$ in part (b) of this exercise is not equivalent to a displacement of $-5/2$. A change of variables to $y =$ argument of delta function is useful for a delta function in which the coefficient of the independent variable of the argument is other than 1.

4–28. Show that $\displaystyle\int \delta(x-a)\, \delta(x-b)\, dx = \delta(a-b)\,.$

Since $\displaystyle\int f(x)\, \delta(x-a)\, dx = f(a)\,,$ let $f(x) = \delta(x-b)$ and evaluate like any other delta function. Dirac[7] provides an alternative argument with "a" used as the variable of integration.

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[7] Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, England, 1958), 4th ed., pp. 60.

4–29. Identify the following functions as even, odd, or neither.

(a) $\sin^2\theta\,\cos\theta$ (b) $\cos^2(r)\,\sin(r)$

(c) $\sqrt{\dfrac{1}{a}}\,\cos\left(\dfrac{\pi x}{2a}\right)\sqrt{\dfrac{3}{2a}}\left[1-\dfrac{|\,x\,|}{a}\right]$ (d) $32\xi^5-160\xi^3+120\xi$

(e) $\sqrt{\dfrac{21}{64\pi}}\,\sin\theta\left(5\cos^2\theta-1\right)$ (f) $32\xi^5-160\xi^3+120\xi-12$

(g) $\dfrac{8}{27\sqrt{6}}\,a_0^{-3/2}\left(1-\dfrac{r}{6a_0}\right)\dfrac{r}{a_0}\,e^{-r/3a_0}$ (h) $A\,\cos(x)\,\sin(x)\,e^{-bx^2}$

See problems 4–8 and 4–9. Multiplicative constants simply increase or decrease the amplitude without changing the symmetry. Additive/subtractive constants, however, shift the graph of a function up or down, often destroying central symmetry that may exist otherwise.

All functions in problem 4–9 and this exercise are functions of one variable. Symmetry can exist in multi-variable functions, where each variable is considered separately. $f(x,\,y)\,=\,xy$ is odd in x and odd in y, $f(x,\,y)\,=\,x^2y^2$ is even in x and even in y, $f(x,\,y)\,=\,x^2y$ is even in x and odd in y, $f(x,\,y)\,=\,x^2y^2+x$ is neither even nor odd in x and is even in y, and $f(x,\,y)\,=\,xy+1$ is neither even nor odd in x and neither even nor odd in y, for instance.

4–30. Show that (a) the product of two even functions is an even function,

(b) the product of two odd functions is an even function, and

(c) the product of an even function and an odd function is an odd function.

An even function means $f(-x)\,=\,f(x)$, and an odd function means $f(-x)\,=\,-f(x)$. Let $f(-x)\,=\,f(x)$ and $g(-x)\,=\,g(x)$, then $f(x)\,g(x)\,=\,h(x)$. Show $h(-x)\,=\,h(x)$ to prove the part (a) assertion, for instance.

4–31. Evaluate (a) $\displaystyle\int 2x^3\,\delta'(x+4)\,dx$ (b) $\displaystyle\int\left(3x^3-5x^2+7x-12\right)\delta'(x-2)\,dx$

(c) $\displaystyle\int A\sqrt{x}\,e^{-x^2}\,\delta'(x-1)\,dx$ (d) $\displaystyle\int\cos^2\theta\,\delta'\left(\theta-\frac{\pi}{6}\right)d\theta$

(e) $\displaystyle\int A\,k^2\,\ln(k)\,\delta'(k-\pi)\,dk$ (f) $\displaystyle\int\sqrt{1-\cos\theta}\,\delta'\left(\theta-\frac{\pi}{3}\right)d\theta$

The integral of a function multiplied by a derivative of a delta function is the negative of the derivative of the function evaluated at the point that makes the argument of the derivative of the delta function zero. Likely the clearest statement is symbolic,

$$\int\delta'(x-a)\,f(x)\,dx\;=\;-f'(a)$$

As indicated in problem 4–11, there are opportunities to encounter derivatives of delta functions in other texts and journal literature. It is addressed here primarily with that in mind.

4–32. Find $\int V_0 \left(e^{-2\alpha x} - 2e^{-\alpha x}\right) \delta'(x-a)\, dx$.

This exercise includes the derivative of a delta function. This potential is realistic and is used to model diatomic molecules where $x = (r - r_0)/r_0$, where r_0 will depend upon the diatomic molecule being modeled. It is known as the **Morse potential**. Calculate the derivative of the function. The integral is the negative of this derivative evaluated at the point where the argument of δ' is zero. You should find that the value of this integral is $2\,V_0\,\alpha\left(e^{-2\alpha a} - e^{-\alpha a}\right)$.

4–33. Express the following brakets in functional notation in the appropriate space.

(a) $<x\,|\,f>$ (b) $<y\,|\,h>$ (c) $<q\,|\,z>$ (d) $<p\,|\,g>$

(e) $<g\,|\,p>$ (f) $<\phi\,|\,p>$ (g) $<E\,|\,\psi>$ (h) $<\Psi\,|\,E>$

This is an exercise in notation. Recognizing and expressing a basis independent braket as a continuous function in the appropriate space is a required skill. The good news is all that is required is to write the answer. The independent variables x, y, and z are the three independent variables of position space. The independent variable p is momentum. When three components are required they will be written p_x, p_y, and p_z, though one component is sufficient until reaching the subject of orbital angular momentum. This text uses a common but non-universal convention of placing a hat over the functional symbol to denote that it is in momentum space. A tilde is placed over the functional symbol to indicate that it is in energy space.

It is important to notice the order of bra and the ket. The location of independent variable in the bra or the ket determines the functional form or a conjugate form, that is

$<y\,|\,g> \;\rightarrow\; g(y)$ but $<g\,|\,y> \;\rightarrow\; g^*(y)$. See problem 4–15.

4–34. Express the following brakets as integrals in both position space and momentum space.

(a) $<g\,|\,f>$ (b) $<\Phi\,|\,h>$ (c) $<\psi\,|\,\phi>$ (d) $<h\,|\,\psi>$

(e) $<\theta\,|\,\mathcal{A}\,|\,\rho>$ (f) $<\phi\,|\,\mathcal{H}\,|\,\psi>$ (g) $<q\,|\,\mathcal{B}^2\,|\,\psi>$ (h) $<\Psi\,|\,\mathcal{L}^2\,|\,\Phi>$

This is a second exercise in notation. There are no independent variables in this exercise, thus each of the brakets is an integral when expressed in continuous position space or momentum space.

For instance, $< f\,|\,g > \;\rightarrow\; \int f^*(x)\; g(x)\, dx$ in continuous position space and $< f\,|\,g > \;\rightarrow\; \int \widehat{f}^*(p)\; \widehat{g}(p)\, dp$ in continuous momentum space. If an operator is part of the braket, $< f\,|\,\mathcal{H}\,|\,g > \;\rightarrow\; \int f^*(x)\; \mathcal{H}\; g(x)\, dx$ and $< f\,|\,\mathcal{H}\,|\,g > \;\rightarrow\; \int \widehat{f}^*(p)\; \mathcal{H}\; \widehat{g}(p)\, dp$ in continuous position and momentum space respectively. The limits on all four of these integrals are $-\infty$ to ∞ implied; all space is understood. See problems 4–16 and 4–17.

Think for a moment about the variety of interpretations already encountered for a braket. Interpretation can be critical. An inner product like $< f \,|\, g >$ may be interpreted as two vectors in $\mathbb{C}^3$ for which arguments from linear algebra may ensue. The same notation $< f \,|\, g >$ in $\mathbb{C}^\infty$ is also an inner product but is an integral in a continuous space. Further, Dirac notation is basis independent. Do you want to go to position space, or momentum space, or energy space, or some other basis? The representation chosen can be critical. Finally, we will later encounter another interpretation of a braket sandwiching an operator that is a matrix element.

4–35. What is the meaning of $< \mathcal{H} >$ in $\mathbb{C}^\infty$ in the position and momentum bases?

This means the expectation value of $\mathcal{H}$ just as it has earlier. Remember that $< \mathcal{H} >$ is simply compact notation for $< \psi \,|\, \mathcal{H} \,|\, \psi >$ where the state vector is implied, which is true in $\mathbb{C}^3$ or $\mathbb{C}^\infty$. All that is left is to write the integrals per the last exercise or problem 4–17.

Just as limits of $-\infty$ to ∞ on an integral are often suppressed when all space is understood, Dirac notation, which is inherently compact, lends itself to further abbreviation. Reading the notation correctly is critical.

4–36. Given the wave function $\psi(x) = 2$ on the interval $-2 < x < 6$,

(a) normalize $\psi(x)$.

(b) Sketch the normalized $\psi(x)$ and $\left|\psi(x)\right|^2$.

(c) What are possible results of a measurement of position?

(d) What is the probability of measuring a position between -2 and 3,?

(e) What is the probability of measuring a position between 3 and 5?

(f) What is the probability of measuring a position between 5 and 6?

(g) What is the expectation value of position?

(h) What is the uncertainty of position?

(i) Annotate the expectation value and uncertainty of position on your part (a) sketches.

The given wave function is not square integrable over all space, but it is square integrable on an interval. The interval constitutes a box in one dimension, so this is an infinite square well like problems 4–19 and 4–20. The given wave function is known as a **uniform** distribution in introductory statistics. Your part (a) sketches should be rectangles. If you have absorbed the interpretive comments from problems 4–20 and 4–21, you should be able to answer parts (c) through (g) by examining your sketches and without a calculation, or more realistically, reinforce your calculations by examining your sketches. Probability is the area under the probability density curve after the wave function is normalized. Also, parts (b) and (d) through (f) all concern rectangles with areas length times width so can be answered from the perspective of area without the requiring the evaluation of an integral. Use procedures from problems 4–19 through 4–21.

4–37. Given the wave function $\psi(x) = 2$ on the interval $-2 < x < 6$,

(a) What is the probability of measuring a position between -2 and 0,?

(b) What is the probability of measuring a position between 1.5 and 4?

(c) What is the probability of measuring a position between 4 and 6?

(d) Find the sum of the parts (a) through (c) probabilities, and explain the result.

The sum of the probabilities for problems 4–19 through 4–21 and exercise 4–36 is 1 because the probability questions partitioned all space without overlap. Should the partitioning not satisfy both criteria, the sum of the probabilities will be 1 only through coincidence.

4–38. Given the wave function $\psi(x) = 2$ on the interval $-2 < x < 6$,

(a) What is the probability of measuring a position between -2 and 1,?

(b) What is the probability of measuring a position between 0 and 5?

(c) What is the probability of measuring a position between 5 and 6?

(d) Find the sum of the parts (a) through (c) probabilities, and explain the result.

The guidance for this exercise is the same as for the last. The sum of the probabilities must be 1 when all space is covered without overlap. If all space is not covered or overlap exists, the sum of the probabilities should not be 1 save for a coincidence.

4–39. Given the wave function $\psi(x) = \sin(x)$ on the interval $-2\pi < x < 2\pi$,

(a) normalize $\psi(x)$.

(b) Sketch the normalized $\psi(x)$ and $|\psi(x)|^2$.

(c) What are possible results of a measurement of position?

(d) What is the probability of measuring a position between -2π and $\pi/2$,?

(e) What is the probability of measuring a position between $\pi/2$ and π?

(f) What is the probability of measuring a position between π and 2π?

(g) What is the expectation value of position?

(h) What is the uncertainty of position?

(i) Annotate the expectation value and uncertainty of position on your part (b) sketches.

Just like the cosine of problem 4–20, $\psi(x) = \sin(x)$ is not square integrable over all space, but it is square integrable on an interval. The interval constitutes an impenetrable box in one dimension, so this also is an infinite square well like problems 4–19 and 4–20 and exercise 4–36. Problem 4–20 may be particularly helpful. Parts (d) through (g) may be answered by inspecting

the sketch for $\left|\psi(x)\right|^2$. The given $\psi(x)$ is an odd function, but $\left|\psi(x)\right|^2$ is an even function. The integrals

$$\int \sin^2(ax)\,dx \;=\; \frac{x}{2} \;-\; \frac{1}{4a}\sin(2ax) \qquad \text{and}$$

$$\int x^2 \sin^2(ax)\,dx \;=\; \frac{x^3}{6} \;-\; \left(\frac{x^2}{4a} - \frac{1}{8a^3}\right)\sin(2ax) \;-\; \frac{x}{4a^2}\cos(2ax)$$

should be of interest. The integral

$$\int x\,\sin^2(ax)\,dx \;=\; \frac{x^2}{4} \;-\; \frac{x}{4a}\sin(2ax) \;-\; \frac{1}{8a^2}\cos(2ax)$$

may also be of interest, but on the interval $-2\pi < x < 2\pi$ it is the integral of an odd function between symmetric limits so is zero. Use procedures from problems 4–19 through 4–21.

Problems 4–19, 4–20, and exercises 4–36, and 4–39 are limited to an interval so that possibilities, probabilities, expectation values, and uncertainties can be addressed using elementary functions. The intervals model a potential energy function often described as an infinite square well in one spatial dimension, or a "particle in a box." The cosine wave function of problem 4–20 and sine wave function of this exercise play significant roles in the more general discussion of the infinite square well that is chapter 8.

4–40. Given the wave function $\psi(x) = \sin(x)$ on the interval $-2\pi < x < 2\pi$,

(a) find $P\left(0 < x < \frac{\pi}{4}\right)$

(b) and $P\left(\frac{\pi}{4} < x < \frac{\pi}{2}\right)$.

This exercise highlights further utility in examining sketches and graphs. The normalized wave function on the interval $-2\pi < x < 2\pi$ is

$$\psi(x) \;=\; \frac{1}{\sqrt{2\pi}}\sin(x)$$

for which probability density is

$$\left|\psi(x)\right|^2 \;=\; \frac{1}{2\pi}\sin^2(x).$$

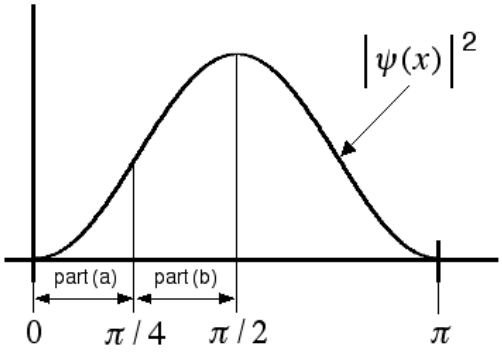

Figure 4–10. $\left|\psi(x)\right|^2$ for $0 < x < \pi$.

The probability density curve for the sub-interval $0 < x < \pi$ is seen in figure 4–10. The probability represented by the area under the probability density curve for this interval must be 1/4 from the symmetry of the sketch of $\left|\psi(x)\right|^2$ in part (b) of the previous exercise. Similarly, the probability represented on the interval $0 < x < \pi/2$ must be 1/8, thus the answers to parts (a) and (b) must sum to 1/8. And since the area corresponding to the probability for part (a) appears smaller than that for part (b), expect that

$$P\left(0 < x < \frac{\pi}{4}\right) \;<\; P\left(\frac{\pi}{4} < x < \frac{\pi}{2}\right).$$

4–41. Given the wave function $\psi(x) = e^{-x^2/2}$, find

(a) $P\big(0 < x < 1.5\big)$,

(b) $P\big(1 < x < 2\big)$,

(c) $P\big(0.5 < x < 1\big)$.

(d) $P\big(-2 < x < 0\big)$, and

(e) $P\big(-1.5 < x < -0.5\big)$.

This exercises probability calculations using error functions. The Gaussian function will be revisited on numerous occasions, so increased familiarity is also intended.

Follow problem 4–21. Normalization is the first step. You can evaluate the appropriate integral or recognize that α from problem 4–21 is $1/2$ for this exercise.

Part (a) is straightforward using the error function table

x	0	0.5	0.7071	1.0	1.4142	1.5	2.0	2.1213
$\text{erf}(x)$	0.0000	0.5205	0.6827	0.8427	0.9545	0.9661	0.9953	0.9973

$$\text{where} \qquad \int_0^u e^{-p^2x^2}dx \;=\; \frac{\sqrt{\pi}}{2p}\,\text{erf}\,(pu)\,, \quad p > 0\,.$$

You should find the parameter $p = 1$ for your probability integrals. Then for parts (b) and (c),

$$\int_a^b e^{-p^2x^2}dx \;=\; \int_0^b e^{-p^2x^2}dx \;-\; \int_0^a e^{-p^2x^2}dx\,.$$

Evaluation and subtraction of the two integrals on the right will yield the desired probability when the normalization constant is applied.

Only positive values are provided in the table, which is a norm. The user of an error function table is <u>required</u> to use the even symmetry of the Gaussian/normal curve. This means, for instance,

$$P\big(-2 < x < 0\big) \;=\; P\big(0 < x < 2\big)\,, \qquad \text{and} \qquad P\big(-1.5 < x < -0.5\big) \;=\; P\big(0.5 < x < 1.5\big)\,.$$

In other words, use the table to find the probability between 0 and $\big|\,x\,\big|$ for negative values of x, and the probability from $-x$ to 0 must be the same.

Chapter 5

Continuous Systems II

This chapter addresses the properties of orthogonality, orthonormality, and Hermiticity as they apply to continuous systems; briefly develops the methods in which polynomial solutions can be used to build continous state functions, and develops the processes of converting from position space to momentum space, or momentum space to position space for continuous systems.

Position space and momentum space are intertwined. Evidence is the Heisenberg uncertainty principle $\triangle x \triangle p \geq \frac{\hbar}{2}$ and the de Broglie relation $p = \frac{h}{\lambda}$. Some applications are addressed more readily in position space, or the **position basis**, while others may be more straightforward in momentum space, or the **momentum basis**. The conversion from one basis to another in $\mathbb{C}^\infty$ is directly analogous to converting from one set of basis vectors to a different set of basis vectors using a unitary transformation in $\mathbb{C}^3$ as seen for discrete systems. The conversion from the position/momentum basis to the momentum/position basis, however, requires a quantum mechanical **Fourier transformation** for continuous systems.

The Fourier transforms are then employed to develop relations in position space including the inner product $<x\,|\,p>$, the relations $\mathcal{X} \rightarrow x$, $\mathcal{P} \rightarrow -i\hbar\frac{d}{dx}$, and the Schrodinger equation.

5–1. Establish $<i\,|\,j> = \delta_{ij}$ in continuous position and momentum space.

It is imperative that eigenvectors, or eigenfunctions in a continuous system, satisfy the orthonormality condition. The orthonormality condition may be expressed $<f_i\,|\,f_j> = \delta_{ij}$ for eigenstates intended to be represented in a continuous space. This problem extends symbolic logic using Dirac notation. Remember that $<x\,|\,f> = f(x)$ and $<f\,|\,x> = f^*(x)$, for instance.

In position space

$$<f_i\,|\,f_j> = \delta_{ij} \quad \Rightarrow \quad <f_i\,|\mathcal{I}|\,f_j> = \delta_{ij} \quad \Rightarrow \quad <f_i\,|\left(\int |\,x><x\,|\,dx\right)|\,f_j> = \delta_{ij}$$

$$\Rightarrow \quad \int <f_i\,|\,x><x\,|\,f_j>\,dx = \delta_{ij} \quad \longrightarrow \quad \int f_i^*(x)\,f_j(x)\,dx = \delta_{ij}\,.$$

In momentum space

$$<f_i\,|\,f_j> = \delta_{ij} \quad \Rightarrow \quad <f_i\,|\mathcal{I}|\,f_j> = \delta_{ij} \quad \Rightarrow \quad <f_i\,|\left(\int |\,p><p\,|\,dp\right)|\,f_j> = \delta_{ij}$$

$$\Rightarrow \quad \int <f_i\,|\,p><p\,|\,f_j>\,dp = \delta_{ij} \quad \longrightarrow \quad \int f_i^*(p)\,f_j(p)\,dp = \delta_{ij}\,.$$

Postscript: The equations $<i\,|\,j> = \delta_{ij}$, $\int f_i^*(x)\,f_j(x)\,dx = \delta_{ij}$, and $\int f_i^*(p)\,f_j(p)\,dp = \delta_{ij}$ assume that the vectors/functions are normalized.

5–2. Show that $f_{n\ \mathrm{odd}}(x) = \cos\left(\frac{n\pi x}{l}\right)$ and $f_{m\ \mathrm{even}}(x) = \sin\left(\frac{m\pi x}{l}\right)$ are orthogonal on the interval $-l < x < l$ for $n = 1$ and $m = 2$.

Sines and cosines are the first continuous orthogonal functions that will serve as eigenfunctions. Sines and cosines are the solutions to the Schrodinger equation for the infinite square well potential energy function (a particle in a one dimensional box in position space).

The statement of the problem means to show $< f_1 \,|\, f_1 > \neq 0$, $< f_2 \,|\, f_2 > \neq 0$, and $< f_1 \,|\, f_2 > = < f_2 \,|\, f_1 > = 0$. The independent variable is x, thus position space is specifically indicated, and the integral form of the first part of problem 5–1 is applicable. The integrals

$$\int \cos^2 ax\, dx = \frac{x}{2} + \frac{1}{4a}\sin 2ax \qquad \text{and} \qquad \int \sin^2 ax\, dx = \frac{x}{2} - \frac{1}{4a}\sin 2ax$$

taken from the 30th edition of CRC Standard Mathematical Tables and Formulae are useful, as is the product relation

$$\cos(\alpha)\,\sin(\beta) = \frac{1}{2}\sin(\alpha+\beta) - \frac{1}{2}\sin(\alpha-\beta).$$

The given $f_i(x)$ do not have an imaginary part so $f_i^*(x) = f_i(x)$. The intent is a limited introduction to the general orthogonality of sines and cosines on an interval. The next problem addresses the unlimited case.

$$< f_1 \,|\, f_1 > \ \rightarrow\ \int f_1^*(x)\, f_1(x)\, dx = \int_{-l}^{l} \cos\left(\frac{\pi x}{l}\right)\cos\left(\frac{\pi x}{l}\right) dx = \int_{-l}^{l} \cos^2\left(\frac{\pi x}{l}\right) dx$$

$$= \left[\frac{x}{2} + \frac{l}{4\pi}\sin\frac{2\pi x}{l}\right]_{-l}^{l} = \frac{l}{2} - \frac{-l}{2} + \frac{l}{4\pi}\Big(\sin(2\pi) - \sin(-2\pi)\Big) = \frac{l}{2} + \frac{l}{2} + \frac{l}{4\pi}\Big(0-0\Big) = l \neq 0.$$

$$< f_2 \,|\, f_2 > \ \rightarrow\ \int f_2^*(x)\, f_2(x)\, dx = \int_{-l}^{l} \sin\left(\frac{2\pi x}{l}\right)\sin\left(\frac{2\pi x}{l}\right) dx = \int_{-l}^{l} \sin^2\left(\frac{2\pi x}{l}\right) dx$$

$$= \left[\frac{x}{2} - \frac{l}{8\pi}\sin\frac{4\pi x}{l}\right]_{-l}^{l} = \frac{l}{2} - \frac{-l}{2} + \frac{l}{8\pi}\Big(\sin(4\pi) - \sin(-4\pi)\Big) = \frac{l}{2} + \frac{l}{2} + \frac{l}{8\pi}\Big(0-0\Big) = l \neq 0.$$

$$< f_1 \,|\, f_2 > \ \rightarrow\ \int f_1^*(x)\, f_2(x)\, dx = \int_{-l}^{l} \cos\left(\frac{\pi x}{l}\right)\sin\left(\frac{2\pi x}{l}\right) dx$$

$$= \int_{-l}^{l}\left(\frac{1}{2}\sin\left(\frac{3\pi x}{l}\right) - \frac{1}{2}\sin\left(-\frac{\pi x}{l}\right)\right) dx = \frac{1}{2}\int_{-l}^{l}\sin\left(\frac{3\pi x}{l}\right) dx + \frac{1}{2}\int_{-l}^{l}\sin\left(\frac{\pi x}{l}\right) dx$$

$$= \frac{1}{2}\left[-\frac{l}{3\pi}\cos\left(\frac{3\pi x}{l}\right)\right]_{-l}^{l} + \frac{1}{2}\left[-\frac{l}{\pi}\cos\left(\frac{\pi x}{l}\right)\right]_{-l}^{l}$$

$$= -\frac{l}{6\pi}\big[\cos(3\pi) - \cos(-3\pi)\big] - \frac{l}{2\pi}\big[\cos(\pi) - \cos(-\pi)\big]$$

$$= -\frac{l}{6\pi}\big[\cos(3\pi) - \cos(3\pi)\big] - \frac{l}{2\pi}\big[\cos(\pi) - \cos(\pi)\big] = -\frac{l}{6\pi}\big[0\big] - \frac{l}{2\pi}\big[0\big] = 0.$$

$$< f_2 \,|\, f_1 > \;\rightarrow\; \int f_2^{*}\,(x)\, f_1\,(x)\, dx \;=\; \int_{-l}^{l} \sin\left(\frac{2\pi x}{l}\right) \cos\left(\frac{\pi x}{l}\right)\, dx$$

$$= \int_{-l}^{l} \cos\left(\frac{\pi x}{l}\right) \sin\left(\frac{2\pi x}{l}\right)\, dx \;=\; < f_1 \,|\, f_2 > \;=\; 0\,,$$

therefore, the given f_i are orthogonal.

Postscript: This calculation could have been shortened by noticing that both $< f_1 \,|\, f_1 >$ and $< f_2 \,|\, f_2 >$ are even functions between symmetric limits, and that $< f_1 \,|\, f_2 >$ and $< f_2 \,|\, f_1 >$ are odd functions between symmetric limits. Notice that even with only two functions of elementary sines and cosines, demonstrating orthogonality for a continuous system is a non-trivial calculation.

Any vectors that are orthogonal can be made orthonormal by the process of normalization. The same is true of any functions that are orthogonal.

5–3. (a) Show that

$\psi_n(x) \;=\; \cos\left(\frac{n\pi x}{l}\right)$ and $\psi_m(x) \;=\; \sin\left(\frac{m\pi x}{l}\right)$ are orthogonal on the interval $-l \,<\, x \,<\, l\,.$

(b) Orthonormalize $\psi_n(x)$ and $\psi_m(x)\,.$

Cosines, sines, and orthogonality are intrinsic to the discussion of Fourier series that follows, and these wave functions are encountered while addressing the infinite square well, orbital angular momentum, and elsewhere. A substantial portion of the reason that sines and cosines are useful in quantum mechanics is the property of orthonormality addressed in part (b).

To show orthogonality for part (a), find that the inner product of each wave function with itself is non-zero, *i.e.*, $< \psi_n \,|\, \psi_n > \;\neq\; 0$ and $< \psi_m \,|\, \psi_m > \neq\; 0$. Then show that

$$< \psi_{n_i} \,|\, \psi_{n_j} > \;=\; < \psi_{m_i} \,|\, \psi_{m_j} > \;=\; < \psi_n \,|\, \psi_m > \;=\; 0\,.$$

Here are some indefinite integrals from Gradshteyn and Ryzhik,

$$\int (\cos\, ax)\,(\cos\, bx)\, dx \;=\; \frac{\sin\,(a-b)\,x}{2\,(a-b)} \;+\; \frac{\sin\,(a+b)\,x}{2\,(a+b)}\,, \qquad a^2 \;\neq\; b^2\,,$$

$$\int (\sin\, ax)\,(\sin\, bx)\, dx \;=\; \frac{\sin\,(a-b)\,x}{2\,(a-b)} \;-\; \frac{\sin\,(a+b)\,x}{2\,(a+b)}\,, \qquad a^2 \;\neq\; b^2\,,$$

$$\int (\sin\, ax)\,(\cos\, bx)\, dx \;=\; -\frac{\cos\,(a-b)\,x}{2\,(a-b)} \;-\; \frac{\cos\,(a+b)\,x}{2\,(a+b)}\,, \qquad a^2 \;\neq\; b^2\,.$$

The appropriate limits on these integrals are $-l$ and $l\,.$ Indices are used only to enumerate eigenstates, thus, all n and m are positive integers. Also remember that cosine is an even function and sine is an odd function.

$$
\begin{aligned}
<\psi_n\,|\,\psi_n> \;&=\; \int_{-l}^{l}\Big(\cos\Big(\frac{n\pi x}{l}\Big)\Big)^*\Big(\cos\Big(\frac{n\pi x}{l}\Big)\Big)\,dx \;=\; \int_{-l}^{l}\cos^2\Big(\frac{n\pi x}{l}\Big)\,dx \\
&=\; \Big[\frac{x}{2}\;+\;\frac{l}{4n\pi}\sin\frac{2n\pi x}{l}\Big]_{-l}^{l} \;=\; \frac{l}{2}\;-\;\frac{-l}{2}\;+\;\frac{l}{4n\pi}\sin\frac{2n\pi l}{l}\;-\;\frac{l}{4n\pi}\sin\frac{-2n\pi l}{l} \\
&=\; l\;+\;\frac{l}{4n\pi}\Big(\sin 2n\pi+\sin 2n\pi\Big) \;=\; l\;+\;\frac{l}{2n\pi}\not{\sin}\,2n\pi \;=\; l\;\neq\;0\,,
\end{aligned}
$$

where the sine is struck because the sine of any integral multiple of π is zero. Similarly

$$
\begin{aligned}
<\psi_m\,|\,\psi_m> \;&=\; \int_{-l}^{l}\Big(\sin\Big(\frac{m\pi x}{l}\Big)\Big)^*\Big(\sin\Big(\frac{m\pi x}{l}\Big)\Big)\,dx \;=\; \int_{-l}^{l}\sin^2\Big(\frac{m\pi x}{l}\Big)\,dx \\
&=\; \Big[\frac{x}{2}\;-\;\frac{l}{4m\pi}\sin\frac{2m\pi x}{l}\Big]_{-l}^{l} \;=\; \frac{l}{2}\;-\;\frac{-l}{2}\;-\;\frac{l}{4m\pi}\sin\frac{2m\pi l}{l}\;+\;\frac{l}{4m\pi}\sin\frac{-2m\pi l}{l} \\
&=\; l\;-\;\frac{l}{4m\pi}\Big(\sin 2m\pi+\sin 2m\pi\Big) \;=\; l\;-\;\frac{l}{2m\pi}\not{\sin}\,2m\pi \;=\; l\;\neq\;0\,.
\end{aligned}
$$

Conjugation is cosmetic when functions are real so is hereafter suppressed. Then

$$
\begin{aligned}
<\psi_{n_i}\,|\,\psi_{n_j}> \;&=\; \int_{-l}^{l}\Big(\cos\;\frac{n_i\pi x}{l}\Big)\Big(\cos\;\frac{n_j\pi x}{l}\Big)\;dx \\
&=\; \left[\;\frac{\sin\Big(\frac{n_i\pi x}{l}-\frac{n_j\pi x}{l}\Big)}{2\Big(\frac{n_i\pi}{l}-\frac{n_j\pi}{l}\Big)}\;+\;\frac{\sin\Big(\frac{n_i\pi x}{l}+\frac{n_j\pi x}{l}\Big)}{2\Big(\frac{n_i\pi}{l}+\frac{n_j\pi}{l}\Big)}\;\right]_{-l}^{l}
\end{aligned}
$$

$$
=\;\frac{l}{2\pi}\frac{\sin\left(n_i-n_j\right)\pi}{\left(n_i-n_j\right)}\;-\;\frac{l}{2\pi}\frac{\sin\left(-n_i+n_j\right)\pi}{\left(n_i-n_j\right)}\;+\;\frac{l}{2\pi}\frac{\sin\left(n_i+n_j\right)\pi}{\left(n_i+n_j\right)}\;-\;\frac{l}{2\pi}\frac{\sin\left(-n_i-n_j\right)\pi}{\left(n_i+n_j\right)}\,.
$$

Remember that $n_i \neq n_j$, because the case $n_i = n_j = n$ is covered by $<\psi_n\,|\,\psi_n>$. The arguments of all the sine functions are sums and differences of integers times π, so are integral multiples of π. The numerators of all terms are therefore zero, so $<\psi_{n_i}\,|\,\psi_{n_j}> \;=\; 0$. Next

$$
\begin{aligned}
<\psi_{m_i}\,|\,\psi_{m_j}> \;&=\int_{-l}^{l}\Big(\sin\;\frac{m_i\pi x}{l}\Big)\Big(\sin\;\frac{m_j\pi x}{l}\Big)\;dx \\
&=\; \left[\;\frac{\sin\Big(\frac{m_i\pi x}{l}-\frac{m_j\pi x}{l}\Big)}{2\Big(\frac{m_i\pi}{l}-\frac{m_j\pi}{l}\Big)}\;-\;\frac{\sin\Big(\frac{m_i\pi x}{l}+\frac{m_j\pi x}{l}\Big)}{2\Big(\frac{m_i\pi}{l}+\frac{m_j\pi}{l}\Big)}\;\right]_{-l}^{l}
\end{aligned}
$$

$$
=\;\frac{l}{2\pi}\frac{\sin\left(m_i-m_j\right)\pi}{\left(m_i-m_j\right)}\;-\;\frac{l}{2\pi}\frac{\sin\left(-m_i+m_j\right)\pi}{\left(m_i-m_j\right)}\;-\;\frac{l}{2\pi}\frac{\sin\left(m_i+m_j\right)\pi}{\left(m_i+m_j\right)}\;+\;\frac{l}{2\pi}\frac{\sin\left(-m_i-m_j\right)\pi}{\left(m_i+m_j\right)}\,.
$$

Again, $m_i \neq m_j$, because the case $m_i = m_j = m$ is addressed by $<\psi_m\,|\,\psi_m>$. Again, the arguments of all the sine functions are sums and differences of integers times π, so are integral

multiples of π. The numerators of all terms are again zero, so $<\psi_{m_i}\,|\,\psi_{m_j}> \;=\; 0$. Then

$$<\psi_m\,|\,\psi_n> \;=\; \int_{-l}^{l}\left(\sin\,\frac{m\pi x}{l}\right)\left(\cos\,\frac{n\pi x}{l}\right)\,dx$$

$$=\;\left[\,-\frac{\cos\left(\dfrac{m\pi x}{l}-\dfrac{n\pi x}{l}\right)}{2\left(\dfrac{m\pi}{l}-\dfrac{n\pi}{l}\right)}\;-\;\frac{\cos\left(\dfrac{m\pi x}{l}+\dfrac{n\pi x}{l}\right)}{2\left(\dfrac{m\pi}{l}+\dfrac{n\pi}{l}\right)}\,\right]_{-l}^{l}$$

$$=\;-\frac{l}{2\pi}\frac{\cos\,(m-n)\,\pi}{(m-n)}\;+\;\frac{l}{2\pi}\frac{\cos\,(-m+n)\,\pi}{(m-n)}\;-\;\frac{l}{2\pi}\frac{\cos\,(m+n)\,\pi}{(m+n)}\;+\;\frac{l}{2\pi}\frac{\cos\,(-m-n)\,\pi}{(m+n)}\,.$$

Cosine is an even function, so

$$\cos\,(-m+n)\,\pi \;=\; \cos\,(m-n)\,\pi \qquad \text{and} \qquad \cos\,(-m-n)\,\pi \;=\; \cos\,(m+n)\,\pi\,.$$

Substituting in the last line,

$$<\psi_m\,|\,\psi_n> \;=\; -\frac{l}{2\pi}\frac{\cos\,(m-n)\,\pi}{(m-n)}\;+\;\frac{l}{2\pi}\frac{\cos\,(m-n)\,\pi}{(m-n)}\;-\;\frac{l}{2\pi}\frac{\cos\,(m+n)\,\pi}{(m+n)}\;+\;\frac{l}{2\pi}\frac{\cos\,(m+n)\,\pi}{(m+n)}\,,$$

where the first and second terms are identical except they have opposite signs so sum to zero. Similarly, the third and fourth terms sum to zero, so $<\psi_m\,|\,\psi_n> \;=\; 0, \quad m \;\neq\; n$. For the case $m \;=\; n$, let $m \;=\; n \;=\; k$

$$<\psi_k\,|\,\psi_k> \;=\; \int_{-l}^{l}\left(\sin\,\frac{k\pi x}{l}\right)\left(\cos\,\frac{k\pi x}{l}\right)\,dx \;=\; \frac{l}{2k\pi}\,\sin^2\,\frac{k\pi x}{l}\Bigg|_{-l}^{l}$$

$$=\;\frac{l}{2k\pi}\,\left(\sin^2\,k\pi-\sin^2\,(-k\pi)\right) \;=\; \frac{l}{2k\pi}\,\left(\sin^2\,k\pi-\sin^2\,k\pi\right) \;=\; 0$$

since $\sin^2$ is an even function. Also, the sine of an integral multiple of π is zero so the squares of integral multiples of π are zero. This exhausts all possibilities for indices that are positive integers. Therefore,

$\psi_n\,(x) \;=\; \cos\left(\dfrac{n\pi x}{l}\right)$ and $\psi_m(x) \;=\; \sin\left(\dfrac{m\pi x}{l}\right)$ are orthogonal on the interval $-l \;<\; x \;<\; l$.

(b) The first two calculations found $<\psi_n\,|\,\psi_n> \;=\; <\psi_m\,|\,\psi_m> \;=\; l$, so

$$<\psi_n\,|\,\mathrm{A}^*\,\mathrm{A}\,|\,\psi_n> \;=\; \left|\,\mathrm{A}\,\right|^2\,<\psi_n\,|\,\psi_n> \;=\; \left|\,\mathrm{A}\,\right|^2 l \;=\; 1 \qquad \Rightarrow \qquad \mathrm{A} \;=\; \frac{1}{\sqrt{l}}$$

$$\Rightarrow \qquad \psi_n(x) \;=\; \frac{1}{\sqrt{l}}\,\cos\left(\frac{n\pi x}{l}\right) \qquad \text{and} \qquad \psi_m(x) \;=\; \frac{1}{\sqrt{l}}\,\sin\left(\frac{n\pi x}{l}\right)$$

are orthonormal on the interval $-l \;<\; x \;<\; l$.

5–4. Show that the Hermite functions associated with the Hermite polynomials $H_1(x) = 2x$ and $H_2(x) = 4x^2 - 2$ are orthogonal.

Orthonormal expressions are obtained through the process of normalization from any system that is orthogonal. The property of orthogonality is a sufficient condition to obtain orthonormality.

Hermite polynomials are solutions to **Hermite's equation**

$$H'' - 2x\,H' + 2\alpha\,H = 0\,, \qquad H = H(x)\,, \qquad \text{and} \qquad \alpha = \text{constant}\,.$$

Hermite polynomials are not themselves orthogonal, however, **Hermite functions** of the form $H_n(x)\,e^{-x^2/2}$ are orthogonal. Hermite functions are used to describe the quantum mechanical simple harmonic oscillator (SHO) in chapter 10.

To demonstrate orthogonality, show $< H_n \,|\, H_m > = \delta_{nm}$ is possible. The integrals

$$\int_{-\infty}^{\infty} e^{-p^2x^2 \pm qx} dx = \exp\left(\frac{q^2}{4p^2}\right)\frac{\sqrt{\pi}}{p}\,, \qquad p > 0\,,$$

form 3.323.2 from Gradshteyn and Ryzhik, and

$$\int_0^{\infty} x^{2n}\, e^{-px^2} dx = \frac{(2n-1)!!}{2\,(2p)^n}\sqrt{\frac{\pi}{p}}\,, \qquad p > 0\,, \quad n = 0\,,1\,,2\,,\ldots$$

form 3.461.2 from Gradshteyn and Ryzhik, are helpful. Arguments about even/odd integrands between symmetric limits are necessary.

$$\begin{aligned} < H_1 \,|\, H_1 > &= \int_{-\infty}^{\infty} 2x\, e^{-x^2/2}\, 2x\, e^{-x^2/2}\, dx = 4\int_{-\infty}^{\infty} x^2\, e^{-x^2}\, dx = 8\int_0^{\infty} x^2\, e^{-x^2}\, dx \\ &= 8\,\frac{(2\cdot 1-1)!!}{2\,(2\cdot 1)^1}\sqrt{\frac{\pi}{1}} = 8\,\frac{1!!}{4}\,\sqrt{\pi} = 2\sqrt{\pi} \neq 0\,. \end{aligned}$$

$$\begin{aligned} < H_2 \,|\, H_2 > &= \int_{-\infty}^{\infty} \left(4x^2-2\right) e^{-x^2/2}\left(4x^2-2\right) e^{-x^2/2}\, dx = \int_{-\infty}^{\infty} \left(16x^4 - 16x^2 + 4\right) e^{-x^2}\, dx \\ &= 16\int_{-\infty}^{\infty} x^4 e^{-x^2}\, dx - 16\int_{-\infty}^{\infty} x^2 e^{-x^2}\, dx + 4\int_{-\infty}^{\infty} e^{-x^2}\, dx \\ &= 32\int_0^{\infty} x^4 e^{-x^2}\, dx - 32\int_0^{\infty} x^2 e^{-x^2}\, dx + 8\,e^0\,\frac{\sqrt{\pi}}{1} \end{aligned}$$

$$= 32\,\frac{(2\cdot 2-1)!!}{2\,(2\cdot 1)^2}\sqrt{\frac{\pi}{1}} - 32\,\frac{\sqrt{\pi}}{4} + 8\sqrt{\pi} = 32\,\frac{3\,!!}{8}\,\sqrt{\pi} - 8\sqrt{\pi} + 8\sqrt{\pi} = 12\sqrt{\pi} \neq 0\,.$$

$$\begin{aligned} < H_1 \,|\, H_2 > &= \int_{-\infty}^{\infty} 2x\, e^{-x^2/2}\left(4x^2-2\right) e^{-x^2/2}\, dx = \int_{-\infty}^{\infty} \left(8x^3 - 4x\right) e^{-x^2}\, dx \\ &= 8\int_{-\infty}^{\infty} x^3\, e^{-x^2}\, dx - 4\int_{-\infty}^{\infty} x\, e^{-x^2}\, dx = 0 - 0 = 0\,, \end{aligned}$$

because both integrals are odd functions between symmetric limits. This is identical to $< H_2 \,|\, H_1 >$ so we conclude H_1 and H_2 are orthogonal.

Postscript: This is a calculation for two specific Hermite functions. Hermite functions are orthogonal in general, so can be made orthonormal, meaning

$$|\, A \,|^2 \int_{-\infty}^{\infty} H_n\,(x)\; e^{-x^2/\,2}\, H_m\,(x)\, e^{-x^2/\,2}\, dx \;=\; \delta_{n,m}.$$

This calculation is done in Byron and Fuller[1], and other texts.

There is no formal definition of **special functions**. Special functions are simply those that are commonly encountered and/or have importance in specific applications. Trigonometric functions, exponentials, and logarithms are considered special functions. The designation also applies to a number of functions that arise from polynomial and trigonometric solutions to commonly encountered differential equations. The Schrodinger equation when expressed for specific $V\,(x)$ often results in a recognizable differential equation, such as Hermite's equation, Legendre's equation, Laplace's equation, and Laguerre's equation, whose solutions are considered special functions.

The polynomial and trigonometric solutions to these differential equations are not generally orthogonal. Appending a **weighting function**, for instance $e^{-x^2/2}$ in the case of Hermite polynomials, can create a family of orthogonal functions. Another strategy is to limit the functions to an interval as is done for sines and cosines in problem 5–3. For any strategy, if a family of functions is orthogonal, it can be made orthonormal.

5–5. Represent (a) $x^2 + 3x\,,$ (b) $2x^3 - 4x^2 + 7\,,$ and (c) $8x^4 - 5x^2 - 4x$ as unique linear combinations of Hermite polynomials.

A general state vector is the superposition or linear combination of all eigenstates,

$$|\,\Psi> \;=\; c_1\,|\,\psi_1> \;+\; c_2\,|\,\psi_2> \;+\; c_3\,|\,\psi_3> \;+\; \cdots \;+\; c_n\,|\,\psi_n> \;=\; \sum_{i=1}^{n} c_i\,|\,\psi_i>$$

where n can be any integer or infinity. For instance, $|\,\Psi> \;=\; c_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \;+\; c_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \;+\; c_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ is a typical representation for a state vector in $\mathbb{C}^3$. The Schrodinger equation in position space for an SHO is a form of Hermite's differential equation with the polynomial solutions

$$f\,(x) \;=\; c_0\,H_0\,(x) \;+\; c_1\,H_1\,(x) \;+\; c_2\,H_3\,(x) \;+\; \cdots \;+\; c_n\,H_n\,(x) \;=\; \sum_{i=0}^{n} c_i\,H_n\,(x)\,.$$

[1] Byron and Fuller *Mathematics of Classical and Quantum Physics* (Dover Publications, New York, 1970), pp 261-273.

These are unique and span polynomial space. In other words, any polynomial can be created from a linear combination of Hermite polynomials for which there is exactly one representation. A method for expressing polynomials in terms of Hermite polynomials is the point of this problem.

The first few Hermite polynomials are

$$\begin{aligned} H_0(x) &= 1 \\ H_1(x) &= 2x \\ H_2(x) &= 4x^2 - 2 \\ H_3(x) &= 8x^3 - 12x \\ H_4(x) &= 16x^4 - 48x^2 + 12 \end{aligned}$$

Table $5-1$. The First Five Hermite Polynomials.

Addressing powers of decreasing degree, for part (a) $f(x) = x^2 + 3x$,

$$H_2 = 4x^2 - 2 \quad \Rightarrow \quad 4x^2 = H_2 + 2 \quad \Rightarrow \quad x^2 = \frac{1}{4}H_2 + \frac{1}{2}$$

so the partial representation is

$$f(x) = \frac{1}{4}H_2 + 3x + \frac{1}{2}. \quad \text{Then}$$

$$H_1 = 2x \quad \Rightarrow \quad 3x = \frac{3}{2}H_1 \quad \Rightarrow \quad f(x) = \frac{1}{4}H_2 + \frac{3}{2}H_1 + \frac{1}{2}H_0.$$

(b) $H_3 = 8x^3 - 12x \Rightarrow 8x^3 = H_3 + 12x \Rightarrow 2x^3 = \frac{1}{4}H_3 + 3x \Rightarrow f(x) = \frac{1}{4}H_3 - 4x^2 + 3x + 7$

$H_2 = 4x^2 - 2 \Rightarrow 4x^2 = H_2 + 2 \Rightarrow -4x^2 = -H_2 - 2 \Rightarrow f(x) = \frac{1}{4}H_3 - H_2 + 3x + 5$

$$H_1 = 2x \quad \Rightarrow \quad 3x = \frac{3}{2}H_1 \quad \Rightarrow \quad f(x) = \frac{1}{4}H_3 - H_2 + \frac{3}{2}H_1 + 5H_0.$$

(c) $H_4 = 16x^4 - 48x^2 + 12 \quad \Rightarrow \quad 16x^4 = H_4 + 48x^2 - 12 \quad \Rightarrow \quad 8x^4 = \frac{1}{2}H_4 + 24x^2 - 6$

$$\Rightarrow \quad f(x) = \frac{1}{2}H_4 + 19x^2 - 4x - 6,$$

$$H_2 = 4x^2 - 2 \quad \Rightarrow \quad 4x^2 = H_2 + 2 \quad \Rightarrow \quad 19x^2 = \frac{19}{4}H_2 + \frac{19}{2}$$

$$f(x) = \frac{1}{2}H_4 + \frac{19}{4}H_2 - 4x + \frac{7}{2}.$$

$$H_1 = 2x \quad \Rightarrow \quad -4x = -2H_1 \quad \Rightarrow \quad f(x) = \frac{1}{2}H_4 + \frac{19}{4}H_2 - 2H_1 + \frac{7}{2}H_0.$$

5–6. Represent (a) x^2+3x, (b) $2x^3-4x^2+7$, and (c) $8x^4-5x^2-4x$ as unique linear combinations of Laguerre polynomials.

This is a second example representing the same three polynomials as linear combinations of Laguerre polynomials so that

$$f(x) \;=\; c_0\,L_0(x) \;+\; c_1\,L_1(x) \;+\; c_2\,L_3(x) \;+\; \cdots \;+\; c_n\,L_n(x) \;=\; \sum_{i=0}^{n} c_i\,L_n(x)\,.$$

The resulting linear combination is unique, and Laguerre polynomials span polynomial space.

The first few Laguerre polynomials are listed in table 5–2.

$$\begin{aligned} L_0(x) &= 1 \\ L_1(x) &= -x+1 \\ L_2(x) &= x^2-4x+2 \\ L_3(x) &= -x^3+9x^2-18x+6 \\ L_4(x) &= x^4-16x^3+72x^2-96x+24 \end{aligned}$$

Table $5-2$. The First Five Laguerre Polynomials.

(a) $f(x) = x^2+3x$: $L_2 = x^2-4x+2 \;\Rightarrow\; x^2 = L_2+4x-2 \;\Rightarrow\; f(x) = L_2+7x-2$

$L_1 = -x+1 \;\Rightarrow\; x = -L_1+1 \;\Rightarrow\; 7x = -7L_1+7 \;\Rightarrow\; f(x) = L_2-7L_1+5L_0\,.$

(b) $f(x) = 2x^3-4x^2+7$: $L_3 = -x^3+9x^2-18x+6 \;\Rightarrow\; x^3 = -L_3+9x^2-18x+6$

$$\Rightarrow\quad 2x^3 = -2L_3+18x^2-36x+12 \quad\Rightarrow\quad f(x) = -2L_3+14x^2-36x+19\,.$$

$$L_2 = x^2-4x+2 \quad\Rightarrow\quad x^2 = L_2+4x-2 \quad\Rightarrow\quad 14x^2 = 14L_2+56x-28$$

$$\Rightarrow\quad f(x) = -2L_3+14L_2+20x-9$$

$$L_1 = -x+1 \quad\Rightarrow\quad x = -L_1+1 \quad\Rightarrow\quad f(x) = -2L_3+14L_2-20L_1+11L_0\,.$$

(c) $f(x) = 8x^4-5x^2-4x$: $L_4 = x^4-16x^3+72x^2-96x+24 \;\Rightarrow\; x^4 = L_4+16x^3-72x^2+96x-24$

$\Rightarrow\quad 8x^4 = 8L_4+128x^3-576x^2+768x-192 \quad\Rightarrow\quad f(x) = 8L_4+128x^3-581x^2+764x-192$

$L_3 = -x^3+9x^2-18x+6 \;\Rightarrow\; x^3 = -L_3+9x^2-18x+6 \;\Rightarrow\; 128x^3 = -128L_3+1152x^2-2304x+768$

$$\Rightarrow\quad f(x) = 8L_4-128L_3+571x^2-1540x+576$$

$$L_2 = x^2-4x+2 \quad\Rightarrow\quad x^2 = L_2+4x-2 \quad\Rightarrow\quad 571x^2 = 571L_2+2284x-1142$$

$$\Rightarrow\quad f(x) = 8L_4-128L_3+571L_2+744x-566$$

$L_1 = -x+1 \quad\Rightarrow\quad 744x = -774L_1+744 \quad\Rightarrow\quad f(x) = 8L_4-128L_3+571L_2-744L_1+178L_0\,.$

Postscript: There are infinite Hermite and Laguerre polynomials, though only five of each are listed in tables 5–1 and 5–2. Hermite and Laguerre polynomials for any n may be generated using

$$H_n(x) \;=\; (-1)^n e^{x^2}\,\frac{d^n}{dx^n}\,e^{-x^2} \qquad \text{and} \qquad L_n(x) \;=\; e^x\,\frac{d^n}{dx^n}\,e^{-x}x^n\,.$$

The index n on both the H_n and L_n corresponds to the highest power of the independent variable. This guarantees the uniqueness of the final expression of a polynomial function in terms of H_n or L_n because there is exactly one way to represent the highest power term of any given polynomial function. Hermite and Laguerre polynomials span the space of polynomials functions. Either family can be used as a basis for polynomial functions.

Hermite polynomials are not themselves orthogonal. Hermite functions of the form $H_n\,e^{-x^2/2}$ are orthogonal. Writing part (a) of problem 5–5 as

$$h(x) \;=\; f(x)\,e^{-x^2/2} \;=\; \left(x^2+3x\right)e^{-x^2/2} \qquad \Rightarrow \qquad h(x) \;=\; \left(\frac{1}{4}\,H_2+\frac{3}{2}\,H_1+\frac{1}{2}\,H_0\right)e^{-x^2/2}$$

establishes that the orthogonal "building blocks" are adjusted functions. Similarly, Laguerre polynomials are not themselves orthogonal. The set of **Laguerre functions** of the form $L_n\,e^{-x/2}$ is orthogonal on the interval $0 \le x < \infty$. Writing part (a) of problem 5–6 as

$$h(x) \;=\; f(x)\,e^{-x/2} \;=\; \left(x^2+3x\right)e^{-x/2} \qquad \Rightarrow \qquad h(x) \;=\; \left(L_2-7L_1+5L_0\right)e^{-x/2}$$

accomplishes the same end for problem 5–6 (a). Laguerre polynomials are used in the solution to the radial equation of the hydrogen atom.

$$\text{Notice} \qquad |\,\Psi> \;=\; c_1\begin{pmatrix}1\\0\\0\end{pmatrix} \;+\; c_2\begin{pmatrix}0\\1\\0\end{pmatrix} \;+\; c_3\begin{pmatrix}0\\0\\1\end{pmatrix}\,, \qquad f(x) \;=\; \frac{1}{4}\,H_2 \;+\; \frac{3}{2}\,H_1 \;+\; \frac{1}{2}\,H_0\,,$$

$f(x) \;=\; L_2 \;-\; 7L_1 \;+\; 5L_0\,,$ are all linear combinations of basis vectors/basis functions.

A Gaussian envelope for H_n, or something like it such as the decreasing exponential on the interval $0 \le x < \infty$ for L_n, is required to make polynomials square integrable.

5–7. What is the meaning of Hermiticity for a continuous system?

An observable quantity is represented by a Hermitian operator per the observables postulate. Hermiticity for a continuous system means

$$\int_{-\infty}^{\infty}\psi_1^*(x)\,\mathcal{A}\,\psi_2(x)\,dx \;\;=\;\; \int_{-\infty}^{\infty}\psi_2(x)\,\mathcal{A}^*\,\psi_1^*(x)\,dx\,.$$

The definition of Hermiticity is $\mathcal{A} \;=\; \mathcal{A}^\dagger$. Remember that $\mathcal{A}^\dagger \;=\; \mathcal{A}^{\mathrm{T}\,*}$. The transpose in continuous space means that the operator acts to the left, or that $\psi_i(x)\,\mathcal{A}^{\mathrm{T}} \;=\; \mathcal{A}\,\psi_i(x)$.

$$\int_{-\infty}^{\infty}\psi_1^*(x)\,\mathcal{A}\,\psi_2(x)\,dx \;\;=\;\; \int_{-\infty}^{\infty}\psi_1^*(x)\,\mathcal{A}^\dagger\,\psi_2(x)\,dx \;\;=\;\; \int_{-\infty}^{\infty}\psi_1^*(x)\,\mathcal{A}^{\mathrm{T}\,*}\,\psi_2(x)\,dx$$

$$=\;\; \int_{-\infty}^{\infty}\left(\mathcal{A}^*\,\psi_1^*(x)\right)\psi_2(x)\,dx \;\;=\;\; \int_{-\infty}^{\infty}\psi_2(x)\left(\mathcal{A}^*\,\psi_1^*(x)\right)dx \;\;=\;\; \int_{-\infty}^{\infty}\psi_2(x)\,\mathcal{A}^*\,\psi_1^*(x)\,dx\,.$$

5–8. Show that the momentum operator in position space, $\mathcal{P}_x = -i\hbar\,\dfrac{d}{dx}$, is Hermitian.

An observable quantity, such as linear momentum, must be represented by a Hermitian operator. Integration by parts is a common technique used to demonstrate Hermiticity for specific operators.

$$<\psi_1\,|\,\mathcal{P}_x\,|\,\psi_2> \;=\; \int_{-\infty}^{\infty}\psi_1^*\left(-i\hbar\,\frac{d}{dx}\right)\psi_2\,dx \;=\; -i\hbar\int_{-\infty}^{\infty}\psi_1^*\,\frac{d\,\psi_2}{dx}\,dx \;=\; -i\hbar\int_{-\infty}^{\infty}\psi_1^*\;d\,\psi_2$$

where the independent variable is understood to be x. Integration by parts means

$$\int u\,dv \;=\; u\,v - \int v\,du\,.\quad \text{Let}\;\; u \;=\; \psi_1^* \quad\Rightarrow\quad du \;=\; d\,\psi_1^* \;\;\text{and}\;\; dv \;=\; d\,\psi_2 \quad\Rightarrow\quad v \;=\; \psi_2$$

$$\Rightarrow\quad -i\hbar\int_{-\infty}^{\infty}\psi_1^*\,d\,\psi_2 \;=\; -i\hbar\left[\psi_1^*\,\psi_2\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\psi_2\,d\,\psi_1^*\right] \;=\; i\hbar\int_{-\infty}^{\infty}\psi_2\,d\,\psi_1^*$$

because $\psi_1^*\,\psi_2\Big|_{-\infty}^{\infty} = 0$ for ψ_i that is square integrable. Then

$$i\hbar\int_{-\infty}^{\infty}\psi_2\,d\,\psi_1^* \;=\; i\hbar\int_{-\infty}^{\infty}\psi_2\,\frac{d\,\psi_1^*}{dx}\,dx \;=\; \int_{-\infty}^{\infty}\psi_2\left(i\hbar\,\frac{d}{dx}\right)\psi_1^*\,dx \;=\; \int_{-\infty}^{\infty}\psi_2\left(-i\hbar\,\frac{d}{dx}\right)^*\psi_1^*\,dx\,.$$

Postscript: Another way to say $\psi_1^*\,\psi_2\Big|_{-\infty}^{\infty} = 0$ for ψ_i that are square integrable is that $\psi_i \to 0$ as $x \to \pm\infty$. Both wave functions must vanish as x approaches positive/negative infinity or the corresponding probability integral diverges.

In three dimensions $\mathcal{P} \;=\; \mathcal{P}_x + \mathcal{P}_y + \mathcal{P}_z \;=\; -i\hbar\left(\dfrac{\partial}{\partial x} + \dfrac{\partial}{\partial y} + \dfrac{\partial}{\partial z}\right) \;=\; -i\hbar\,\nabla\,.$

Problems 5–9 through 5–19 develop and employ the quantum mechanical Fourier transforms

$$\psi\,(x) \;=\; \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\widehat{\psi}\,(p)\,e^{ipx/\hbar}\,dp, \qquad \widehat{\psi}\,(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi\,(x)\,e^{-ipx/\hbar}\,dx$$

used to convert from the position basis to the momentum basis, or vice versa.

5–9. What is a basic Fourier series?

A **Fourier series** is a representation of a periodic function as a linear combination of all cosine and sine functions that have the same period. The periodic function $f(x) = f(x+2l)$, has a period of $2l$, or repeats itself every $2l$. In a basic Fourier series,

$$f(x) \;=\; \frac{a_0}{2} \;+\; \sum_{n=1}^{\infty} a_n \cos\left(\frac{n\pi x}{l}\right) \;+\; \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{l}\right), \qquad \text{where the coefficients are}$$

$$a_n \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\cos\left(\frac{n\pi x}{l}\right)dx, \qquad b_n \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\sin\left(\frac{n\pi x}{l}\right)dx, \qquad \text{and the period is } 2l.$$

5–10. Expand the function

$$f(x) \;=\; \begin{cases} 1 & \text{if} \quad -\pi < x < 0, \\ 0 & \text{if} \quad 0 < x < \pi, \end{cases}$$

using a basic Fourier series given that it has a period of 2π.

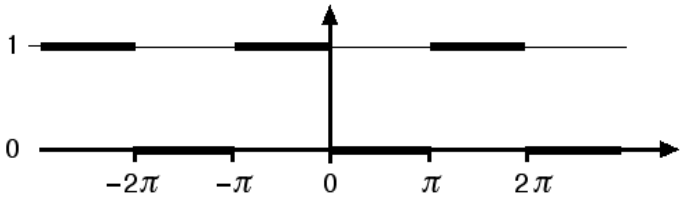

Figure 5–1. Sketch of given $f(x)$.

An example attempting to convey the meaning of problem 5–9 is warranted.

First addressing a_n,

$$\begin{aligned} a_n \;&=\; \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos\left(\frac{n\pi x}{\pi}\right)dx \;=\; \frac{1}{\pi}\left[\int_{-\pi}^{0} 1\cdot\cos(nx)\,dx \;+\; \int_{0}^{\pi} 0\cdot\cos(nx)\,dx\right] \\ &=\; \frac{1}{\pi}\int_{-\pi}^{0}\cos(nx)\,dx, \end{aligned}$$

$$n = 0 \;\Rightarrow\; a_0 \;=\; \frac{1}{\pi}\int_{-\pi}^{0}\cos(0)\,dx \;=\; \frac{1}{\pi}\int_{-\pi}^{0} dx \;=\; \frac{1}{\pi}\,x\Big|_{-\pi}^{0} = \frac{1}{\pi}\left(0 - -\pi\right) \;=\; 1,$$

$$n > 0 \;\Rightarrow\; a_n \;=\; \frac{1}{n\pi}\sin(nx)\Big|_{-\pi}^{0} \;=\; \frac{1}{n\pi}\left[\sin(n\cdot 0) \;-\; \sin(-n\pi)\right] \;=\; \frac{1}{n\pi}\left[0-0\right] \;=\; 0.$$

Then for b_n,

$$\begin{aligned} b_n \;&=\; \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin\left(\frac{n\pi x}{\pi}\right)dx \;=\; \frac{1}{\pi}\left[\int_{-\pi}^{0} 1\cdot\sin(nx)\,dx \;+\; \int_{0}^{\pi} 0\cdot\sin(nx)\,dx\right] \\ &=\; \frac{1}{\pi}\int_{-\pi}^{0}\sin(nx)\,dx, \end{aligned}$$

$$\begin{aligned} n > 0 \;\Rightarrow\; b_n \;&=\; \frac{1}{n\pi}\left[-\cos(nx)\right]_{-\pi}^{0} \;=\; \frac{1}{n\pi}\left[-\cos(0) \;+\; \cos(-n\pi)\right] \\ &=\; \frac{1}{n\pi}\left[-1+\cos(n\pi)\right] \;=\; \begin{cases} 0 & \text{if} \quad n \;\text{ even} \\ -\dfrac{2}{n\pi} & \text{if} \quad n \;\text{ odd} \end{cases} \end{aligned}$$

The function can then be expressed

$$f(x) \;=\; \frac{1}{2} - \sum_{n\ \text{odd}}^{\infty} \frac{2}{n\pi} \sin(nx) \;=\; \frac{1}{2} - \frac{2}{\pi}\left(\frac{\sin(x)}{1} \;+\; \frac{\sin(3x)}{3} \;+\; \frac{\sin(5x)}{5} \;+\; \frac{\sin(7x)}{7} \;+\; \cdots\right).$$

The function can be approximated to arbitrary precision with partial sums. Convergence toward figure 5–1 can be seen in the following figures for $n = 5$, $n = 15$, $n = 25$, and $n = 35$.

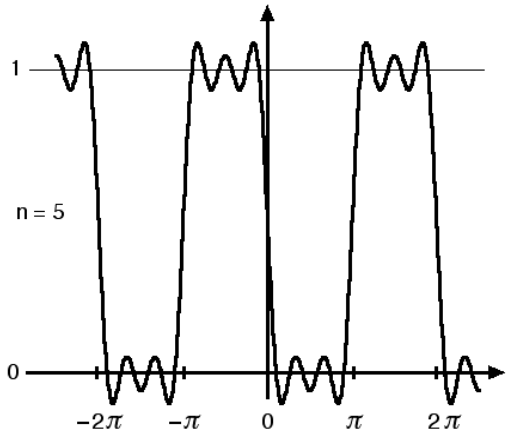

Figure 5–2 (a). $f(x)$ for $n = 5$.

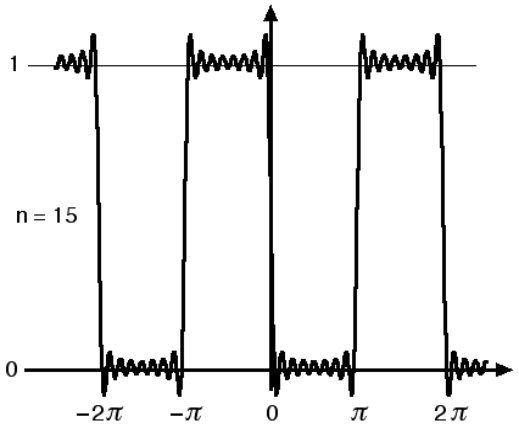

Figure 5–2 (b). $f(x)$ for $n = 15$.

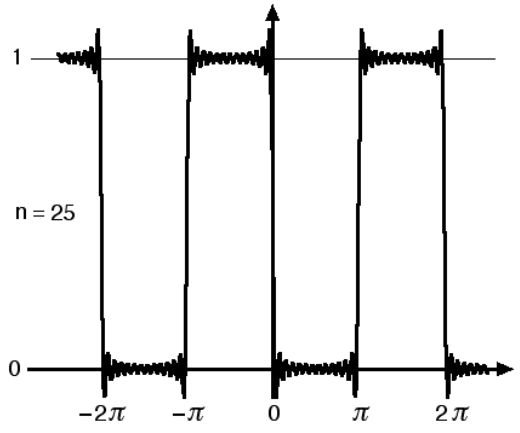

Figure 5–2 (c). $f(x)$ for $n = 25$.

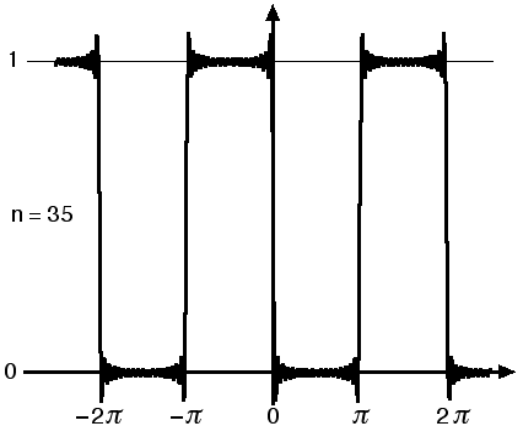

Figure 5–2 (d). $f(x)$ for $n = 35$.

5–11. Show for a basic Fourier series if indices of $n < 0$ were to apply,

(a) $a_{-n} \;=\; a_n$, and that $a_0 \;=\; \dfrac{1}{l}\displaystyle\int_{-l}^{l} f(x)\,dx$, and

(b) $b_{-n} \;=\; -b_n$, and that $b_0 \;=\; 0$.

The basic Fourier series is limited to $n \geq 0$. This problem removes this constraint. Use the defining integrals for a_n and b_n. Remember $\cos(-x) = \cos(x)$ and $\sin(-x) = -\sin(x)$.

(a) $$a_{-n} \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\,\cos\left(\frac{-n\pi x}{l}\right)\,dx \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\,\cos\left(\frac{n\pi x}{l}\right)\,dx \;=\; a_n\,,$$

$$\text{and} \qquad a_0 \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\,\cos(0)\,dx \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\,dx\,.$$

(b) $$b_{-n} \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\,\sin\left(\frac{-n\pi x}{l}\right)\,dx \;=\; -\frac{1}{l}\int_{-l}^{l} f(x)\,\sin\left(\frac{n\pi x}{l}\right)\,dx \;=\; -b_n\,,$$

$$\text{and} \qquad b_0 \;=\; \frac{1}{l}\int_{-l}^{l} f(x)\,\sin(0)\,dx \;=\; 0\,.$$

5–12. Express the c_n that are the coefficients of the exponential format of the Fourier series in terms of the basic Fourier coefficients a_n and b_n, and show that $c_0 = a_0/2$.

The Fourier series in an exponential format for a function that is periodic over the length $2l$ is

$$f(x) \;=\; \sum_{-\infty}^{\infty} c_n\,e^{in\pi x/l}, \qquad \text{where} \qquad c_n \;=\; \frac{1}{2l}\int_{-l}^{l} f(x)\,e^{-in\pi x/l}\,dx\,.$$

Notice that the lower limit of the summation is negative infinity.

$$c_n \;=\; \frac{1}{2l}\int_{-l}^{l} f(x)\,e^{-in\pi x/l}\,dx \;=\; \frac{1}{2l}\int_{-l}^{l} f(x)\left[\cos\left(\frac{n\pi x}{l}\right) \;-\; i\sin\left(\frac{n\pi x}{l}\right)\right]\,dx$$

$$=\; \frac{1}{2l}\int_{-l}^{l} f(x)\,\cos\left(\frac{n\pi x}{l}\right)\,dx \;-\; \frac{i}{2l}\int_{-l}^{l} f(x)\,\sin\left(\frac{n\pi x}{l}\right)\,dx \;=\; \frac{1}{2}\,(a_n - ib_n)\,.$$

When $n = 0$, the argument of the exponential is zero, so

$$c_0 \;=\; \frac{1}{2l}\int_{-l}^{l} f(x)\,e^{0}\,dx \;=\; \frac{1}{2l}\int_{-l}^{l} f(x)\,dx \;=\; \frac{1}{2}\,a_0\,.$$

5–13. Demonstrate the equivalence of the basic and exponential formats of a Fourier series.

Substituting previous results into the summation that defines the exponential form yields the basic Fourier series required. It is wise to divide the summation into three parts that coincide with the three cases, namely: $n < 0$ implies a summation from $-\infty$ to -1, $n = 0$ is one term of the summation, and $n > 0$ implies a summation from 1 to ∞. Switching the indices on the summation from $-\infty$ to -1 may require some reflection, but realize that

$$\sum_{-\infty}^{-1} \frac{1}{2}\,(a_n - ib_n)\,e^{in\pi x/l} \;=\; \sum_{1}^{\infty} \frac{1}{2}\,(a_n + ib_n)\,e^{-in\pi x/l}$$

because $b_{-n} = -b_n$ from problem 5–11, and the argument of the exponential that is positive for $n < 0$ is negative for $n > 0$. Remember $\cos x = \dfrac{e^{ix} + e^{-ix}}{2}$, $\sin x = \dfrac{e^{ix} - e^{-ix}}{2i}$.

For convenience, let $\theta = \pi x/l$. The summation is

$$\begin{aligned}
f(\theta) &= \sum_{-\infty}^{\infty} c_n\, e^{in\theta} = \sum_{-\infty}^{-1} \frac{1}{2}\,(a_n - ib_n)\, e^{in\theta} + \frac{1}{2}\,a_0 + \sum_{1}^{\infty} \frac{1}{2}\,(a_n - ib_n)\, e^{in\theta} \\
&= \frac{1}{2}\,a_0 + \sum_{1}^{\infty} \left(\frac{a_n}{2} + \frac{ib_n}{2} \right) e^{-in\theta} + \sum_{1}^{\infty} \left(\frac{a_n}{2} - \frac{ib_n}{2} \right) e^{in\theta} \\
&= \frac{1}{2}\,a_0 + \sum_{1}^{\infty} \left[\frac{a_n}{2}\, e^{-in\theta} + \frac{ib_n}{2} e^{-in\theta} + \frac{a_n}{2}\, e^{in\theta} - \frac{ib_n}{2} e^{in\theta} \right] \\
&= \frac{1}{2}\,a_0 + \sum_{1}^{\infty} \left[a_n \left(\frac{e^{in\theta} + e^{-in\theta}}{2} \right) + b_n \left(\frac{e^{in\theta} - e^{-in\theta}}{2i} \right) \right] \\
&= \frac{1}{2}\,a_0 + \sum_{1}^{\infty} \left(a_n \cos n\theta + b_n \sin n\theta \right)
\end{aligned}$$

which is identical to the basic Fourier series upon the substitution of $\theta = \pi x/l$.

Postscript: The exponential format of the Fourier series, also known as the **complex Fourier series**, is of interest because it is the form from which Fourier transforms are most readily obtained, and the form that is most readily generalized to the **Fourier integral**.

5–14. Derive the Fourier transforms from the complex Fourier series.

Start with the notation

$$F(y) = \sum_{-\infty}^{\infty} c_n\, e^{in\pi y/l}, \qquad \text{where} \qquad c_n = \frac{1}{2l} \int_{-l}^{l} F(y)\, e^{-in\pi y/l}\, dy\,.$$

Substitute the integral form of c_n into the summation. Symmetrize the factor of $\dfrac{1}{2l}$. This means to rearrange the summation so a factor of $\dfrac{1}{\sqrt{2l}}$ is in both the $F(y)$ and the c_n so $F(y)$ and c_n are different than originally defined. Change variables by letting

$$x = \sqrt{\frac{\pi}{l}}\, y\,. \qquad \text{Also, let} \qquad k_n = n\sqrt{\frac{\pi}{l}} \qquad \text{to find that}$$

$$\Delta k_n = \sqrt{\frac{\pi}{l}} \qquad \text{and} \qquad \frac{n\pi y}{l} = k_n x\,.$$

Let $F(y) = F\left(\sqrt{\frac{l}{\pi}}\,x\right) = f(x)$. Introduce a new symbol for the coefficients that indicates the index k_n replaces n, so $c_n \to g_{k_n}$. Finally, let $l \to \infty$, so that the Fourier transforms

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k)\,e^{ikx}\,dk \qquad \text{and} \qquad g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\,e^{-ikx}\,dx \qquad \text{are exposed.}$$

$$\begin{aligned} F(y) &= \sum_{n=-\infty}^{\infty}\left(\frac{1}{2l}\int_{-l}^{l} F(y)\,e^{-in\pi y/l}\,dy\right)e^{in\pi y/l} \\ &= \sum_{n=-\infty}^{\infty}\left(\frac{1}{\sqrt{2l}}\int_{-l}^{l} F(y)\,e^{-in\pi y/l}\,dy\right)\frac{1}{\sqrt{2l}}\,e^{in\pi y/l}\,. \end{aligned}$$

Identify a symmetrized function and coefficient as

$$F(y) = \sum_{n=-\infty}^{\infty} c_n \frac{1}{\sqrt{2l}}\,e^{in\pi y/l} \qquad \text{and} \qquad c_n = \frac{1}{\sqrt{2l}}\int_{-l}^{l} F(y)\,e^{-in\pi y/l}\,dy\,. \tag{1}$$

Change variables to

$$\sqrt{\frac{\pi}{l}}\,y = x \quad \Rightarrow \quad y = \sqrt{\frac{l}{\pi}}\,x \quad \Rightarrow \quad dy = \sqrt{\frac{l}{\pi}}\,dx\,.$$

Use

$$k_n = n\sqrt{\frac{\pi}{l}} \quad \Rightarrow \quad \Delta k_n = k_{n+1} - k_n = (n+1)\sqrt{\frac{\pi}{l}} - n\sqrt{\frac{\pi}{l}} = \sqrt{\frac{\pi}{l}}\,.$$

These substitutions allow

$$\frac{n\pi y}{l} = n\sqrt{\frac{\pi}{l}}\sqrt{\frac{\pi}{l}}\,y = k_n x\,.$$

The difference in the new index is

$$\Delta k_n = \sqrt{\frac{\pi}{l}} \quad \Rightarrow \quad \frac{\Delta k_n}{\sqrt{2\pi}} = \frac{1}{\sqrt{2l}}\,.$$

Limits on the integral are $y = l \;\Rightarrow\; x = \sqrt{\frac{\pi}{l}}\,l = \sqrt{\pi l}\,,$ and $y = -l \;\Rightarrow\; x = -\sqrt{\pi l}\,.$

Introduce a new symbol that indicates the index is now k_n vice n, so $c_n \to g_{k_n}$. Using these substitutions and developments in equation (1),

$$\begin{aligned} F(y) = F\left(\sqrt{\frac{l}{\pi}}\,x\right) &= \sum_{k_n=-\infty}^{\infty} g_{k_n}\,\frac{1}{\sqrt{2\pi}}\,e^{ik_n x}\,\Delta k_n \\ &= \frac{1}{\sqrt{2\pi}}\sum_{k_n=-\infty}^{\infty} g_{k_n}\,e^{ik_n x}\,\Delta k_n \end{aligned}$$

and

$$g_{k_n} = \frac{1}{\sqrt{2l}} \int_{-\sqrt{\pi l}}^{\sqrt{\pi l}} F\left(\sqrt{\frac{l}{\pi}}\, x\right) e^{-ik_n x} \sqrt{\frac{l}{\pi}}\, dx$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\sqrt{\pi l}}^{\sqrt{\pi l}} F\left(\sqrt{\frac{l}{\pi}}\, x\right) e^{-ik_n x}\, dx$$

Redefine $F\left(\sqrt{\frac{l}{\pi}}\, x\right) = f(x)$. Now let the period $l \to \infty \quad \Rightarrow \quad \Delta k_n = \sqrt{\frac{\pi}{l}} \to 0$. The difference between successive $k_n \to 0$ so that k_n assumes all real values and thus becomes a continuous variable. The summation over discrete k_n becomes an integral over the continuous variable k, the coefficients g_{k_n} become a continuous function $g(k)$, the difference Δk_n becomes the differential dk, and

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k)\, e^{ikx}\, dk \qquad \text{and} \qquad g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx\,.$$

5–15. Sketch the graphs of the following functions and their the Fourier transforms.

(a) $f(x) = \begin{cases} 1\,, & -a < x < a\,, \\ 0\,, & \text{elsewhere, and} \end{cases}$

(b) $h(x) = \begin{cases} 1/2\,, & -b < x < b\,, \\ 0\,, & \text{elsewhere, where} \quad b = 2a\,. \end{cases}$

(c) Comment on the similarities and differences between the two Fourier transforms.

The functions given for parts (a) and (b) are constants for specified intervals and zero elsewhere which means to find $g(k)$ for part (a) and $j(k)$ for part (b) by integrating between $-a$ and a, and $-b$ and b instead of using infinite limits. Express the answer for part (b) in terms of the constant a and look for relations between the graphs of parts (a) and (b). This problem uses constant functions which are among the easiest functions to integrate both as an appropriate place to start and to highlight relations between parts (a) and (b). Remember

$$\sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}$$

from Euler's equation. For part (c), notice that $f(x)$ and $h(x)$ have the same basic rectangular shape and the same area. The function $h(x)$ is wider than $f(x)$. What impact does this have on the Fourier transforms?

(a)
$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx = \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} 1 \cdot e^{-ikx}\, dx$$
$$= \frac{1}{\sqrt{2\pi}} \frac{1}{(-ik)}\, e^{-ikx}\Big|_{-a}^{a} = \frac{1}{\sqrt{2\pi}} \frac{e^{-ika} - e^{ika}}{-ik}$$
$$= \frac{2}{\sqrt{2\pi}\, k} \frac{e^{-ika} - e^{ika}}{-2i} = \frac{2}{\sqrt{2\pi}\, k} \frac{e^{ika} - e^{-ika}}{2i} = \frac{2}{\sqrt{2\pi}} \frac{\sin(ka)}{k}\,.$$

The graphs of $f(x)$ and $g(k)$ are

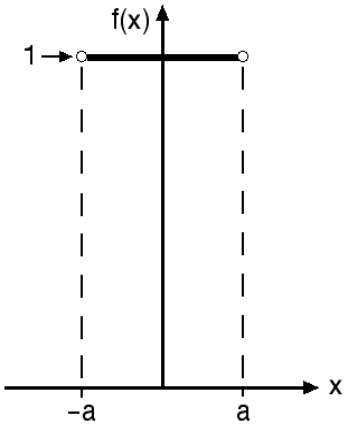

Figure 5–3 (a). Graph of $f(x)$.

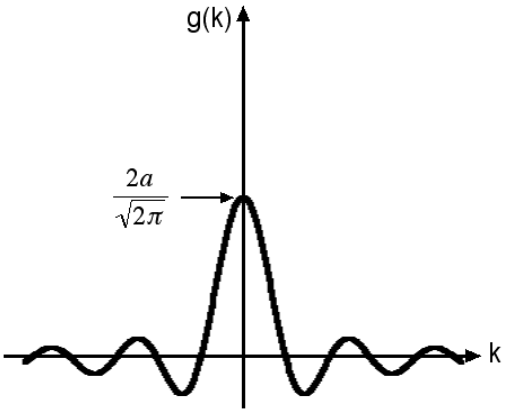

Figure 5–3 (b). Graph of $g(k)$.

Zeroes for $g(k)$ are at $k = \dfrac{n\pi}{a}$.

(b) The Fourier transform of the given function where $b = 2a$, double the width and half the height, so that the area under the curve is equal for both $f(x)$ and $h(x)$, is

$$j(k) = \frac{2}{\sqrt{2\pi}}\,\frac{1}{2}\,\frac{\sin(kb)}{k} = \frac{1}{\sqrt{2\pi}}\,\frac{\sin(2ka)}{k}.$$

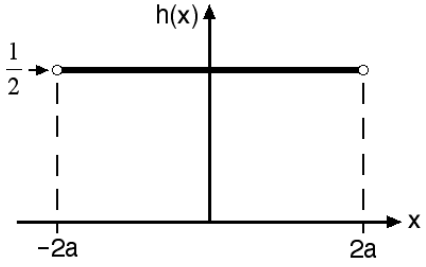

Figure 5–3 (c). Graph of $h(x)$.

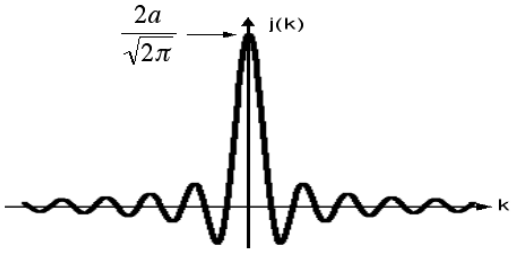

Figure 5–3 (d). Graph of $j(k)$.

Zeroes for $j(k)$ are at $k = \dfrac{n\pi}{2a}$.

(c) The graph of $h(x)$ is broader than the graph of $f(x)$, but the graph of $j(k)$ is sharper than the graph of $g(k)$. If one of the Fourier transforms is distributed and broad, the other will be localized and sharp. This phenomena is a precursor of the Heisenberg uncertainty relations.

While both $f(x)$ and $h(x)$ have a limited domain, the domains of $g(k)$ and $j(k)$ are infinite. This is another general feature of Fourier transforms.

Postscript: A sine function divided by the argument of the sine is a **sinc function**. The graph of a sinc function is characterized by a large central maximum or minimum with periodic relative maxima/minima that decrease in amplitude as distance from the origin increases.

5–16. Find the momentum space wave function corresponding to $\psi(x) = A e^{-bx^2}$.

Quantum mechanical Fourier transforms are the means to change from position space to momentum space and vice versa. This problem is a change to momentum space from position space.

The de Broglie relation associates wavelength or wavenumber, and momentum,

$$\lambda = \frac{h}{p} \quad \Rightarrow \quad \frac{2\pi}{k} = \frac{h}{p} \quad \Rightarrow \quad k = \frac{p}{\hbar}.$$

Substitute $p/\hbar$ for k in both Fourier transforms. This means the differential $dk = dp/\hbar$ in the integral for $f(x)$. Symmetrize the $1/\hbar$ from this differential by placing a factor $1/\sqrt{\hbar}$ in both integrals, and the result is the quantum mechanical form of the Fourier transforms,

$$f(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{g}(p)\, e^{ipx/\hbar}\, dp, \qquad \widehat{g}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} f(x)\, e^{-ipx/\hbar}\, dx.$$

The usual use of these relations is to transform a wave function in position space to momentum space (or vice versa), so will be applied

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}(p)\, e^{ipx/\hbar}\, dp, \qquad \widehat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dx.$$

There are a number of subtleties associated with the quantum mechanical analog of the Fourier transforms, so our heuristic argument should be regarded as a useful mnemonic.

Form 3.323.2 from Gradshteyn and Ryzhik,

$$\int_{-\infty}^{\infty} e^{-\alpha^2 x^2 - \beta x}\, dx = \frac{\sqrt{\pi}}{\alpha}\, e^{\beta^2/4\alpha^2},$$

should be useful. Do you recognize the functional form of the momentum space wave function?

$$\widehat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dx = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} A e^{-bx^2}\, e^{-ipx/\hbar}\, dx$$
$$= \frac{A}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-bx^2 - ipx/\hbar}\, dx.$$

Using $\alpha = \sqrt{b}$, and $\beta = ip/\hbar$, our integral is

$$\widehat{\psi}(p) = \frac{A}{\sqrt{2\pi\hbar}} \frac{\sqrt{\pi}}{\sqrt{b}} \exp\left(\frac{(ip/\hbar)^2}{4(\sqrt{b})^2}\right) = \frac{A}{\sqrt{2\hbar b}}\, e^{-p^2/4b\hbar^2}.$$

Postscript: Notice that $\widehat{\psi}(p)$ is also an exponential function with a negative argument that is a constant times the independent variable squared. In fact, $\widehat{\psi}(p)$ is also a Gaussian wave function. The Fourier transform of a Gaussian function is another Gaussian function.

5–17. Given $\psi(x) = \mathrm{A}\, e^{ik_0 x}$, $-\dfrac{4\pi}{k_0} \le x \le \dfrac{4\pi}{k_0}$, and 0 otherwise,

(a) normalize $\psi(x)$,

(b) find $\widehat{\psi}(p)$, and

(c) sketch $\psi(x)$ and $\widehat{\psi}(p)$.

The physical system described by the given $\psi(x)$ is a plane wave that is confined. An unconfined plane wave is not square integrable, thus cannot be normalized to be consistent with the probability postulate, so cannot by itself be a wave function. Part (a) means to solve for the constant A using the normalization condition on the interval to which the system is confined. In other words, the confinement allows use of $-4\pi/k_0$ and $4\pi/k_0$ as the limits of integration. Again, integrate between the limits of $-4\pi/k_0$ and $4\pi/k_0$ for part (b). "Sketch" means to understand the shape of the curves. Draw or plot only the real part of $\psi(x)$. Set the constants k_0 and $\hbar$ equal to 1 to obtain the shapes of $\psi(x)$ and $\widehat{\psi}(p)$ for part (c). You should find that the real part of $\psi(x)$ is an evenly distributed cosine curve but that $\widehat{\psi}(p)$ is distinctly peaked.

(a) The normalization condition for a continuous system on the interval given is

$$1 = \int_{-4\pi/k_0}^{4\pi/k_0} \mathrm{A}^*\, e^{-ik_0 x}\, \mathrm{A}\, e^{ik_0 x}\, dx = |\,\mathrm{A}\,|^2 \int_{-4\pi/k_0}^{4\pi/k_0} e^0\, dx = |\,\mathrm{A}\,|^2 \int_{-4\pi/k_0}^{4\pi/k_0} dx$$

$$= |\,\mathrm{A}\,|^2 \left(x \Big|_{-4\pi/k_0}^{4\pi/k_0} \right) = |\,\mathrm{A}\,|^2 \left(\frac{4\pi}{k_0} - -\frac{4\pi}{k_0} \right) = |\,\mathrm{A}\,|^2\, \frac{8\pi}{k_0} \quad \Rightarrow \quad \mathrm{A} = \sqrt{\frac{k_0}{8\pi}}$$

$$\Rightarrow \quad \psi(x) = \sqrt{\frac{k_0}{8\pi}}\, e^{ik_0 x} = \frac{1}{2} \sqrt{\frac{k_0}{2\pi}}\, e^{ik_0 x}\,.$$

$$(b) \quad \widehat{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dx = \frac{1}{\sqrt{2\pi\hbar}}\, \frac{1}{2} \sqrt{\frac{k_0}{2\pi}} \int_{-4\pi/k_0}^{4\pi/k_0} e^{ik_0 x}\, e^{-ipx/\hbar}\, dx$$

after substituting the results of part (a). So

$$\widehat{\psi}(p) = \frac{1}{4\pi} \sqrt{\frac{k_0}{\hbar}} \int_{-4\pi/k_0}^{4\pi/k_0} e^{i(k_0 - p/\hbar)x}\, dx = \frac{1}{4\pi} \sqrt{\frac{k_0}{\hbar}}\, \frac{1}{i\,(k_0 - p/\hbar)}\, e^{i(k_0 - p/\hbar)x} \Big|_{-4\pi/k_0}^{4\pi/k_0}$$

$$= \frac{1}{4\pi} \sqrt{\frac{k_0}{\hbar}}\, \frac{1}{i\,(k_0 - p/\hbar)} \left(e^{i(k_0 - p/\hbar)(4\pi/k_0)} - e^{i(k_0 - p/\hbar)(-4\pi/k_0)} \right)$$

$$= \frac{1}{2\pi} \sqrt{\frac{k_0}{\hbar}}\, \frac{1}{2i\,(k_0 - p/\hbar)} \left(e^{i4\pi(1 - p/k_0\hbar)} - e^{-i4\pi(1 - p/k_0\hbar)} \right)$$

$$= \frac{1}{2\pi} \sqrt{\frac{1}{k_0\hbar}}\, \frac{1}{(1 - p/k_0\hbar)}\, \frac{e^{i4\pi(1 - p/k_0\hbar)} - e^{-i4\pi(1 - p/k_0\hbar)}}{2i}$$

$$= \frac{1}{2\pi} \sqrt{\frac{1}{k_0\hbar}}\, \frac{\sin\left(4\pi\,(1 - p/k_0\hbar)\right)}{(1 - p/k_0\hbar)} \quad \Rightarrow \quad \widehat{\psi}(p) = 2 \sqrt{\frac{1}{k_0\hbar}}\, \frac{\sin\left(4\pi - \dfrac{4\pi p}{k_0\hbar}\right)}{\left(4\pi - \dfrac{4\pi p}{k_0\hbar}\right)}\,.$$

The domain is $-\infty < p < \infty$ in momentum space.

(c)

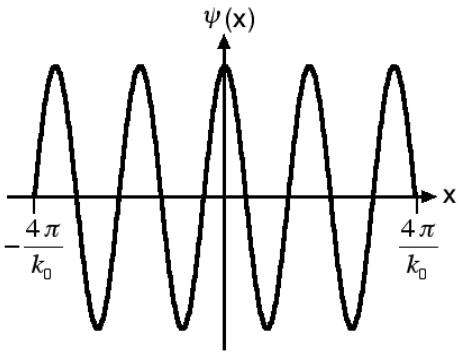

Figure 5–4 (a). Sketch of $\psi(x)$.

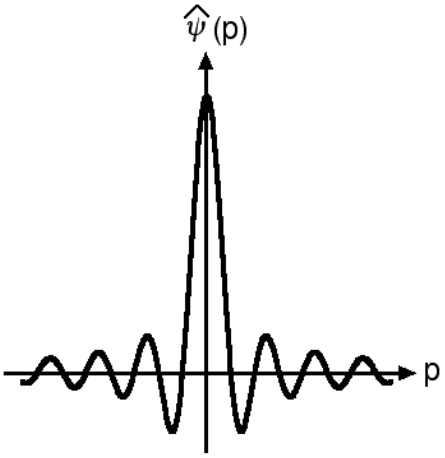

Figure 5–4 (b). Sketch of $\widehat{\psi}(p)$.

5–18. Given $|\psi>$ such that $<p|\psi> \rightarrow \widehat{\psi}(p) = \dfrac{\hbar \sin\left(\frac{ap}{\hbar}\right)}{p}$, $\qquad a \in \mathbb{R}$,

(a) normalize $\widehat{\psi}(p)$,

(b) find $\psi(x)$, and

(c) sketch $\widehat{\psi}(p)$ and $\psi(x)$.

This problem differs from the last only in that it emphasizes momentum space. Though arguments in position space are most common, momentum space can be a preferred environment.

Two integrals are of interest. Form 611 from the 30th edition of the CRC tables,

$$\int_0^\infty \frac{\sin^2(ax)}{x^2}\,dx = \frac{\pi\,|\,a\,|}{2}$$

for part (a). Assume that $a > 0$ so that you do not have to carry the absolute value symbols. Changing variables to $y = ap/\hbar$ means that the above integral is useful for normalization, given proper use of the even/odd function arguments. The second integral of interest is

$$\int_0^\infty \frac{\sin bx \cos cx}{x}\,dx = \begin{cases} 0\,, & c > b > 0\,, \\ \pi/2\,, & b > c > 0\,, \\ \pi/4\,, & b = c > 0\,, \end{cases}$$

from the 30th edition of the CRC tables, form 615. The Euler equation is $e^{i\theta} = \cos\theta + i \sin\theta$.

You should find $$\psi(x) = \frac{1}{\pi\hbar}\sqrt{\frac{2}{a}}\int_0^\infty \frac{\sin\left(\frac{ap}{\hbar}\right)\cos\left(\frac{px}{\hbar}\right)}{p/\hbar}\,dp$$

and this integral can be caste into the desired form by changing variables using $y = p/\hbar$.

(a) The normalization condition in momentum space is

$$1 = \int_{-\infty}^{\infty} \widehat{\psi}^{*}(p)\,\mathrm{A}^{*}\,\mathrm{A}\,\widehat{\psi}(p)\,dp = |\,\mathrm{A}\,|^{2}\int_{-\infty}^{\infty}\frac{\hbar\,\sin\left(\frac{ap}{\hbar}\right)}{p}\,\frac{\hbar\,\sin\left(\frac{ap}{\hbar}\right)}{p}\,dp$$

$$= |\,\mathrm{A}\,|^{2}\int_{-\infty}^{\infty}\frac{\hbar^{2}\,\sin^{2}\left(\frac{ap}{\hbar}\right)}{p^{2}}\,dp = |\,\mathrm{A}\,|^{2}\,a^{2}\int_{-\infty}^{\infty}\frac{\sin^{2}\left(\frac{ap}{\hbar}\right)}{\frac{a^{2}p^{2}}{\hbar^{2}}}\,dp\,.$$

Let $y = \frac{ap}{\hbar} \Rightarrow dy = \frac{a}{\hbar}\,dp \Rightarrow dp = \frac{\hbar}{a}\,dy\,,$ and integral limits are identical,

$$\Rightarrow\ 1 = |\,\mathrm{A}\,|^{2}\,a\hbar\int_{-\infty}^{\infty}\frac{\sin^{2}(y)}{y^{2}}\,dy = |\,\mathrm{A}\,|^{2}\,2a\hbar\int_{0}^{\infty}\frac{\sin^{2}(y)}{y^{2}}\,dy = |\,\mathrm{A}\,|^{2}\,2a\hbar\,\frac{\pi}{2}$$

$$\Rightarrow\ \mathrm{A} = \frac{1}{\sqrt{a\pi\hbar}} \Rightarrow \widehat{\psi}(p) = \frac{1}{\sqrt{a\pi\hbar}}\,\frac{\hbar\,\sin\left(\frac{ap}{\hbar}\right)}{p}\,.$$

(b) The wave function in position space is

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\,\frac{1}{\sqrt{a\pi\hbar}}\int_{-\infty}^{\infty}\frac{\hbar\,\sin\left(\frac{ap}{\hbar}\right)}{p}\,e^{ipx/\hbar}\,dp$$

$$= \frac{1}{\pi\hbar}\,\frac{1}{\sqrt{2a}}\int_{-\infty}^{\infty}\frac{\sin\left(\frac{ap}{\hbar}\right)}{p/\hbar}\,\left[\cos\left(\frac{px}{\hbar}\right) + i\sin\left(\frac{px}{\hbar}\right)\right]\,dp$$

$$= \frac{1}{\pi\hbar}\,\frac{1}{\sqrt{2a}}\int_{-\infty}^{\infty}\frac{\sin\left(\frac{ap}{\hbar}\right)\,\cos\left(\frac{px}{\hbar}\right)}{p/\hbar}\,dp + \frac{1}{\pi\hbar}\,\frac{1}{\sqrt{2a}}\,i\int_{-\infty}^{\infty}\frac{\sin\left(\frac{ap}{\hbar}\right)\,\sin\left(\frac{px}{\hbar}\right)}{p/\hbar}\,dp$$

where the last integral is zero because the product of three odd functions is an odd function, both sines and $1/p$ are odd functions, and the integral of an odd integrand between symmetric limits is zero. The other integrand is the product of two odd and one even functions so is an even function. An even integrand between symmetric limits is twice the integral from zero to the upper limit so

$$\psi(x) = \frac{1}{\pi\hbar}\,\frac{2}{\sqrt{2a}}\int_{0}^{\infty}\frac{\sin\left(\frac{ap}{\hbar}\right)\,\cos\left(\frac{px}{\hbar}\right)}{p/\hbar}\,dp\,.$$

Changing variables to $y = \frac{p}{\hbar} \Rightarrow p = \hbar y \Rightarrow dp = \hbar\,dy\,,$ so the limits are the same under this change of variables. Then

$$\psi(x) = \frac{1}{\pi\hbar}\,\frac{2}{\sqrt{2a}}\int_{0}^{\infty}\frac{\sin(ay)\,\cos(xy)}{y}\,\hbar\,dy = \begin{cases} 0\,, & x > a > 0\,, \\ \frac{1}{\sqrt{2a}}\,, & a > x > 0\,, \\ \frac{1}{2\sqrt{2a}}\,, & a = x > 0\,. \end{cases}$$

(c) The constant a has the dimension of length, which is pertinent to the graph of $\psi(x)$.

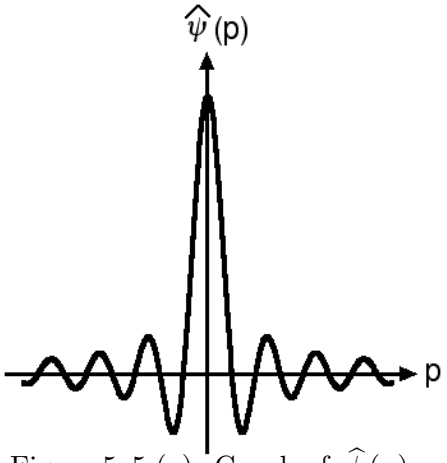

Figure 5–5 (a). Graph of $\widehat{\psi}(p)$.

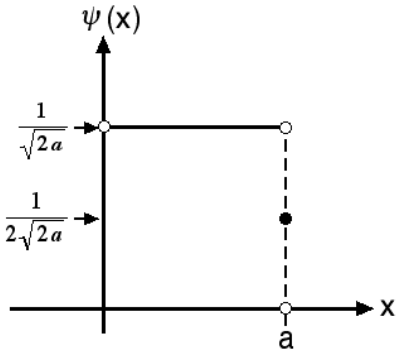

Figure 5–5 (b). Graph of $\psi(x)$.

Postscript: The momentum space wave function for this problem is a sinc function (or can be caste in the form of a sinc function by multiplying top and bottom by a). This problem shows that the Fourier transform of a sinc function is a constant function. Constants and sinc functions are related by their Fourier transforms in general.

The position space wave function of the previous problem is a confined plane wave. The only part that survives the integral transform is the periodic cosine portion. The cosine function spread uniformly throughout the interval is closely enough related to a constant function that its Fourier transform on a finite interval is also a sinc function.

5–19. Consider a particle described by the wave function

$$\psi(x) = \mathrm{N} \quad \text{when} \quad -10\ \text{Å} \leq x \leq +10\ \text{Å}, \qquad \psi(x) = 0 \quad \text{otherwise.}$$

(a) Calculate the normalization constant N.

(b) What are the possible results of a measurement of position?

(c) Calculate the probability that the particle will be found between $x = -3$ Å and $x = +5$ Å.

(d) The particle is found at $x = 3.5$ Å. Sketch the wave function subsequent to the measurement.

(e) Calculate the associated momentum space wave function $\widehat{\psi}(p)$. Sketch $\widehat{\psi}(p)$.

(f) What results can be obtained for a measurement of momentum?

(g) Suppose $p = 0$ is obtained. Sketch $\widehat{\psi}(p)$ immediately after the measurement.

This problem intends to reinforce some previously encountered material and introduces modeling using delta functions. A delta function is an idealization. Nevertheless, a delta function does properly describe the philosophy embedded in the eigenvalue and eigenvector postulates.

A position measured to be 3.5 Å means only that the measurement is made to 3.5 Å $\pm$ 0.05 Å. This is actually an interval rather than a delta function at a point. Further, the probability of measuring any given eigenvalue x_i is zero because there are an infinite number

of points on any continuous curve. The mathematics is $\int_a^a f(x)\,dx = 0$, any integral with the same upper and lower limit is zero. That said, parts (d) and (g) intend to expose how delta functions are often depicted. The eigenvalue postulate says x_i rather than an interval. The eigenvector postulate says that it stays at x_i rather than wandering within an interval.

Notice that the given wave function is a constant so the Fourier transform is anticipated to be a sinc function per previous discussions.

(a) Calculate the normalization constant

$$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 1 \quad \Rightarrow \quad \int_{-10\,\mathring{\text{A}}}^{+10\,\mathring{\text{A}}} \text{N}^*\text{N}\,dx = 1 \quad \Rightarrow \quad \int_{-10\,\mathring{\text{A}}}^{+10\,\mathring{\text{A}}} |\,\text{N}\,|^2\,dx = 1$$

$$\Rightarrow \quad |\,\text{N}\,|^2 \int_{-10\,\mathring{\text{A}}}^{+10\,\mathring{\text{A}}} dx = 1 \quad \Rightarrow \quad |\,\text{N}\,|^2\, x\Big|_{-10\,\mathring{\text{A}}}^{+10\,\mathring{\text{A}}} = 1 \quad \Rightarrow \quad |\,\text{N}\,|^2\big(+10\,\text{Å} - (-10\,\text{Å})\big) = 1$$

$$\Rightarrow \quad 20\,\text{Å}\,|\,\text{N}\,|^2 = 1 \quad \Rightarrow \quad |\,\text{N}\,|^2 = \frac{1}{20\,\text{Å}} \quad \Rightarrow \quad \text{N} = \frac{1}{\sqrt{20\,\text{Å}}}.$$

The normalization constant will always have units of $1/\sqrt{\text{length}}$ in one dimension in position space. A popular procedure is to minimize clutter by excluding units during calculation, and then carefully placing the units back into the final answer.

(b) The possible results of a position measurement are any x in the interval $-10\,\text{Å} \le x \le 10\,\text{Å}$.

(c) Calculate the probability

$$P(-3\text{Å} < x < 5\text{Å}) = \int_{-3}^{5} \psi^*(x)\,\psi(x)\,dx = \int_{-3}^{5} |\,\text{N}\,|^2\,dx$$

$$= \frac{1}{20\,\text{Å}}\, x\Big|_{-3\,\mathring{\text{A}}}^{+5\,\mathring{\text{A}}} = \frac{1}{20\,\text{Å}}\big(+5\,\text{Å} - -3\,\text{Å}\big) = \frac{8}{20} = \frac{2}{5} = 0.4.$$

(d) If the particle is at $x = 3.5\,\text{Å}$, then the wave function can be modeled by a delta function centered at $x = 3.5\,\text{Å}$, which is sketched at the right. Though this model may be mathematically suspect, it does depict the eigenvalue and eigenvector postulates justifying the sketch.

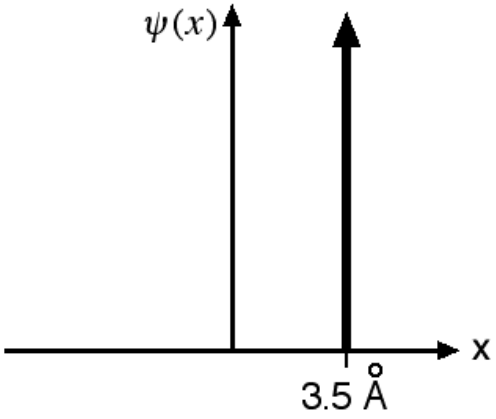

Figure 5–6 (a). Sketch of $\psi(x)$ after measurement.

(e) The wave function in momentum space is given by the Fourier transform

$$\begin{aligned}
\widehat{\psi}\,(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\,\psi\,(x)\,dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\int_{-10}^{10} e^{-ipx/\hbar}\,\mathrm{N}\,dx = \frac{\mathrm{N}}{\sqrt{2\pi\hbar}}\int_{-10}^{10} e^{-ipx/\hbar}\,dx \\
&= \frac{\mathrm{N}}{\sqrt{2\pi\hbar}}\frac{\hbar}{(-ip)}\Big(e^{-ip10/\hbar} - e^{+ip10/\hbar}\Big) \\
&= \frac{\mathrm{N}\sqrt{2}}{\sqrt{\pi\hbar}}\,\frac{\hbar}{p}\left(\frac{e^{+ip10/\hbar} - e^{-ip10/\hbar}}{2i}\right) \\
&= \frac{\sqrt{2}}{\sqrt{20\,\text{Å}}}\,\frac{1}{\sqrt{\pi\hbar}}\,\frac{\hbar}{p}\,\sin\Big(\frac{p}{\hbar}10\,\text{Å}\Big) \\
&= \frac{1}{\sqrt{10\pi\hbar\,\text{Å}}}\frac{\sin\Big(\frac{p}{\hbar}\,(10\,\text{Å})\Big)}{p/\hbar}.
\end{aligned}$$

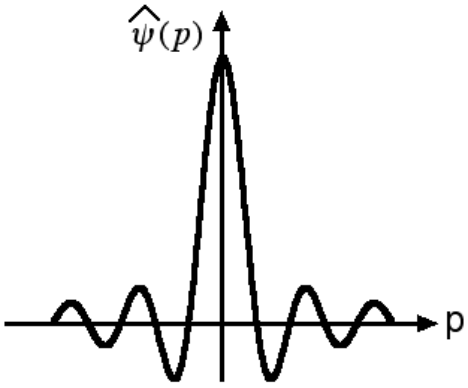

Figure 5–6 (b). Sketch of $\widehat{\psi}\,(p)$.

This is a sinc function with the independent variable p. The constants $\hbar$ and $10\,\text{Å}$ serve only to compress or expand the horizontal and vertical scales.

(f) The possible results of a momentum measurement are any p in the interval $-\infty \le p \le \infty$. The probability density in momentum space is $|\,\widehat{\psi}\,(p)\,|^{\,2}$, and

$$P\,(p_a < p < p_b) = \frac{1}{10\pi\hbar\,\text{Å}}\int_{p_a}^{p_b}\frac{\sin^2\Big(\frac{p}{\hbar}\,(10\,\text{Å})\Big)}{p^2/\hbar^2}\,dp$$

is a relation to calculate probability in momentum space.

(g) Finding $p = 0$, the momentum wave function can be modeled by a delta function located at $p = 0$.

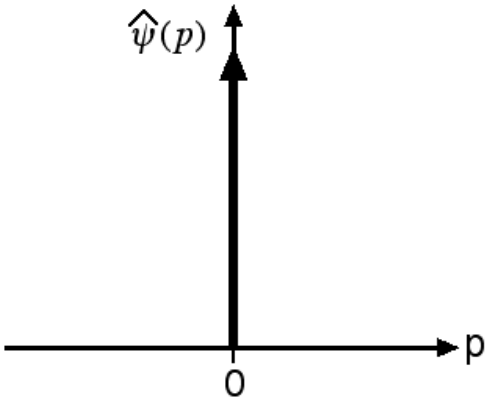

Figure 5–6 (c). Sketch of $\widehat{\psi}\,(p)$ after measurement.

Postscript: The probability of measuring any individual x_i is zero. The probability of obtaining a value between the limits a and b is $P\,(a < x < b) = \dfrac{1}{20\,\text{Å}}\displaystyle\int_a^b dx$, for this problem where a and b are in angstroms. The region of interest can be very small, for instance if $a = 3.499999\,\text{Å}$ and $b = 3.500001\,\text{Å}$. There is a small probability of finding the particle between these limits, and this is realistically what is meant by a measurement of $x = 3.5\,\text{Å}$. Nevertheless, delta functions are often used as depictions in continuous space because they do reflect the statements of the eigenvalue and eigenvector postulates.

5–20. What is the Fourier integral?

The sole reason for this problem is to discuss different conventions that may be encountered in other discussions concerning Fourier transforms.

Fourier integrals are generalizations of Fourier series. A **Fourier integral** is a representation of a non-periodic function that may be regarded as the limit of the Fourier series as the period approaches infinity. Two Fourier transforms compose the Fourier integral.

In the limit of $l \to \infty$, the complex Fourier series becomes

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k)\, e^{ikx}\, dk\,, \qquad g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx\,.$$

The function $f(x)$ is the Fourier transform of $g(k)$, and $g(k)$ is the Fourier transform of $f(x)$. Substitution of one transform into the other expressing the combination as one relation, *i.e.*,

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x')\, e^{-ikx'}\, dx' \right) e^{ikx}\, dk \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} f(x')\, e^{ik(x-x')}\, dx' \quad \text{is the Fourier integral.} \end{aligned}$$

We refer the reader to Byron and Fuller[2], or other texts on mathematical physics for greater depth.

Postscript: The factor of $1/2\pi$ must be in the Fourier integral but it does not need to be symmetrized in the Fourier transforms as presented. Some place the entire factor of $1/2\pi$ with one integral so that the other integral is without a coefficient. The signs of the exponentials may differ from what has been presented here. Asymmetric treatment of the factor of $1/2\pi$ and/or use of a different sign convention result in slightly different functional forms for Fourier transforms.

5–21. What is the meaning of $\mathcal{X}\,|\,x> \;=\; x\,|\,x>$?

The eigenvalue/eigenvector equation for the position operator in position space is essentially a definition[3]. Nevertheless, some justification is appropriate.

Position is an observable quantity, therefore $\mathcal{X}$ is Hermitian. All Hermitian operators can be diagonalized. If $\mathcal{X}$ is not diagonal, an appropriate unitary transformation $\mathcal{U}^\dagger\,\mathcal{X}\,\mathcal{U} = \mathcal{X}'$ is diagonal, or for the purposes of notational consistency, $\mathcal{U}^\dagger\,\mathcal{X}'\,\mathcal{U} = \mathcal{X}$ is diagonal. In the basis in

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[2] Byron and Fuller, *Mathematics of Classical and Quantum Physics* (Dover Publications, Inc., New York, 1970), pp. 239–253, 566–570.

[3] Cohen-Tannoudji, Diu, & Laloe, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), 4th ed., pp. 149.

which $\mathcal{X}$ is diagonal, the eigenvalues are on the main diagonal and the basis vectors are infinite dimensional unit vectors. In position space, the matrix representation could be denoted

$$\mathcal{X}\,|\,x> \;=\; x\,|\,x> \quad \Rightarrow \quad \begin{pmatrix} x_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & x_2 & 0 & 0 & 0 & \dots \\ 0 & 0 & x_3 & 0 & 0 & \dots \\ 0 & 0 & 0 & x_4 & 0 & \dots \\ 0 & 0 & 0 & 0 & x_5 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix} \;=\; x_n \begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix}$$

where the 1 in the unit vector is the nth component. This is an infinity of eigenvalue/eigenvector equations that may be denoted $\mathcal{X}\,|\,x_n> \;=\; x_n\,|\,x_n>$ but is usually written $\mathcal{X}\,|\,x> \;=\; x\,|\,x>$.

Postscript: The same argument applies to the momentum operator in momentum space, that is

$$\mathcal{P}\,|\,p> \;=\; p\,|\,p> \quad \Rightarrow \quad \begin{pmatrix} p_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & p_2 & 0 & 0 & 0 & \dots \\ 0 & 0 & p_3 & 0 & 0 & \dots \\ 0 & 0 & 0 & p_4 & 0 & \dots \\ 0 & 0 & 0 & 0 & p_5 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix} \;=\; p_n \begin{pmatrix} \vdots \\ 1 \\ \vdots \end{pmatrix}.$$

The eigenvalues of position are on the main diagonal in position space (times the unit vectors), and the eigenvalues of momentum are on the main diagonal in momentum space (times the unit vectors). The meanings of the momentum operator in position space and the position operator in momentum space are less clear and must be developed.

5–22. Show that $<x\,|\,p> \;\rightarrow\; \dfrac{1}{\sqrt{2\pi\hbar}}\,e^{ipx/\hbar}$.

The state functions in position and momentum space are related by the quantum mechanical Fourier transforms. The relation $<x\,|\,\psi> \rightarrow\; \psi\,(x)$ says only that an abstract state functions picks appropriate positions from Hilbert space to represent a conventional function of position. The relation $<p\,|\,\psi> \rightarrow\; \widehat{\psi}\,(p)$ is a comparable statement in momentum space. The inner product $<x\,|\,p>$, however, is different because position and momentum are related.

$$\psi\,(x) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}\,(p)\,e^{ipx/\hbar}\,dp \quad \Rightarrow \quad <x\,|\,\psi> \;\rightarrow\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widehat{\psi}\,(p)\,e^{ipx/\hbar}\,dp$$

$$<x\,|\,\psi> \;=\; <x\,|\,\mathcal{I}\,|\,\psi> \;=\; <x\,|\left(\int_{-\infty}^{\infty} |\,p><p\,|\,dp\right)|\,\psi>$$

$$= \int_{-\infty}^{\infty} <x\,|\,p><p\,|\,\psi>\,dp \;=\; \int_{-\infty}^{\infty} <x\,|\,p>\,\widehat{\psi}\,(p)\,dp\,, \qquad \text{thus}$$

$$\int_{-\infty}^{\infty} <x\,|\,p>\,\widehat{\psi}\,(p)\,dp \;\;\rightarrow\;\; \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\widehat{\psi}\,(p)\,e^{ipx/\hbar}\,dp\,. \qquad \text{Then}$$

$$<x\,|\,p>\,\widehat{\psi}\,(p) \;\;\rightarrow\;\; \frac{1}{\sqrt{2\pi\hbar}}\,\widehat{\psi}\,(p)\,e^{ipx/\hbar} \qquad \text{and} \qquad <x\,|\,p> \;\rightarrow\; \frac{1}{\sqrt{2\pi\hbar}}\,e^{ipx/\hbar}\,.$$

Postscript: This also means the conjugate quantity $\quad <p\,|\,x> \;\rightarrow\; \dfrac{1}{\sqrt{2\pi\hbar}}\,e^{-ipx/\hbar}\,.$

5–23. Show that (a) $<x\,|\,\mathcal{X}\,|\,x'> \;=\; x\,\delta\,(x-x')$ and (b) $<x\,|\,\mathcal{P}\,|\,x'> \;=\; -i\hbar\,\delta'\,(x-x')\,.$

The observables postulate requires that $\mathcal{X}$ is Hermitian. Hermitian operators can operate to the right or to the left. The eigenvalue/eigenvector relation is $<x\,|\,\mathcal{X} \;=\; <x\,|\,x$ when $\mathcal{X}$ operates to the left. The part (a) is a one line application of the eigenvalue/eigenvector equation requiring the recognition of a delta function.

Part (b) uses the quantum mechanical Fourier transforms to form a Fourier integral for $\psi\,(x)\,.$ Write $\quad \psi\,(x) \;=\; \displaystyle\int_{-\infty}^{\infty}\delta\,(x-x')\,\psi\,(x')\,dx'\,,$ set the two expressions equal, and develop relations for $\delta\,(x-x')$ and finally $\delta'\,(x-x')\,.$ Then

$$<x\,|\,\mathcal{P}\,|\,x'> \;=\; <x\,|\,\mathcal{I}\,|\,\mathcal{P}\,|\,x'> \;=\; <x\,|\left(\int\,|\,p><p\,|\,dp\right)|\,\mathcal{P}\,|\,x'>\,,$$

and use the relations of $<x\,|\,p>$ and $<p\,|\,x>$ from the previous problem to eventually arrive at expressions that can be recognized as $\delta'\,(x-x')\,.$

(a) Letting $\mathcal{X}$ operate to the left and recognizing that $\;<x\,|\,x'> \;=\; \delta\,(x-x')\,,$

$$<x\,|\,\mathcal{X}\,|\,x'> \;=\; <x\,|\,x\,|\,x'> \;=\; x<x\,|\,x'> \;=\; x\,\delta\,(x-x')\,.$$

(b) The quantum mechanical Fourier integral is

$$\psi\,(x) \;=\; \frac{1}{\sqrt{2\pi\hbar}}\int\!\left(\frac{1}{\sqrt{2\pi\hbar}}\int\psi\,(x')\,e^{-ipx'/\hbar}\,dx'\right)e^{ipx/\hbar}\,dp \;=\; \frac{1}{2\pi\hbar}\int dp\int\psi\,(x')\,e^{ip(x-x')/\hbar}\,dx'.$$

The wave function in position space can be written $\quad \psi\,(x) \;=\; \displaystyle\int\delta\,(x-x')\,\psi\,(x')\,dx' \quad$ so

$$\int\delta\,(x-x')\,\psi\,(x')\,dx' \;=\; \frac{1}{2\pi\hbar}\int dp\int\psi\,(x')\,e^{ip(x-x')/\hbar}\,dx'\,.$$

$$\Rightarrow \quad \delta\,(x-x')\,\psi\,(x') \;=\; \frac{1}{2\pi\hbar}\int\psi\,(x')\,e^{ip(x-x')/\hbar}\,dp \;=\; \frac{1}{2\pi\hbar}\,\psi\,(x')\int e^{ip(x-x')/\hbar}\,dp \qquad (1)$$

$$\Rightarrow \quad \delta\,(x-x') \;=\; \frac{1}{2\pi\hbar}\int e^{ip(x-x')/\hbar}\,dp$$

$$\Rightarrow \quad \delta'(x-x') \;=\; \frac{1}{2\pi\hbar}\int \frac{i}{\hbar}\, p\, e^{ip(x-x')/\hbar}\, dp\,. \tag{2}$$

$$\begin{aligned}
<x\,|\,\mathcal{P}\,|\,x'> \;&=\; <x\,|\,\mathcal{I}\,|\,\mathcal{P}\,|\,x'> \;=\; <x\,|\left(\int\,|\,p><p\,|\,dp\right)|\,\mathcal{P}\,|\,x'> \\
&=\; \int <x\,|\,p><p\,|\,\mathcal{P}\,|\,x'>\,dp \\
&=\; \int <x\,|\,p><p\,|\,p\,|\,x'>\,dp \;=\; \int p\,<x\,|\,p><p\,|\,x'>\,dp \qquad (3)\\
&=\; \int p\left(\frac{1}{\sqrt{2\pi\hbar}}\,e^{ipx/\hbar}\right)\left(\frac{1}{\sqrt{2\pi\hbar}}\,e^{-ipx'/\hbar}\right)dp \qquad (4)\\
&=\; \frac{1}{2\pi\hbar}\int p\,e^{ip(x-x')/\hbar}\,dp \;=\; \frac{\hbar}{i}\,\delta'(x-x') \;=\; -i\hbar\,\delta'(x-x')\,. \qquad (5)
\end{aligned}$$

The function solely of position $\psi(x')$ is removed from the integral with respect to dp in line (1). Line (2) is differentiation with respect to x. The first expression in line (3) is the result of the eigenvalue/eigenvector equation, $<p\,|\,\mathcal{P} \;=\; <p\,|\,p$. Line (4) employs the expressions developed for $<x\,|\,p>$ and $<p\,|\,x>$ in the previous problem. The second expression in line (5) is obtained by comparing the first expression in line (5) with equation (2).

Postscript: The relations above are in the position basis. Analogous relations in the momentum basis are $<p\,|\,\mathcal{P}\,|\,p'> \;=\; p\,\delta(p-p')$ and $<p\,|\,\mathcal{X}\,|\,p'> \;=\; i\hbar\,\delta'(p-p')$. The absence of a negative sign in the last equation is a choice of phase. A choice of phase is necessary.

These relations involving delta functions and their derivatives have been used to state portions of the postulates of quantum mechanics[4].

5–24. Find the form of an expectation value of the position operator in position space.

The expectation value of position is $<\psi\,|\,\mathcal{X}\,|\,\psi>$ in Dirac notation. Insert the identity in terms of $|\,x'>$ on the left and $|\,x>$ on the right of the abstract position operator. Rearrange the expression to find a factor of $<x'\,|\,\mathcal{X}\,|\,x> \;=\; x'\,\delta(x'-x)$. One of the two integrations can be done using this delta function to find $<\psi\,|\,\mathcal{X}\,|\,\psi> \;=\; \int \psi^*(x)\,x\,\psi(x)\,dx$.

$$\begin{aligned}
<\psi\,|\,\mathcal{X}\,|\,\psi> \;&=\; <\psi\,|\,\mathcal{I}\,|\,\mathcal{X}\,|\,\mathcal{I}\,|\,\psi> \qquad (1)\\
&=\; <\psi\,|\left(\int\,|\,x'><x'\,|\,dx'\right)|\,\mathcal{X}\,|\left(\int\,|\,x><x\,|\,dx\right)|\,\psi> \qquad (2)\\
&=\; \int\int <\psi\,|\,x'><x'\,|\,\mathcal{X}\,|\,x><x\,|\,\psi>\,dx'\,dx
\end{aligned}$$

[4] Shankar, *Principles of Quantum Mechanics* (Plenum Press, New York, 1994), 2nd ed., pp. 115-116.

$$= \int\int \psi^*(x')\, x'\, \delta(x'-x)\, \psi(x)\, dx'\, dx \tag{3}$$

$$= \int \left(\int \psi^*(x')\, x'\, \delta(x'-x)\, dx' \right) \psi(x)\, dx \quad = \quad \int \psi^*(x)\, x\, \psi(x)\, dx\,.$$

The identity is inserted twice in line (1), two different forms of the identity are used in line (2), inner products and the braket (per problem 5–23 (a)) are represented in position space in line (3).

Postscript: This is evidence $\mathcal{X} \rightarrow x$ in position space. Similarly, if more than one spatial dimension is required, $\mathcal{Y} \rightarrow y$, and $\mathcal{Z} \rightarrow z$.

5–25. Find the form of the expectation value of the momentum operator in position space.

This is similar to the last problem except it addresses momentum. Start with $<\psi\,|\,\mathcal{P}\,|\,\psi>$, insert identities in the same form as the last problem but you will need to use the relation $<x\,|\,\mathcal{P}\,|\,x'> \;=\; -i\hbar\,\delta'(x-x')$ addressed in problem 5–23 (b). The delta function is an even function but the derivative of the delta function is an odd function so $<x'\,|\,\mathcal{P}\,|\,x> \;=\; i\hbar\,\delta'(x'-x)$ is the form to use. The derivative of a delta function is the negative of the derivative of the function.

$$\begin{aligned}
<\psi\,|\,\mathcal{P}\,|\,\psi> \;&=\; <\psi\,|\,\mathcal{I}\,|\,\mathcal{P}\,|\,\mathcal{I}\,|\,\psi> \\
&=\; <\psi\,|\left(\int\,|\,x'><x'\,|\,dx'\right)|\,\mathcal{P}\,|\left(\int\,|\,x><x\,|\,dx\right)|\,\psi> \\
&=\; \int\int <\psi\,|\,x'><x'\,|\,\mathcal{P}\,|\,x><x\,|\,\psi>\, dx'\, dx \\
&=\; \int\int \psi^*(x')\Big(i\hbar\,\delta'(x'-x)\Big)\,\psi(x)\, dx'\, dx \qquad (1) \\
&=\; \int \psi^*(x)\Big(-i\hbar\,\frac{d}{dx}\Big)\,\psi(x)\, dx \quad = \quad -i\hbar\int \psi^*(x)\,\frac{d}{dx}\,\psi(x)\, dx\,. \qquad (2)
\end{aligned}$$

The inner products and the derivative of the delta function are both represented in position space in line (1). Evaluating the derivative of the delta function results in the first expression in line (2).

Postscript: This problem is evidence that $\mathcal{P} \;\rightarrow\; -i\hbar\,\dfrac{d}{dx}$ in position space.

These relations are readily generalized to two or three dimensions by working two or three one-dimensional problems. If more than one spatial component is required,

$$\mathcal{P} \;\rightarrow\; -i\hbar\nabla \;=\; -i\hbar\left(\frac{\partial}{\partial x} \;+\; \frac{\partial}{\partial y} \;+\; \frac{\partial}{\partial z}\right), \quad \text{in three spatial dimensions, for instance.}$$

The analogous relations in momentum space are $\mathcal{X} \;\rightarrow\; i\hbar\dfrac{d}{dp}$ and $\mathcal{P} \;\rightarrow\; p$. In three dimensions

$$\mathcal{X} \;\rightarrow\; i\hbar\frac{d}{dp_x}, \quad \mathcal{Y} \;\rightarrow\; i\hbar\frac{d}{dp_y}, \quad \mathcal{Z} \;\rightarrow\; i\hbar\frac{d}{dp_z}, \quad \text{and} \quad \mathcal{P}_x \;\rightarrow\; p_x, \quad \mathcal{P}_y \;\rightarrow\; p_y, \quad \mathcal{P}_z \;\rightarrow\; p_z\,.$$

The absence of a negative sign in momentum operators reflects the popular choice of phase.

5–26. Derive the position space form of the time-independent Schrodinger equation in one dimension. Assume that potential energy is a function of position only.

Basis-independent statements of the Schrodinger equation offer generality and flexibility and can provide physical insight, but they are not often useful to obtain functional or numeric solutions to real problems. Representations of the Schrodinger equation in position space and momentum space are the tools generally used to address specific systems.

Start with the eigenvalue/eigenvector equation for the time-independent, quantum mechanical Hamiltonian, $\mathcal{H}\,|\,\psi> \;=\; E\,|\,\psi>$. Form the quantum mechanical Hamiltonian,

$$H_{\text{classical}} \;=\; T \,+\, V \;=\; \frac{p^2}{2m} \,+\, V \qquad \longrightarrow \qquad \mathcal{H} \;=\; \frac{\mathcal{P}^2}{2m} \,+\, \mathcal{V}\,.$$

Potential energy is a function of position only $\;\Rightarrow\;\mathcal{V} \,\rightarrow \mathcal{V}\,(\mathcal{X})$ and $\mathcal{X} \,\rightarrow\, x \;\Rightarrow\; \mathcal{V}\,(\mathcal{X}) \rightarrow V\,(x)$ for this problem. Form a braket of both sides using $<x\,|$. Assume that this bra commutes with the Hamiltonian to find

$$-\frac{\hbar^2}{2m}\,\frac{d^2}{d^2x}\,\psi\,(x) \;+\; V\,(x)\,\psi\,(x) \;\;=\;\; E\,\psi\,(x)\,.$$

$$\begin{aligned}
\mathcal{H}\,|\,\psi> \;=\; E\,|\,\psi> \quad &\Rightarrow \quad \left(\frac{\mathcal{P}^2}{2m} \,+\, \mathcal{V}\right)|\,\psi> \;=\; E\,|\,\psi> \\
&\Rightarrow \quad \left(\frac{\mathcal{P}^2}{2m} \,+\, \mathcal{V}\,(\mathcal{X})\right)|\,\psi> \;=\; E\,|\,\psi> \qquad (1) \\
&\Rightarrow \quad <x\,|\left(\frac{\mathcal{P}^2}{2m} \,+\, \mathcal{V}\,(\mathcal{X})\right)|\,\psi> \;=\; <x\,|\,E\,|\,\psi> \qquad (2) \\
&\Rightarrow \quad \left(\frac{1}{2m}\,\mathcal{P}^2 \,+\, \mathcal{V}\,(\mathcal{X})\right)<x\,|\,\psi> \;=\; E<x\,|\,\psi> \qquad (3) \\
&\Rightarrow \quad \left[\frac{1}{2m}\left(-i\hbar\,\frac{d}{dx}\right)\left(-i\hbar\,\frac{d}{dx}\right) \,+\, V(x)\right]\psi\,(x) \;=\; E\,\psi\,(x) \qquad (4) \\
&\Rightarrow \quad -\frac{\hbar^2}{2m}\,\frac{d^2}{d^2x}\,\psi\,(x) \;+\; V\,(x)\,\psi\,(x) \;\;=\;\; E\,\psi\,(x)\,.
\end{aligned}$$

Equation (1) embeds the assumption that potential energy is a function of position only. Brakets are formed with $<x\,|$ so as to obtain a position space representation in equation (2). The E on the right side of equation (3) is an eigenvalue and any constant can be removed from a braket. The expression in parenthesis on the left side of equation (3) is simply a different form of the Hamiltonian operator. The position space representations of the momentum operator, the potential energy operator, and the inner products are substituted in equation (4).

Postscript: That $<x\,|$ commutes with the Hamiltonian is founded by the requirement for eigenstates to be unique, a property that follows from the orthogonality of the eigenstates. There are an infinite number of $\psi\,(x)$'s or $\psi_i\,(x)$'s. The right side of equation (2) becomes a constant times an eigenfunction. In order for the left side of equation (2) to be the same in an infinite number of cases, it also must become a constant times a function, thus $<x\,|$ commutes with $\mathcal{H}$.

Exercises

5–27. Show that

(a) $\psi_n(\phi) = e^{in\phi}$ and $\psi_m(\phi) = e^{im\phi}$, $-\pi < \phi < \pi$, are orthogonal, n and $m \in \mathbb{Z}$.

(b) Orthonormalize $\psi_n(\phi)$ and $\psi_m(\phi)$.

The intent of this exercise is similar to problem 5–3. Demonstrating orthogonality for any set of functions in continuous space can be challenging. The exponentials in this exercise are likely more straightforward than the sines and cosines of problem 5–3.

The notation n and $m \in \mathbb{Z}$ means that n and m are in the set of integers. ($\mathbb{Z}$ is from the German word "zahl" meaning number or numeral). Show that $<\psi_n \,|\, \psi_n> \neq 0$ and $<\psi_m \,|\, \psi_m> \neq 0$. Establish that $<\psi_n \,|\, \psi_m> = 0$ for all integer $n \neq m$. Convert the inner products to integrals for the actual calculation for the functional forms given. The "particle" is confined to the interval $-\pi < \phi < \pi$, so $-\pi$ and π are the limits of integration.

5–28. Show that if $|\,\psi>$ is normalized, so is $|\,\psi'> = e^{i\phi}\,|\,\psi>$ in position space.

This exercise reinforces the meaning of normalization but also addresses the concept of phase. The factor $e^{i\phi}$ is the phase and the scalar ϕ is the phase angle, though at times the scalar ϕ is called the phase because it is the only portion of the exponential that can vary. Remember $<\psi \,|\, \psi> = 1 \;\Rightarrow\; \int \psi^*(x)\,\psi(x)\,dx = 1$ in position space to show that $<\psi' \,|\, \psi'> = 1$.

5–29. Show that Legendre polynomials $P_2(x)$ and $P_3(x)$ are orthogonal on $-1 < x < 1$.

Legendre's equation is

$$\left(1 - x^2\right) y'' \;-\; 2xy' \;+\; l\left(l+1\right) y \;=\; 0\,.$$

The solutions to Legendre's equation are **Legendre polynomials**. The first six Legendre polynomials, usually denoted by a subscripted upper case P_n, are listed in table 5–3.

$P_0(x) = 1$		$P_3(x) = \frac{1}{2}\left(5x^3 - 3x\right)$	
$P_1(x) = x$		$P_4(x) = \frac{1}{8}\left(35x^4 - 30x^2 + 3\right)$	
$P_2(x) = \frac{1}{2}\left(3x^2 - 1\right)$		$P_5(x) = \frac{1}{8}\left(63x^5 - 70x^3 + 15x\right)$	

Table 5 – 3. The First Six Legendre Polynomials.

Hermite and Laguerre polynomials are not themselves orthogonal, however, appending an exponential weighting factor creates related functions which are orthogonal over all space. The weighting

factor diminishes quickly enough to overpower the polynomials as $|x| \to \infty$. A different technique is applied to Legendre polynomials. Like the sines and cosines of problem 5–3, they are orthogonal on an interval. Thus, the problem asks you to show

$$\int_{-1}^{1} P_m(x)\,P_n(x)\,dx \;=\; 0\,, \quad m \neq n\,, \qquad \text{and} \qquad \int_{-1}^{1} P_i(x)\,P_i(x)\,dx \;\neq\; 0\,, \quad \text{for} \quad i \,=\, 2\,,\; 3\,.$$

Use even/odd integrand between symmetric limits arguments. See problem 5–4.

5–30. Represent (a) $x^2 + 3x\,,$ (b) $2x^3 - 4x^2 + 7\,,$ and (c) $8x^4 - 5x^2 - 4x$ as unique linear combinations of Legendre polynomials.

Like problems 5–5 and 5–6. Work from the highest power to the lowest power to ensure uniqueness. Legendre polynomials are used to describe orbital angular momentum.

5–31. Represent x^4 as unique linear combinations of (a) Hermite, (b) Laguerre, and (c) Legendre polynomials.

The first five Hermite and Laguerre polynomials are reproduced for your convenience.

$$\begin{aligned} H_0\,(x) &= 1 & L_0(x) &= 1 \\ H_1\,(x) &= 2x & L_1(x) &= -x + 1 \\ H_2\,(x) &= 4x^2 - 2 & L_2(x) &= x^2 - 4x + 2 \\ H_3\,(x) &= 8x^3 - 12x & L_3(x) &= -x^3 + 9x^2 - 18x + 6 \\ H_4\,(x) &= 16x^4 - 48x^2 + 12 & L_4(x) &= x^4 - 16x^3 + 72x^2 - 96x + 24 \end{aligned}$$

Each part will contain as many as five (a) Hermite, (b) Laguerre, or (c) Legendre polynomials because representation of x^4 introduces terms with powers less than 4.

5–32. Use the generating functions

$$H_n\,(x) \;=\; (-1)^n e^{x^2}\,\frac{d^n}{dx^n}\,e^{-x^2} \qquad \text{and} \qquad L_n\,(x) \;=\; e^{x}\,\frac{d^n}{dx^n}\,e^{-x}x^n$$

to obtain $H_2\,(x)$ and $L_2\,(x)\,.$

The generating functions require the chain rule of differentiation. For example,

$$H_2 \;=\; (-1)^2 e^{x^2}\,\frac{d^2}{dx^2}\,e^{-x^2} \;=\; e^{x^2}\,\frac{d}{dx}\,e^{-x^2}(-2x)$$

$$=\; e^{x^2}\left(e^{-x^2}(-2x)(-2x) + e^{-x^2}(-2)\right) \;=\; e^{x^2}e^{-x^2}\left(4x^2 - 2\right) \;=\; 4x^2 - 2 \quad \text{per table 5–1.}$$

5–33. Obtain $H_5(x)$ and $H_6(x)$.

Both may be obtained using the generating function, rather, a **recursion relation** such as

$$H_{n+1}(x) \;=\; 2x\,H_n(x) \;-\; 2n\,H_{n-1}(x)$$

is more efficient for Hermite polynomials with large, or even moderately sized, indices. Thus

$$H_5(x) \;=\; 2x\,H_4(x) \;-\; 2\cdot 4\,H_3(x) \;=\; 2x\big(16x^4 - 48x^2 + 12\big) \;-\; 8\big(8x^3 - 12x\big)$$

$$=\; 32x^5 - 96x^3 + 24x - 64x^3 + 96x \;=\; 32x^5 - 160x^3 + 120x\,.$$

You now have $H_5(x)$ and $H_4(x)$ to calculate $H_6(x)$.

5–34. (a) Show that the operator x is Hermitian.

(b) Show that the differential operator $\mathcal{D} \;=\; i\dfrac{d}{dx}$ is Hermitian.

These are intended to be straightforward introductions to the process of establishing Hermiticity for operators for continuous systems. Part (a) is nearly proof by notation. The operator x is a real valued function, thus $x = x^*$, and functions, whether real or complex valued, commute. Said another way, a function returns a scalar and scalars commute. The "proof" is essentially writing the appropriate integral in both orders along with the justification given in the last two sentences.

Use integration by parts for part (b). Remember that $\psi_1^*\,\psi_2\Big|_{-\infty}^{\infty} = 0$ for ψ_i that are square integrable. See problems 5–7 and 5–8.

5–35. Show that $\mathcal{H} \;\rightarrow\; -\dfrac{\hbar^2}{2m}\,\dfrac{d^2}{dx^2}$ is Hermitian.

The Hamiltonian operator is that for a free particle ($V(x) = 0$). This is meatier than the previous exercise. The proof uses integration by parts twice. Integration by parts is frequently seen

$$\int u\,dv \;\;=\;\; u\,v - \int v\,du$$

where partitioning the original integrand can be challenging. Using $dv = d\left(\dfrac{d\psi_2}{dx}\right)$ in the first integration by parts, and $u = \dfrac{d\psi_1^*}{dx} \;\Rightarrow\; du = d\left(\dfrac{d\psi_1^*}{dx}\right)$ in the second leads to the desired end.

The product $u\,v$ is zero for both integrations. Each wave function must go to zero at $\pm\infty$ to be square integrable. Also, the product $u\,v$ will contain a derivative in both integrations. The first derivative of a function that superimposes the horizontal axis at $\pm\infty$ is also zero (*i.e.* slope = 0).

5–36. Discuss the significance of the orthogonality of sines and cosines to the basic Fourier series.

This exercise concerns the meaning of orthogonality for a continuous system. Consider the Cartesian coordinates of introductory physics. Can a vector be uniquely described in $\mathbb{R}^3$ if $\widehat{x}$, $\widehat{y}$, and $\widehat{z}$ are not mutually perpendicular? (The answer is maybe, but it is vastly easier if they are). Generalize to $\mathbb{R}^5$ or $\mathbb{C}^5$. Consider unit vectors in ket notation in those spaces. Does each individual unit vector make a unique contribution? Can you then generalize to a continuous system?

Problem 5–3 establishes the orthogonality of sines and cosines on the interval $-l < x < l$. Notice that this is an interval of $2l$. Problem 5–9 denotes the basic Fourier series as

$$f(x) \;=\; \frac{a_0}{2} \;+\; \sum_{n=1}^{\infty} a_n \cos\Big(\frac{n\pi x}{l}\Big) \;+\; \sum_{n=1}^{\infty} b_n \sin\Big(\frac{n\pi x}{l}\Big) \qquad \text{given that the period is } 2l\,.$$

Examine the progression of the four sketches in figures 5–2. Will the sum converge if contributions from different n do not add something previous n could not? The meaning of orthogonality in a continuous system is that every n contributes something unique. Our answer is nine lines.

5–37. Sketch the function

$$f(x) \;=\; \begin{cases} 0 & \text{if} \quad -\pi < x < 0\,, \\ 1 & \text{if} \quad 0 < x < \pi\,, \end{cases}$$

then expand it using a basic Fourier series given that it has a period of 2π.

This is a straightforward modification of problem 5–10 appropriate to an introduction to Fourier analysis. Comparing a sketch of the given function to figure 5–1 may be illustrative.

5–38. Sketch the function

$$f(x) \;=\; \begin{cases} 0 & \text{if} \quad -\pi < x < -\pi/2\,, \\ 1 & \text{if} \quad -\pi/2 < x < \pi/2\,, \\ 0 & \text{if} \quad \pi/2 < x < \pi\,, \end{cases}$$

then expand it using a basic Fourier series given that it has a period of 2π.

Like 5–10 and 5–37, however, this will contain alternating cosine terms.

5–39. Sketch the function

$$f(x) \;=\; x\,, \qquad 0 < x < 2\pi\,,$$

then expand it using a basic Fourier series given that it has a period of 2π.

A sketch is that of a sawtooth function. One exercise where the function is other than a periodic constant is appropriate. The integrals

$$\int x\,\cos(nx)\,dx \;=\; \frac{1}{n^2}\cos(nx) \;+\; \frac{x}{n}\sin(nx) \qquad \int x\,\sin(nx)\,dx \;=\; \frac{1}{n^2}\sin(nx) \;-\; \frac{x}{n}\cos(nx)$$

pertain. The $n = 0$ integral is unlike those for $n > 0$, though it is straightforward.

5–40. Consider a particle described by the wave function $\psi(x) = \dfrac{\mathrm{A}}{x^2+1}$.

(a) Normalize $\psi(x)$. Sketch $\psi(x)$.

(b) Calculate $P(0 < x < 1)$.

(c) What are the possible results of a measurement of position?

(d) The particle is found at $x = \pi$. Sketch the wave function immediately after the measurement.

(e) Calculate the momentum space wave function $\widehat{\psi}(p)$. Sketch $\widehat{\psi}(p)$.

(f) The momentum of the particle is measured. What results can be obtained?

(g) Suppose $p = 0$ is measured. Sketch $\widehat{\psi}(p)$ immediately after the measurement.

The wave function is a Lorentzian curve which is used frequently in spectral analysis. The integrals

$$\int \frac{dx}{(a^2+b^2x^2)^2} = \frac{x}{2a^2(a^2+b^2x^2)} + \frac{1}{2a^3b}\arctan\left(\frac{bx}{a}\right) \qquad \int_{-\infty}^{\infty} \frac{e^{-iqx}}{x^2+a^2}\,dx = \frac{\pi}{a}\,e^{-|aq|}$$

will be of interest. You should find

$$P(0 < x < 1) = \frac{1}{2\pi} + \frac{1}{4} \approx 0.4092 \quad \text{for part (b), and} \quad \widehat{\psi}(p) = \frac{e^{-|p|/\hbar}}{\sqrt{\hbar}} \quad \text{for part (e).}$$

Also, $\arctan\infty = \pi/2$, $\arctan -\infty = -\pi/2$, $\arctan 0 = 0$, and $\arctan 1 = \pi/4$. The post measurement sketches for parts (d) and (g) are delta functions.

5–41. (a) Represent the expectation value of the momentum operator in momentum space.

(b) Represent the expectation value of the position operator in momentum space.

Use procedures similar to those seen in problems 5–24 and 5–25. Use the relations

$$<p\,|\,\mathcal{P}\,|\,p'> = p\,\delta(p-p') \qquad \text{and} \qquad <p\,|\,\mathcal{X}\,|\,p'> = i\hbar\,\delta'(p-p')$$

per the postscript to problem 5–23.

Obtaining the "correct" $\pm$ signs for problems 5–24 and 5–25 and this exercise can be puzzling. The signs are a choice of phase. Part (b) requires the use of the primed bras and kets in the left identity as done in problems 5–24 and 5–25, and use of the fact that the derivative of the delta function is odd, that is $\delta'(p-p') = -\delta'(p'-p)$, per the prescript of problem 5–25. The postscript to problem 5–25 discusses the necessary results using the popular phase convention.

Chapter 6

Ehrenfest, Heisenberg, and Gauss

Part 1, Ehrenfest's Theorem

Quantum mechanics must give the same results as classical mechanics in a classical regime. Bohr's correspondence principle, which states the relations of quantum mechanics reduce to the relations of classical mechanics for large quantum numbers, is often cited. Paul Ehrenfest originated a different answer. Ehrenfest said replace the dynamical variables of classical mechanics with the expectation values of quantum mechanics and you obtain the same relations.

6–1. Derive Ehrenfest's Theorem.

This derivation assumes that an operator representing an observable quantity is time independent, and that the state vector is time dependent. Observable quantities are functions of position only in this text, and time evolution of a state vector has been discussed in previous chapters. Notice that the derivation is for a general operator $\mathcal{A}$, which may represent position, momentum, energy, or any other observable quantity. Remember that a commutator is defined $\left[\mathcal{A}, \mathcal{B}\right] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}$.

Start with the expectation value of a time independent operator, $<\mathcal{A}> \;=\; <\psi|\,\mathcal{A}\,|\psi>$, and take a time derivative. The wave function is assumed to be a function of time, so using the chain rule to take the derivative,

$$\frac{d}{dt}<\mathcal{A}> \;=\; <\dot{\psi}|\,\mathcal{A}\,|\psi> \;+\; <\psi|\,\dot{\mathcal{A}}\,|\psi> \;+\; <\psi|\,\mathcal{A}\,|\dot{\psi}>\,.$$

Since the operator is assumed to be time independent, the middle term is zero so this reduces to

$$\frac{d}{dt}<\mathcal{A}> \;=\; <\dot{\psi}|\,\mathcal{A}\,|\psi> \;+\; <\psi|\,\mathcal{A}\,|\dot{\psi}>\;. \tag{1}$$

The Schrodinger postulate is

$$\mathcal{H}\,|\psi> \;=\; i\hbar\,|\dot{\psi}> \quad\Rightarrow\quad |\dot{\psi}> \;=\; \frac{1}{i\hbar}\mathcal{H}\,|\psi> \;=\; -\frac{i}{\hbar}\mathcal{H}\,|\psi>\,.$$

Forming the adjoint of the last relation, $<\dot{\psi}| \;=\; <\psi|\,\mathcal{H}^{\dagger}\left(\frac{i}{\hbar}\right)$, and since the Hamiltonian is Hermitian, this is $<\dot{\psi}| \;=\; \frac{i}{\hbar}<\psi|\,\mathcal{H}$. Using these in equation (1),

$$\begin{aligned}
\frac{d}{dt}<\mathcal{A}> \;&=\; \frac{i}{\hbar}<\psi|\,\mathcal{H}\mathcal{A}\,|\psi> \;-\; \frac{i}{\hbar}<\psi|\,\mathcal{A}\mathcal{H}\,|\psi> \\
&=\; \frac{i}{\hbar}\left(<\psi|\,\mathcal{H}\mathcal{A}\,|\psi> \;-\; <\psi|\,\mathcal{A}\mathcal{H}\,|\psi>\right) \\
&=\; \frac{i}{\hbar}<\psi|\,\Big[\mathcal{H},\,\mathcal{A}\Big]\,|\psi> \\
&=\; \frac{i}{\hbar}<\Big[\mathcal{H},\,\mathcal{A}\Big]>
\end{aligned}$$

which is Ehrenfest's theorem.

6–2. What is the fundamental canonical commutation relation?

A commutator equivalent to multiplication by the factor $i\hbar$ is a **canonical commutator**, *i.e.*, if

$$\big[\,\mathcal{A},\,\mathcal{B}\,\big] \;=\; \mathcal{A}\mathcal{B} \;-\; \mathcal{B}\mathcal{A} \;=\; i\hbar\,,$$

then $\big[\,\mathcal{A}\,,\mathcal{B}\,\big]$ is a canonical commutation relation. Realize $i\hbar \;\rightarrow\; i\hbar\mathcal{I}$ in more than one dimension. The **fundamental canonical commutator**[1] is $\big[\,\mathcal{X},\,\mathcal{P}\,\big] \;=\; i\hbar\,.$

Postscript: The fundamental commutation relations in three dimensions are

$$\big[\,\mathcal{X},\,\mathcal{P}_x\,\big] \;=\; i\hbar\,, \qquad \big[\,\mathcal{Y},\,\mathcal{P}_y\,\big] \;=\; i\hbar\,, \qquad \big[\,\mathcal{Z},\,\mathcal{P}_z\,\big] \;=\; i\hbar\,.$$

6–3. Show $\big[\,\mathcal{X},\,\mathcal{P}\,\big] \;=\; i\hbar$ in position space.

This derivation relies on representations previously discussed. In position space,

$$\mathcal{X} \;\rightarrow\; x \qquad \text{and} \qquad \mathcal{P} \;\rightarrow\; -i\hbar\,\frac{d}{dx} \qquad \text{in one dimension.}$$

The commutator is an operator so give it an arbitrary function in position space, $f(x)$, on which to operate, so

$$\begin{aligned}\big[\,\mathcal{X},\,\mathcal{P}\,\big]\,f(x) \;&=\; \Big(\mathcal{X}\,\mathcal{P} - \mathcal{P}\,\mathcal{X}\Big)f(x) \\ &=\; \mathcal{X}\,\mathcal{P}\,f(x) - \mathcal{P}\,\mathcal{X}\,f(x)\,.\end{aligned}$$

Representing this in position space, this is

$$\big[\,\mathcal{X},\,\mathcal{P}\,\big]\,f(x) \;=\; (x)\left(-i\hbar\frac{d}{dx}\right)f(x) \;-\; \left(-i\hbar\frac{d}{dx}\right)x\,f(x)$$

where it is necessary to use the chain rule to evaluate the last term. Differentiating,

$$\big[\,\mathcal{X},\,\mathcal{P}\,\big]\,f(x) \;=\; -i\hbar\,x\frac{d\,\cancel{f(x)}}{\cancel{dx}} \;+\; i\hbar\,f(x) \;+\; i\hbar\,x\frac{d\,\cancel{f(x)}}{\cancel{dx}} \;=\; i\hbar\,f(x)\,.$$

Since $f(x)$ is an arbitrary function, the effect of the commutator is $\big[\,\mathcal{X},\,\mathcal{P}\,\big] \;=\; i\hbar\,.$

Postscript: The fundamental commutation relations are summarized $\big[\,\mathcal{X}_i\,,\,\mathcal{P}_j\,\big] \;=\; i\hbar\,\delta_{ij}$ in three dimensions. Along the same lines, $\big[\,\mathcal{X}_i\,,\,\mathcal{X}_j\,\big] \;=\; 0\,,$ and $\big[\,\mathcal{P}_i\,,\,\mathcal{P}_j\,\big] \;=\; 0\,.$

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[1] Cohen-Tannoudji, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), pp 149 – 151.

6–4. Calculate $<\dot{\mathcal{X}}>$ for a particle.

Calculate $<\dot{\mathcal{X}}>$ using Ehrenfest's theorem, which for the choice of the operator $\mathcal{X}$ is

$$<\dot{\mathcal{X}}> \;=\; \frac{i}{\hbar}<\Big[\mathcal{H}\,,\,\mathcal{X}\Big]>,$$

where we need an explicit form of a Hamiltonian. The Hamiltonian for a particle is

$$H \;=\; T \;+\; V \;\;\rightarrow\;\; \mathcal{H} \;=\; \frac{\mathcal{P}^2}{2m} \;+\; \mathcal{V}(\mathcal{X})$$

Assume $\mathcal{V}(\mathcal{X})$ is a function of $\mathcal{X}$ only or powers of $\mathcal{X}$, such as $-k\,\mathcal{X}$ or $\frac{1}{2}\,k\,\mathcal{X}^2$. This assumption means that $\mathcal{V}(\mathcal{X})$ commutes with $\mathcal{X}$ per problem 3–25.

$$<\dot{\mathcal{X}}> \;=\; \frac{i}{\hbar}<\Big[\frac{\mathcal{P}^2}{2m} \;+\; \mathcal{V}(\mathcal{X})\,,\,\mathcal{X}\Big]> \;=\; \frac{i}{\hbar}<\Big[\frac{\mathcal{P}^2}{2m}\,,\,\mathcal{X}\Big] \;+\; \Big[\mathcal{V}(\mathcal{X})\,,\,\mathcal{X}\Big]> .$$

The second commutator in the expectation value is zero, so the time derivative is

$$<\dot{\mathcal{X}}> \;=\; \frac{i}{\hbar}<\Big[\frac{\mathcal{P}^2}{2m}\,,\,\mathcal{X}\Big]> \;=\; \frac{i}{2m\hbar}<\Big[\mathcal{P}^2\,,\,\mathcal{X}\Big]> . \qquad (1)$$

Evaluating the commutator,

$$\Big[\mathcal{P}^2\,,\,\mathcal{X}\Big] \;=\; \mathcal{P}^2\mathcal{X} \;-\; \mathcal{X}\mathcal{P}^2 \;=\; \mathcal{P}\,\mathcal{P}\,\mathcal{X} \;-\; \mathcal{X}\,\mathcal{P}\,\mathcal{P}\,.$$

Add zero with the intent of putting the last expression in some form related to the fundamental commutator. In other words, if we add and subtract $\mathcal{P}\,\mathcal{X}\,\mathcal{P}$, the last commutator becomes

$$\begin{aligned}
\Big[\mathcal{P}^2,\mathcal{X}\Big] \;&=\; \mathcal{P}\,\mathcal{P}\,\mathcal{X} \;-\; \mathcal{X}\,\mathcal{P}\,\mathcal{P} \;+\; \mathcal{P}\,\mathcal{X}\,\mathcal{P} \;-\; \mathcal{P}\,\mathcal{X}\,\mathcal{P} \\
&=\; \mathcal{P}\,\mathcal{P}\,\mathcal{X} \;-\; \mathcal{P}\,\mathcal{X}\,\mathcal{P} \;+\; \mathcal{P}\,\mathcal{X}\,\mathcal{P} \;-\; \mathcal{X}\,\mathcal{P}\,\mathcal{P} \\
&=\; \mathcal{P}\Big(\mathcal{P}\,\mathcal{X}-\mathcal{X}\,\mathcal{P}\Big) \;+\; \Big(\mathcal{P}\,\mathcal{X}-\mathcal{X}\,\mathcal{P}\Big)\mathcal{P} \\
&=\; \mathcal{P}\Big[\mathcal{P}\,,\,\mathcal{X}\Big] \;+\; \Big[\mathcal{P}\,,\,\mathcal{X}\Big]\mathcal{P} \\
&=\; \mathcal{P}\big(-i\hbar\big) \;+\; \big(-i\hbar\big)\mathcal{P} \;=\; -2i\hbar\,\mathcal{P}\,.
\end{aligned}$$

Using this in equation (1),

$$<\dot{\mathcal{X}}> \;=\; \frac{i}{2m\hbar}<\big(-2i\hbar\,\mathcal{P}\big)> \;=\; \frac{i}{2m\hbar}\big(-2i\hbar\big)<\mathcal{P}> \;=\; \frac{<\mathcal{P}>}{m}\,.$$

Postscript: A naive interpretation is that the expectation value of the momentum operator may be mv_0, so that $<\dot{\mathcal{X}}> = v_0$. Mixing classical and quantum mechanical arguments into a "semi-classical" model is dangerous, at best. The thought is intriguing, nevertheless. Problem 6–30 toward the end of this chapter provides a purely quantum mechanical calculation with the same outcome using a result from the next problem.

6–5. Construct quantum mechanical expressions for $<\dot{\mathcal{X}}>$ in

(a) continuous position space, and

(b) continuous momentum space.

The expectation value of the time rate of change of the position operator is equal to the expectation value of the momentum operator divided by mass. In position space, $\mathcal{X} \rightarrow x$ and $\mathcal{P} \rightarrow -i\hbar \dfrac{d}{dx}$. In momentum space, $\mathcal{P} \rightarrow p$ and $\mathcal{X} \rightarrow i\hbar \dfrac{d}{dp}$. Remember for the general operator $\mathcal{A}$,

$$<\mathcal{A}> \rightarrow \int_{-\infty}^{\infty} \psi^*(x)\, \mathcal{A}\, \psi(x)\, dx \qquad \text{in position space, for instance.}$$

Two expressions are written for each space.

(a) In continuous position space,

$$<\dot{\mathcal{X}}> \rightarrow \int_{-\infty}^{\infty} \psi^*(x) \left(\frac{d}{dt}\, x \right) \psi(x)\, dx \qquad \text{when substituting } x\text{, and}$$

$$<\dot{\mathcal{X}}> \rightarrow \int_{-\infty}^{\infty} \psi^*(x)\, \frac{1}{m} \left(-i\hbar \frac{d}{dx} \right) \psi(x)\, dx \qquad \text{using problem 6–4 and the representation of } \mathcal{P}.$$

(b) In momentum space, the results are

$$<\dot{\mathcal{X}}> \rightarrow \int_{-\infty}^{\infty} \widehat{\psi}^*(p) \left(\frac{d}{dt} \right) \left(i\hbar \frac{d}{dp} \right) \widehat{\psi}(p)\, dp \qquad \text{using } \mathcal{X} \rightarrow i\hbar \frac{d}{dp}\text{, and}$$

$$<\dot{\mathcal{X}}> \rightarrow \int_{-\infty}^{\infty} \widehat{\psi}^*(p)\, \frac{p}{m}\, \widehat{\psi}(p)\, dp \qquad \text{using the result of problem 6–4 and } \mathcal{P} \rightarrow p\,.$$

Postscript: Paul Ehrenfest published his theorem in 1927. It deserves mention, though it's primary uses are only to create quantum mechanical analogies to $p = mv$ and $F = ma$ in most introductory expositions. The connection Ehrenfest's theorem makes between quantum and classical mechanics had "...great appeal to many physicists and did much to further the acceptance of the theory. For it made possible to describe the particle by a localized **wave packet** which, though eventually spreading out in space, follows the trajectory of the classical motion[2]." Wave packets are central concepts in part 3 of this chapter.

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[2] Max Jammer from *Concepts of Mass* (1961), as quoted by Nicholas Wheeler, *Remarks Concerning the Status and Some Ramifications of Ehrenfest's Theorem* (Reed College Physics Department, 1998), page 1.

Part 2, The Heisenberg Uncertainty Relations

Expectation values and uncertainties are statistical measures of central tendency that follow from the eigenvalue and probability postulates. Expectation value was used at the end of the last chapter to show that $\mathcal{X} \rightarrow x$ and $\mathcal{P} \rightarrow -i\hbar\frac{d}{dx}$ in position space. Problem 6–3 has used these to show $\left[\mathcal{X}, \mathcal{P}\right] = i\hbar$, which is the fundamental canonical commutator. Canonically conjugate commutators other than position and momentum occur. In general, canonically conjugate commutators are of the form $\left[\mathcal{A}, \mathcal{B}\right] = i\hbar = i\hbar\mathcal{I}$. The minimal uncertainty relation for canonically conjugate Hermitian operators is

$$\triangle\mathcal{A}\,\triangle\mathcal{B} \geq \frac{\hbar}{2}. \qquad \text{This becomes} \qquad \triangle\mathcal{X}\,\triangle\mathcal{P} \geq \frac{\hbar}{2}$$

for position and momentum. Both are statements of the Heisenberg uncertainty principle.

The observables postulate plays a central role in our development. An observable quantity is represented by a Hermitian operator. The eigenvalues of Hermitian operators are real numbers, thus the expectation values and uncertainties of Hermitian operators are real numbers.

There exist pairs of operators that are not canonically conjugate of the form

$$\left[\mathcal{A}, \mathcal{B}\right] = \beta\mathcal{K}$$

such as the component angular momentum/spin operators. Problem 6–16 examines one of the consequences of such a relationship.

6–6. Show that if $\left[\mathcal{A}, \mathcal{B}\right] = i\mathcal{C}$ where $\mathcal{A}$ and $\mathcal{B}$ are Hermitian, the operator $\mathcal{C}$ is Hermitian.

A commutator is an operator. Labeling that operator $\mathcal{C}$ is cosmetic notation. That the commutator of two Hermitian operators can be i times another Hermitian operator is significant, and is the case for canonically conjugate Hermitian operators.

$$\begin{aligned}
\left[\mathcal{A}, \mathcal{B}\right] = i\mathcal{C} \quad &\Leftrightarrow \quad \left[\mathcal{A}, \mathcal{B}\right]^\dagger = \left(i\mathcal{C}\right)^\dagger \\
&\Leftrightarrow \quad \left(\mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}\right)^\dagger = i^\dagger\mathcal{C}^\dagger \\
&\Leftrightarrow \quad \left(\mathcal{A}\mathcal{B}\right)^\dagger - \left(\mathcal{B}\mathcal{A}\right)^\dagger = -i\mathcal{C}^\dagger \\
&\Leftrightarrow \quad \mathcal{B}^\dagger\mathcal{A}^\dagger - \mathcal{A}^\dagger\mathcal{B}^\dagger = -i\mathcal{C}^\dagger \\
&\Leftrightarrow \quad \mathcal{B}\mathcal{A} - \mathcal{A}\mathcal{B} = -i\mathcal{C}^\dagger \\
&\Leftrightarrow \quad -\left[\mathcal{A}, \mathcal{B}\right] = -i\mathcal{C}^\dagger \\
&\Leftrightarrow \quad \left[\mathcal{A}, \mathcal{B}\right] = i\mathcal{C}^\dagger
\end{aligned}$$

but the given relation $\left[\mathcal{A}, \mathcal{B}\right] = i\mathcal{C}$ means $i\mathcal{C} = i\mathcal{C}^\dagger \Leftrightarrow \mathcal{C} = \mathcal{C}^\dagger$, thus, $\mathcal{C}$ is Hermitian.

6–7. Given $\widehat{\mathcal{A}} = \mathcal{A} - <\mathcal{A}> \mathcal{I}$, show that $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right] = \left[\mathcal{A}, \mathcal{B}\right]$.

Remember that $\triangle \mathcal{A}_\psi = <\psi| \left(\mathcal{A} - <\mathcal{A}> \mathcal{I}\right)^2 |\psi>^{1/2}$ is one definition of uncertainty. The "hatted" operator is the expression in parentheses. This step in the development of the Heisenberg uncertainty principle is not strictly necessary but is fairly conventional and enables clean and economical notation for what follows. Remember that an expectation value is a scalar so commutes with everything, and the identity operator also commutes with everything.

$$\begin{aligned}
\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right] &= \widehat{\mathcal{A}}\widehat{\mathcal{B}} - \widehat{\mathcal{B}}\widehat{\mathcal{A}} \\
&= \left(\mathcal{A} - <\mathcal{A}> \mathcal{I}\right)\left(\mathcal{B} - <\mathcal{B}> \mathcal{I}\right) - \left(\mathcal{B} - <\mathcal{B}> \mathcal{I}\right)\left(\mathcal{A} - <\mathcal{A}> \mathcal{I}\right) \\
&= \mathcal{A}\mathcal{B} - \mathcal{A} <\mathcal{B}> \mathcal{I} - <\mathcal{A}> \mathcal{I}\mathcal{B} + <\mathcal{A}> \mathcal{I} <\mathcal{B}> \mathcal{I} \\
&\qquad - \mathcal{B}\mathcal{A} + \mathcal{B} <\mathcal{A}> \mathcal{I} + <\mathcal{B}> \mathcal{I}\mathcal{A} - <\mathcal{B}> \mathcal{I} <\mathcal{A}> \mathcal{I} \\
&= \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A} + \left(- <\mathcal{B}> \mathcal{I}\mathcal{A} + <\mathcal{B}> \mathcal{I}\mathcal{A}\right) + \left(- <\mathcal{A}> \mathcal{I}\mathcal{B} + <\mathcal{A}> \mathcal{I}\mathcal{B}\right) \\
&\qquad + \left(<\mathcal{A}><\mathcal{B}> \mathcal{I}^2 - <\mathcal{A}><\mathcal{B}> \mathcal{I}^2\right)
\end{aligned}$$

where all the grouped terms sum to zero, so

$$\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A} = \left[\mathcal{A}, \mathcal{B}\right].$$

6–8. Show that if $\mathcal{A}$ is Hermitian, $\widehat{\mathcal{A}}$ is Hermitian.

You know that $\mathcal{A}$ is Hermitian and that $\mathcal{I}$ is Hermitian. Is the expectation value $<\mathcal{A}>$ of a Hermitian operator a real number? (Yes, though the proof is left as an exercise).

$$\begin{aligned}
\widehat{\mathcal{A}} &= \mathcal{A} - <\mathcal{A}> \mathcal{I} \\
\Rightarrow \quad \widehat{\mathcal{A}}^\dagger &= \left(\mathcal{A} - <\mathcal{A}> \mathcal{I}\right)^\dagger \\
&= \mathcal{A}^\dagger - <\mathcal{A}>^* \mathcal{I}^\dagger.
\end{aligned}$$

Now $\mathcal{I}^\dagger = \mathcal{I}$ because of the nature of the identity, and $\mathcal{A}^\dagger = \mathcal{A}$ because it is given to be Hermitian. The expectation value $<\mathcal{A}>$ is of Hermitian operator, so must be a real number. The complex conjugate of a real number is the same real number, that is $<\mathcal{A}>^* = <\mathcal{A}>$, so

$$\widehat{\mathcal{A}}^\dagger = \mathcal{A}^\dagger - <\mathcal{A}>^* \mathcal{I}^\dagger = \mathcal{A} - <\mathcal{A}> \mathcal{I} = \widehat{\mathcal{A}},$$

therefore, $\widehat{\mathcal{A}}^\dagger = \widehat{\mathcal{A}}$ and $\widehat{\mathcal{A}}$ is Hermitian.

6–9. Show that $\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 = \left|\,|\,\widehat{\mathcal{A}}\psi>\,\right|^2\left|\,|\,\widehat{\mathcal{B}}\psi>\,\right|^2$, given that $\mathcal{A}$ and $\mathcal{B}$ are Hermitian.

This is the reason for problem 6–8.

$$\begin{aligned}\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 &= <\psi\,|\left(\mathcal{A}-<\mathcal{A}>\mathcal{I}\right)^2|\,\psi><\psi\,|\left(\mathcal{B}-<\mathcal{B}>\mathcal{I}\right)^2|\,\psi> \\ &= <\psi\,|\left(\widehat{\mathcal{A}}\right)^2|\,\psi><\psi\,|\left(\widehat{\mathcal{B}}\right)^2|\,\psi> \\ &= <\psi\,|\,\widehat{\mathcal{A}}\,\widehat{\mathcal{A}}\,|\,\psi><\psi\,|\,\widehat{\mathcal{B}}\,\widehat{\mathcal{B}}\,|\,\psi> \\ &= <\psi\,|\,\widehat{\mathcal{A}}^\dagger\,\widehat{\mathcal{A}}\,|\,\psi><\psi\,|\,\widehat{\mathcal{B}}^\dagger\,\widehat{\mathcal{B}}\,|\,\psi> \\ &= \left|\,\widehat{\mathcal{A}}\,|\,\psi>\,\right|^2\left|\,\widehat{\mathcal{B}}\,|\,\psi>\,\right|^2\end{aligned}$$

where the next to last step uses the fact the operators are Hermitian.

6–10. Show that an anti-commutator of Hermitian operators is Hermitian.

The **anti-commutator** is defined $\left[\mathcal{A}\,,\,\mathcal{B}\right]_+ = \mathcal{A}\mathcal{B}+\mathcal{B}\mathcal{A}$. The **general uncertainty relation** is expressed as a difference of an anti-commutator and a commutator.

$$\begin{aligned}\left[\mathcal{A}\,,\,\mathcal{B}\right]_+^\dagger &= \left(\mathcal{A}\mathcal{B}+\mathcal{B}\mathcal{A}\right)^\dagger = \left(\mathcal{A}\mathcal{B}\right)^\dagger + \left(\mathcal{B}\mathcal{A}\right)^\dagger = \mathcal{B}^\dagger\,\mathcal{A}^\dagger + \mathcal{A}^\dagger\,\mathcal{B}^\dagger \\ &= \mathcal{B}\mathcal{A} + \mathcal{A}\mathcal{B} = \mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A} = \left[\mathcal{A}\,,\,\mathcal{B}\right]_+\end{aligned}$$

Postscript: This result will be used in the form $\left[\widehat{\mathcal{A}}\,,\,\widehat{\mathcal{B}}\right]_+^\dagger = \left[\widehat{\mathcal{A}}\,,\,\widehat{\mathcal{B}}\right]_+$.

6–11. Prove the Schwarz inequality.

The **Schwarz inequality** is $\left|\,|\,v_1>\,\right|\left|\,|\,v_2>\,\right| \geq \left|\,<v_1\,|\,v_2>\,\right|$.

Form a vector from two others such that

$$|\,3> \;=\; |\,1> \;-\; \frac{<2\,|\,1>}{\left|\,|\,2>\,\right|^2}\,|\,2> \;.$$

An inner product is a scalar, a norm is a scalar, so the vector $|\,3>$ is an arbitrary linear combination of one vector minus the second vector scaled. Form the adjoint of $|\,3>$. The inner product $<3\,|\,3>$ is necessarily non-negative meaning that $<3\,|\,3> \geq 0$, which is the sole purpose of defining the arbitrary vector $|\,3>$. Having introduced the relationship of inequality, the rest is the algebra of bras, kets, and norms.

Let $|3> = |1> - \dfrac{<2|1>}{||2>|^2}|2> \;\Rightarrow\; <3| = <1| - <2|\dfrac{<2|1>^*}{||2>|^2}$. Then $<3|3> \geq 0$,

$$\text{and} \qquad <3|3> = \left(<1| - <2|\frac{<2|1>^*}{||2>|^2}\right)\left(|1> - \frac{<2|1>}{||2>|^2}|2>\right) \geq 0$$

$$\Rightarrow \quad <1|1> - <1|2>\frac{<2|1>}{||2>|^2} - \frac{<2|1>^*}{||2>|^2}<2|1> + \frac{<2|1>^*<2|1>}{||2>|^4}<2|2> \geq 0.$$

Now $<2|2> = ||2>|^2$, and using $<2|1>^* = <1|2>$ selectively on the last term,

$$<1|1> - \frac{<1|2>\cancel{<2|1>}}{||\cancel{2}>|^2} - \frac{<2|1>^*<2|1>}{||2>|^2} + \frac{<1|2>\cancel{<2|1>}}{||\cancel{2}>|^2} \geq 0$$

$$\Rightarrow \quad <1|1> \geq \frac{<2|1>^*<2|1>}{||2>|^2}$$

$$\Rightarrow \quad ||1>|^2||2>|^2 \geq |<2|1>|^2$$

where $<2|1>^*<2|1> = |<2|1>|^2$. Taking a square root of both sides yields

$$||1>|\,||2>| \geq |<2|1>|.$$

6–12. Apply the Schwarz inequality to the result of problem 6–9.

Since the product of an operator and a vector is a vector, both $\widehat{\mathcal{A}}|\psi>$ and $\widehat{\mathcal{B}}|\psi>$ are vectors, and the Schwarz inequality applied to the result of problem 6–9 is

$$\left|\widehat{\mathcal{A}}|\psi>\right|^2\left|\widehat{\mathcal{B}}|\psi>\right|^2 \geq \left|<\psi|\,\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}\,|\psi>\right|^2$$

The "hatted" operators accommodate clean notation, but they also encode the uncertainties, thus

$$(\triangle\mathcal{A})^2(\triangle\mathcal{B})^2 \geq \left|<\psi|\,\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}\,|\psi>\right|^2$$

is an undeveloped statement of the general uncertainty relation.

The operator $\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}$ may be expressed $\widehat{\mathcal{A}}\,\widehat{\mathcal{B}} = \frac{1}{2}\widehat{\mathcal{A}}\,\widehat{\mathcal{B}} + \frac{1}{2}\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}$. Adding zero in the form $\frac{1}{2}\widehat{\mathcal{B}}\,\widehat{\mathcal{A}} - \frac{1}{2}\widehat{\mathcal{B}}\,\widehat{\mathcal{A}}$ allows $\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}$ to be described as a sum of an anti-commutator and a commutator,

$$\begin{aligned}\widehat{\mathcal{A}}\,\widehat{\mathcal{B}} &= \frac{1}{2}\widehat{\mathcal{A}}\,\widehat{\mathcal{B}} + \frac{1}{2}\widehat{\mathcal{A}}\,\widehat{\mathcal{B}} + \frac{1}{2}\widehat{\mathcal{B}}\,\widehat{\mathcal{A}} - \frac{1}{2}\widehat{\mathcal{B}}\,\widehat{\mathcal{A}} \\ &= \frac{1}{2}\left(\widehat{\mathcal{A}}\,\widehat{\mathcal{B}} + \widehat{\mathcal{B}}\,\widehat{\mathcal{A}}\right) + \frac{1}{2}\left(\widehat{\mathcal{A}}\,\widehat{\mathcal{B}} - \widehat{\mathcal{B}}\,\widehat{\mathcal{A}}\right) = \frac{1}{2}\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+ + \frac{1}{2}\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right].\end{aligned}$$

Since $\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \left|<\psi|\,\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}\,|\psi>\right|^2$,

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \left|<\psi|\,\frac{1}{2}\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+ \;+\; \frac{1}{2}\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]\,|\psi>\right|^2$$

$$\Leftrightarrow\quad \left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\left|<\psi|\,\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+ \;+\; \left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]\,|\psi>\right|^2$$

is another preliminary statement of the generalized uncertainty relation.

6–13. Use problems 6–6, 6–7, and 6–10 to further develop the general uncertainty relation.

A primary intent of part 2 of chapter 6 is to derive $\triangle\mathcal{A}\,\triangle\mathcal{B} \;\geq\; \frac{\hbar}{2}$ for canonically conjugate operators, completed in this and the next problem using elements thus far developed.

Using the result of problem 6–7 directly, the general uncertainty relation is

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\left|<\psi|\,\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+ \;+\; \left[\mathcal{A},\mathcal{B}\right]\,|\psi>\right|^2$$

which can be written

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\left|<\psi|\,\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+|\psi> \;+\; <\psi|\,\left[\mathcal{A},\mathcal{B}\right]\,|\psi>\right|^2$$

The anti-commutator $\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+$ is Hermitian from problem 6–10, and the expectation value of a Hermitian operator is a real number. The commutator $\left[\mathcal{A},\mathcal{B}\right] = i\mathcal{C}$ from problem 6–6, where $\mathcal{C}$ is Hermitian. The expectation value of $\mathcal{C}$ is a real number, so $i\mathcal{C}$ is an imaginary number. Thus, the right side of the last inequality contains a magnitude squared of the form

$$\left|\,a+ib\,\right|^2 \;=\; \left(a+ib\right)\left(a-ib\right) \;=\; a^2+b^2\,,\quad \text{so}$$

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+|\psi>^2 \;+\; \frac{1}{4}\,<\psi|\,\mathcal{C}\,|\psi>^2$$

which is the general uncertainty relation between any two Hermitian operators.

6–14. What is the general uncertainty relation between canonically conjugate Hermitian operators?

The meaning of canonically conjugate operators is $\left[\mathcal{A},\mathcal{B}\right] \;=\; i\hbar \;=\; i\hbar\mathcal{I} \;=\; i\mathcal{C}\,,\;\;\text{so}\;\;\mathcal{C} \;=\; \hbar\mathcal{I}\,.$

$$\begin{aligned}\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;&\geq\; \frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+|\psi>^2 \;+\; \frac{1}{4}\,<\psi|\,\hbar\mathcal{I}\,|\psi>^2 \\ &=\; \frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+|\psi>^2 \;+\; \frac{\hbar^2}{4}\,<\psi|\psi>^2 = \;\frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\widehat{\mathcal{B}}\right]_+|\psi>^2 \;+\; \frac{\hbar^2}{4}\end{aligned}$$

employing the orthonormality of eigenstates in the last step. Summarizing,

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2 \;+\; \frac{\hbar^2}{4}$$

is the general uncertainty relation between two canonically conjugate Hermitian operators.

Postscript: The expression $\frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2$ is positive definite, that is

$$\frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2 \geq\; 0$$

since the expectation value of any real number squared is greater than or equal to zero. Thus,

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2 \;+\; \frac{\hbar^2}{4} \;\geq\; \frac{\hbar^2}{4}$$

and this means

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{\hbar^2}{4} \quad\Rightarrow\quad \triangle\mathcal{A}\,\triangle\mathcal{B} \;\geq\; \frac{\hbar}{2}$$

for all possible state vectors. For $\left[\,\mathcal{X}\,,\,\mathcal{P}\,\right] \;=\; i\hbar \;=\; i\hbar\mathcal{I}\,,$ this becomes

$$\triangle\mathcal{X}\;\triangle\mathcal{P} \;\geq\; \frac{\hbar}{2}.$$

6–15. Show that the general uncertainty relation becomes an equality when both

$$<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi> \;=\; 0 \qquad \text{and} \qquad \widehat{\mathcal{A}}\,|\,\psi> \;=\; \beta\,\widehat{\mathcal{B}}\,|\,\psi>,$$

where β is a scalar. $\mathcal{A}$ and $\mathcal{B}$ are given to be canonically conjugate and Hermitian.

This problem reveals the conditions under which a minimal uncertainty relation is obtained.

For Hermitian $\mathcal{A}$ and $\mathcal{B}$, $\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right] \;=\; \left[\mathcal{A},\,\mathcal{B}\right]$, however, $\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+ \;\neq\; \left[\mathcal{A},\,\mathcal{B}\right]_+$ in general, so it is appropriate to work with "hatted" operators. That $<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi> \;=\; 0$ is a necessary, but insufficient, condition for a minimal uncertainty relation. The substance of the problem is the rearrangement of the proportionality condition using bra/ket algebra.

The anti-commutator $\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+$ is a Hermitian operator. A Hermitian operator has real eigenvalues. The expectation value $<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>$ is therefore a real scalar which means that $<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2 \geq\; 0\,.$ Since this quantity is greater than or equal to zero,

$$\frac{1}{4}<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2 \;+\; \frac{1}{4}\,<\psi|\,\mathcal{C}\,|\,\psi>^2 = \;\frac{1}{4}\,<\psi|\,\mathcal{C}\,|\,\psi>^2,$$

if and only if

$$<\psi\,|\,\big[\,\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\,\big]_+\,|\,\psi>^2\;=\;0\quad\Rightarrow\quad<\psi\,|\,\big[\,\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\,\big]_+\,|\,\psi>\;=\;0\,.$$

Then $\widehat{\mathcal{A}}\,|\,\psi>\;=\;\beta\,\widehat{\mathcal{B}}\,|\,\psi>\quad\Rightarrow\quad<\psi\,|\,\widehat{\mathcal{A}}\;=\;<\psi\,|\,\widehat{\mathcal{B}}\,\beta^*$. The product of the norms squared is

$$\begin{aligned}
\Big|\,|\,\widehat{\mathcal{A}}\,\psi>\Big|^2\Big|\,|\,\widehat{\mathcal{B}}\,\psi>\Big|^2 \;&=\; \Big|\,|\,\beta\,\widehat{\mathcal{B}}\,\psi>\Big|^2\Big|\,|\,\widehat{\mathcal{B}}\,\psi>\Big|^2\\
&=\; <\psi\,\widehat{\mathcal{B}}\,\beta\,|\,\beta\,\widehat{\mathcal{B}}\,\psi><\psi\,\widehat{\mathcal{B}}\,|\,\widehat{\mathcal{B}}\,\psi>\\
&=\; |\,\beta\,|^2<\psi\,\widehat{\mathcal{B}}\,|\,\widehat{\mathcal{B}}\,\psi><\psi\,\widehat{\mathcal{B}}\,|\,\widehat{\mathcal{B}}\,\psi>\\
&=\; <\psi\,\widehat{\mathcal{B}}\,\beta\,|\,\widehat{\mathcal{B}}\,\psi><\psi\,\widehat{\mathcal{B}}\,|\,\beta\,\widehat{\mathcal{B}}\,\psi>\\
&=\; <\psi\,\widehat{\mathcal{A}}\,|\,\widehat{\mathcal{B}}\,\psi><\psi\,\widehat{\mathcal{B}}\,|\,\widehat{\mathcal{A}}\,\psi>\\
&=\; <\psi\,\widehat{\mathcal{A}}\,|\,\widehat{\mathcal{B}}\,\psi><\psi\,\widehat{\mathcal{A}}\,|\,\widehat{\mathcal{B}}\,\psi>^*\\
&=\; \Big|\,<\psi\,|\,\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}\,|\,\psi>\,\Big|^2,
\end{aligned}$$

using the result of problem 6–9,

$$\big(\triangle\mathcal{A}\big)^2\big(\triangle\mathcal{B}\big)^2\;=\;\Big|\,|\,\widehat{\mathcal{A}}\,\psi>\Big|^2\Big|\,|\,\widehat{\mathcal{B}}\,\psi>\Big|^2\;=\;\Big|\,<\psi\,|\,\widehat{\mathcal{A}}\,\widehat{\mathcal{B}}\,|\,\psi>\,\Big|^2,$$

the relation of equality is warranted for calculations paralleling problems 6–12, 6–13, and 6–14,

$$\Rightarrow\quad\big(\triangle\mathcal{A}\big)\big(\triangle\mathcal{B}\big)\;=\;\frac{1}{2}\,\hbar$$

is a minimal uncertainty relation for $\mathcal{A}$ and $\mathcal{B}$ that are canonically conjugate and Hermitian, and also subject to the two conditions given.

Postscript: The fact that $\big[\,\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\,\big]_+\;\neq\;\big[\,\mathcal{A},\,\mathcal{B}\,\big]_+$ is left as an exercise.

The two conditions of problem 6–15 are said to saturate the inequality. They are the conditions for the minimum in the product of uncertainties. Following a short general discussion of Gaussian functions, the same two conditions will be shown to require a Gaussian wave function.

Notice that $<\psi\,|\,\big[\,\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\,\big]_+\,|\,\psi>\;=\;0$ is a necessary condition for the Heisenberg uncertainty relation to be an equality, but it is not sufficient. The condition of proportionality must also be satisfied for sufficient conditions to exist.

6–16. What is the minimal uncertainty relation for $\big[\,\mathcal{A}\,,\,\mathcal{B}\,\big]\;=\;i\beta\,\mathcal{K}$?

This problem addresses operators that are not canonically conjugate.

The product of uncertainties can only be minimized only if $\dfrac{1}{4}\,<\psi\,|\,\big[\,\widehat{\mathcal{A}}\,,\,\widehat{\mathcal{B}}\,\big]_+\,|\,\psi>^2\;=\;0\,,$

thus consider only $\qquad\big(\,\triangle\,\mathcal{A}\,\big)^2\big(\,\triangle\,\mathcal{B}\,\big)^2\;\geq\;\dfrac{1}{4}\,<\psi\,|\,\mathcal{C}\,|\,\psi>^2\,.$

For canonically conjugate pairs $\mathcal{C} \rightarrow \hbar\mathcal{I}$, but in this case $\mathcal{C} \rightarrow \beta\mathcal{K}$, so

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \geq \frac{1}{4} <\psi|\, \beta\mathcal{K}\, |\psi>^2$$

$$\Rightarrow \quad \triangle\mathcal{A}\triangle\mathcal{B} \geq \frac{\beta}{2}\left|<\mathcal{K}>\right|$$

where the absolute value is appropriate because its square is positive definite. The expectation value $<\mathcal{K}>$ may be negative, but the product of uncertainties must be non-negative.

Postscript: A commutator is an operator. If that operator is $\mathcal{I}$, as it is for canonically conjugate pairs, then the minimal uncertainty relation in general is

$$\triangle\mathcal{A}\,\triangle\mathcal{B} \geq \frac{\hbar}{2}.$$

If the commutator is other than an identity operator, the minimal uncertainty relation contains the absolute value of an expectation value of that operator. In particular,

$$\left[\mathcal{L}_x, \mathcal{L}_y\right] = i\hbar\,\mathcal{L}_z, \qquad \left[\mathcal{L}_y, \mathcal{L}_z\right] = i\hbar\,\mathcal{L}_x, \qquad \text{and} \qquad \left[\mathcal{L}_z, \mathcal{L}_x\right] = i\hbar\,\mathcal{L}_y$$

for component orbital angular momentum operators, and for component spin angular momentum

$$\left[\mathcal{S}_x, \mathcal{S}_y\right] = i\hbar\,\mathcal{S}_z, \qquad \left[\mathcal{S}_y, \mathcal{S}_z\right] = i\hbar\,\mathcal{S}_x, \qquad \text{and} \qquad \left[\mathcal{S}_z, \mathcal{S}_x\right] = i\hbar\,\mathcal{S}_y.$$

Said another way, the condition of proportionality addressed in problem 6–15 cannot be satisfied by the component angular momentum/spin operators for any non-zero state vector.

This phenomena is discussed in more detail when orbital/spin angular momentum is addressed.

6–17. Use the Heisenberg uncertainty principle to show that the Bohr model of the hydrogen atom is technically flawed.

The statement $\triangle x\,\triangle p \geq \hbar/2$ in position space is often used to demonstrate implausibility or impossibility, as seen in this problem.

One fundamental premise of the Bohr atom is that "orbits" are quantized such that $pr = n\hbar$, for $n = 1, 2, 3, \ldots$ We expect that $\triangle x \ll r$, (or $\triangle r \ll r$), and $\triangle p \ll p$ in these precisely defined orbits. Rewriting these relations

$$\frac{\triangle x}{r} \ll 1, \quad \text{and} \quad \frac{\triangle p}{p} \ll 1 \quad \Rightarrow \quad \frac{\triangle x\,\triangle p}{rp} \ll 1. \tag{1}$$

The premise $pr = n\hbar \quad \Rightarrow \quad \hbar/2 = pr/2n$, so the uncertainty principle states

$$\triangle x\,\triangle p \geq \frac{\hbar}{2} = \frac{pr}{2n} \qquad \Rightarrow \qquad \frac{\triangle x\,\triangle p}{rp} \geq \frac{1}{2n}$$

which is inconsistent with statement (1) except for large n. Since hydrogen appears to be stable in its ground state, $n = 1$, the Heisenberg uncertainty principle indicates that the Bohr model of the hydrogen atom is technically flawed.

Part 3, Gaussian Functions and Wave Packets

The bell-shaped envelopes of normal distributions in the field of statistics are called normal functions. It would be just as correct to call them Gaussian distributions and Gaussian functions. The Gaussian wave functions of quantum mechanics are closely related to the normal functions of statistics, though they are not the same things. Further, standard deviation, commonly denoted σ in statistics, is comparable to uncertainty in position, $\triangle x$ in quantum mechanics.

The matter waves of particles or electromagnetic waves of photons seem quantized. As Feynman said, "They come in lumps." The normal mathematical model is that of a **wave packet**. The idea is that the amplitude of the wave is greatest at and around where the "lump" is perceived, and diminishes farther away from the where the "lump" is perceived, so that the amplitude approaches zero at locations not near the "lump."

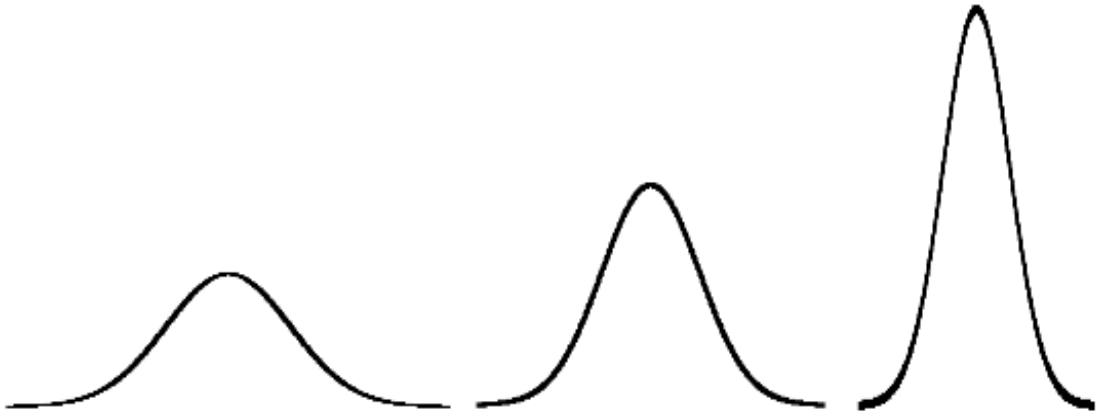
Finally, a Gaussian wave function is the form that minimizes the uncertainty in position $\triangle x$.

6–18. What is a Gaussian function?

A **Gaussian function** is of the form $f(x) = A\,b^{-cx^2}$ where b is a real constant greater than 1, c is a real constant greater than zero, and A is a normalization constant. It will be a bell-shaped curve under these conditions. It is called a **normal function** in the field of statistics.

6–19. What gives a normal/Gaussian function its bell shape?

The factor giving the curve its bell shape is b^{-x^2}, where b is any real constant including e.



small b medium b large b

Figure 6–1. Normalized Gaussian curves for increasing base b.

Notice all three illustrations have a bell shape. A Gaussian curve can be short and wide, or tall and thin. All the constants do not affect the basic bell shape of a Gaussian function. The b^{-x^2} determines that it has a bell shape.

6–20. Normalize the Gaussian wave function $\psi(x) = A\,e^{-bx^2}$.

Per problem 4–21, the Gaussian function of the form

$$f(x) = A\,e^{-bx^2} \quad \Rightarrow \quad A = \left(\frac{2b}{\pi}\right)^{1/4}$$

A second method to obtain this result is presented here. Form the square of $I = \displaystyle\int_{-\infty}^{\infty} e^{-ax^2}\,dx$, change to polar coordinates where the square of the integral is easily evaluated because of the symmetry of the Gaussian function, and then a square root yields the value of the original integral.

Let $I = \displaystyle\int_{-\infty}^{\infty} e^{-ax^2}\,dx \quad \Rightarrow \quad I^2 = \int_{-\infty}^{\infty} e^{-ax^2}\,dx \int_{-\infty}^{\infty} e^{-ay^2}\,dy = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-a(x^2+y^2)}\,dx\,dy.$

We can express this in polar coordinates, where $x^2 + y^2 = r^2$ and $dx\,dy = r\,dr\,d\phi$, so

$$I^2 = \int_0^{\infty}\int_0^{2\pi} e^{-ar^2} r\,dr\,d\phi = \int_0^{\infty} r\,e^{-ar^2}\,dr \int_0^{2\pi} d\phi$$

$$= \int_0^{\infty} r\,e^{-ar^2}\,dr \left[\phi\right]_0^{2\pi} = 2\pi \int_0^{\infty} r\,e^{-ar^2}\,dr$$

$$= 2\pi\left[-\frac{1}{2a}\,e^{-ar^2}\right]_0^{\infty} = \frac{2\pi}{2a}\left[-\cancel{e^{-a(\infty)^2}} + e^0\right] = \frac{\pi}{a} \quad \Rightarrow \quad I = \sqrt{\frac{\pi}{a}}.$$

Then knowing the value of the integral,

$$<\psi\,|\,\psi> = 1 \quad \rightarrow \quad \int \left(A\,e^{-bx^2}\right)^* A\,e^{-bx^2}\,dx = 1 \quad \Rightarrow \quad |\,A\,|^2 \int e^{-2bx^2}\,dx = 1$$

$$\Rightarrow \quad |\,A\,|^2 \sqrt{\frac{\pi}{a}} = 1 \quad \text{where } a = 2b \text{ here, thus } \quad |\,A\,|^2 \sqrt{\frac{\pi}{2b}} = 1 \quad \Rightarrow \quad A = \left(\frac{2b}{\pi}\right)^{1/4}$$

consistent with the earlier result, and $\psi(x) = \left(\dfrac{2b}{\pi}\right)^{1/4} e^{-bx^2}$.

Postscript: A Gaussian wave function of quantum mechanics is often written $\psi(x) = A\,e^{-x^2/2\alpha^2}$. Thus, if the constant b is $\dfrac{1}{2\alpha^2}$, $\psi(x) = \dfrac{1}{(\pi\,\alpha^2)^{1/4}}\,e^{-x^2/\,2\alpha^2}$.

6–21. Compare a normal function of statistics to a Gaussian wave function of quantum mechanics.

A general normal function in statistics is

$$f\,(x) \;=\; \frac{1}{\sqrt{2\pi}\;\sigma}\,e^{-(x-\mu)^2/2\sigma^2}$$

where μ is the mean and σ is the standard deviation. The independent variable is x. The constants $\dfrac{1}{\sqrt{2\pi}\;\sigma}$ ensure the area under the curve is 1. In effect, these constants determine the height of a normalized bell-shaped curve. The mean, μ, will shift the bell shape to the right or the left. The $2\sigma^2$ in the denominator of the exponential determine whether the bell shape is narrow or wide. The choice of the base of e is essentially arbitrary and is used in statistics primarily for the purpose of standardization.

The base e in quantum mechanics is from the integral of $\dfrac{d\,\psi(x)}{\psi(x)}$, so is not arbitrary.

The expectation value $<x>$ of quantum mechanics is the same as the mean μ of statistics.

$$\psi\,(x) \;=\; \frac{1}{(\pi\,\alpha^2)^{1/4}}\,e^{-(x-<x>)^2/\,2\alpha^2}$$

when the wave function is centered at $<x>$ rather the than the origin. Consider $<x> \,=\, \mu \,=\, 0$ for the rest of this discussion. Should $<x> \,\neq\, 0$, changes to the following argument are cosmetic.

The primary difference between the normal function of statistics and the Gaussian wave functions of quantum mechanics is the manner in which probability is calculated. In statistics,

$$P(a<x<b) \;=\; \int_a^b f(x)\,dx \;=\; \int_a^b \frac{1}{\sqrt{2\pi}\;\sigma}\,e^{-x^2/2\sigma^2}\,dx \;=\; \frac{1}{\sqrt{2\pi}\;\sigma}\int_a^b e^{-x^2/2\sigma^2}\,dx \qquad (1)$$

while quantum mechanically,

$$\begin{aligned} P(a<x<b) \;&=\; \int_a^b \left|\,\psi(x)\right|^2 dx \;=\; \int_a^b \left(\frac{1}{(\pi\,\alpha^2)^{1/4}}\,e^{-x^2/\,2\alpha^2}\right)^{*} \frac{1}{(\pi\,\alpha^2)^{1/4}}\,e^{-x^2/\,2\alpha^2}\,dx \\ &=\; \frac{1}{\sqrt{\pi}\,\alpha}\int_a^b e^{-x^2/\alpha^2}\,dx \qquad (2) \end{aligned}$$

A simple comparison of the final integrals in lines (1) and (2) reveals these are precisely the same, to include the normalization constants, if $\quad \alpha^2 \;=\; 2\sigma^2 \quad \Rightarrow \quad \sigma \;=\; \dfrac{\alpha}{\sqrt{2}}$.

Postscript: The probability density $\left|\,\psi(x)\right|^2$, rather than the wave function $\psi(x)$, is comparable to a general normal function of statistics. We shall find that $\triangle x \;=\; \dfrac{\alpha}{\sqrt{2}}$ for the minimum uncertainty wave function (which is Gaussian). It is tempting to combine this with the last equation to conclude that uncertainty in position is the same as standard deviation. This is correct in this case and for discrete systems, but other wave functions are possible. Thinking of uncertainty in position as related to standard deviation, rather than the same as standard deviation, is a healthy approach and may be useful in developing understanding of uncertainty.

6–22. What is a Gaussian wave packet?

A particle has a wave nature but is somewhat localized in space and time (they come in lumps). A wave packet is a model using a functional form as an envelope to contain a wave whose amplitude varies with position within the envelope. A function of the form $A\,b^{-cx^2}$ where $b > 1$ and $c > 0$ creates a Gaussian curve as seen in figure 6–2. Multiply by negative 1 to obtain its reflection in the x-axis, and together they form an envelope as seen in figure 6–3. Figure 6–4 attempts to illustrate a plane wave bounded by this envelope. The envelope itself is not physical, so an illustration of a Gaussian wave packet in two dimensions is attempted in figure 6–5 without the envelope. What is "waving" is related to the probability amplitude of a photon or an electron, proton, or other particle. Euler's number is commonly used as the base of a Gaussian function per problem 6–24.

Figure 6–2. A Gaussian curve.

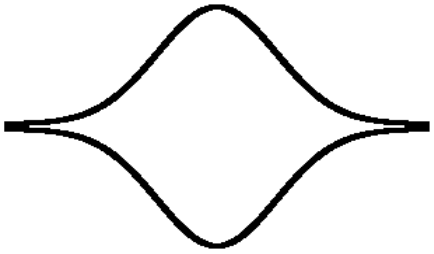


Figure 6–3. A Gaussian envelope.

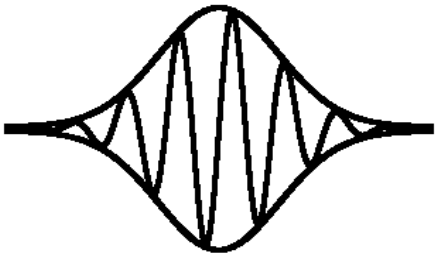


Figure 6–4. A Gaussian wave packet within an envelope.

Figure 6–5. A Gaussian wave packet.

Postscript: There are dozens, if not hundreds, of wave packet models in addition to a Gaussian form, for instance, rectangular, triangular, Lorentzian, etc. The Gaussian wave packet is the most useful. The minimum uncertainty wave function is a Gaussian wave function.

6–23. Where does Ehrenfest's theorem apply?

Ehrenfest's theorem is applicable when a classical force is uniform over the width of the particle wave packet. Classical force is the derivative of the potential, $F = -\dfrac{d}{dx}V(x)$. If the packet is large compared to variations in the potential, the derivative varies over its width. If the wave packet is small compared to variations in the potential, the "particle" experiences a uniform force since the derivative over its width is constant, or almost constant.

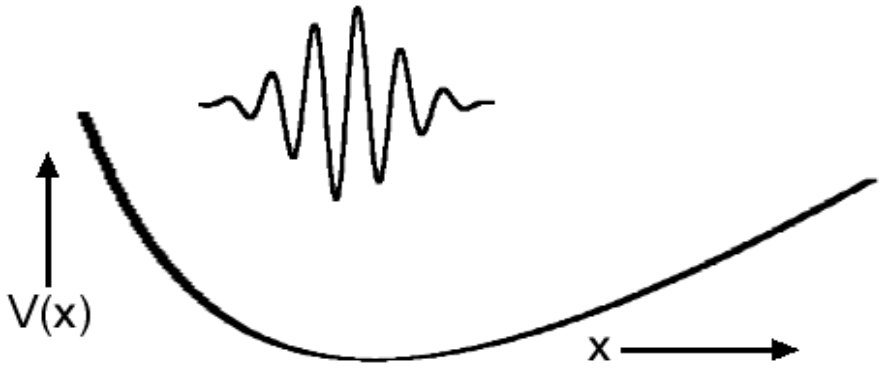


Figure 6–6. Derivative varies over width of wave packet. Ehrenfest's theorem does not apply.

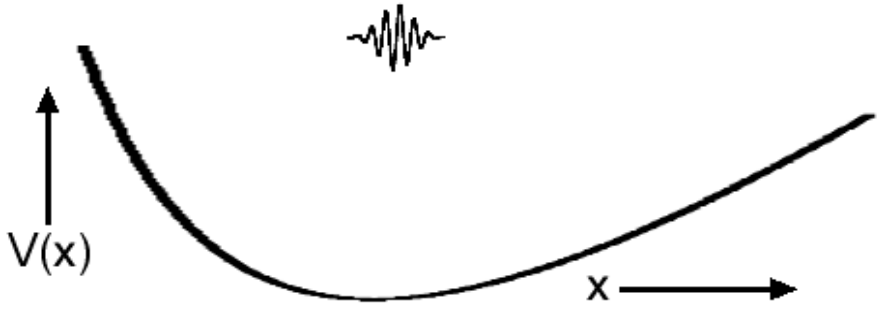


Figure 6–7. Derivative varies little over width of wave packet. Ehrenfest's theorem applies.

6–24. Assume that $<\psi|\left[\mathcal{X},\mathcal{P}\right]_+|\psi> \;=\; 0$ and $\mathcal{P}\,|\psi> \;=\; \beta\,\mathcal{X}\,|\psi>$.

(a) Show that these conditions require that the wave function in position space is Gaussian.

(b) Substitute $\beta \;=\; i\hbar/\alpha^2$ and interpret the result.

This problem joins the Gaussian wave function and the uncertainty relations to canonical operators under conditions that require the relation of equality in the general uncertainty principle. Act with $<x|$ to establish the second condition in position space. Use the position space representations of $\mathcal{X}$ and $\mathcal{P}$. This results in a variables separable differential equation $\Rightarrow \quad \psi(x) \;=\; e^{i\beta x^2/\,2\hbar}$. Substitute the expression given for β to realize a Gaussian function.

(a) Acting with $<x|$ to establish the second condition in position space, and using the position space representations of $\mathcal{X}$ and $\mathcal{P}$,

$$<x|\,\mathcal{P}\,|\psi> \;=\; <x|\,\beta\,\mathcal{X}\,|\psi> \qquad \Rightarrow \qquad -i\hbar\,\frac{d}{dx}\,<x|\,\psi> \;=\; \beta\,x\,<x|\,\psi>$$

$$\Rightarrow \qquad -i\hbar\,\frac{d}{dx}\,\psi(x) \;=\; \beta\,x\,\psi(x) \qquad \Rightarrow \qquad \frac{d\,\psi(x)}{dx} \;=\; \frac{i}{\hbar}\,\beta\,x\,\psi(x) \qquad \Rightarrow \qquad \frac{d\,\psi(x)}{\psi(x)} \;=\; \frac{i}{\hbar}\,\beta\,x\,dx$$

$$\Rightarrow \qquad \ln\psi(x) \;=\; \frac{i}{\hbar}\,\beta\,\frac{x^2}{2} \qquad \Rightarrow \qquad \psi(x) \;=\; e^{i\beta x^2/\,2\hbar}\,.$$

(b) $\beta \;=\; i\,\dfrac{\hbar}{\alpha^2} \qquad \Rightarrow \qquad \psi\,(x) \;=\; e^{-\hbar x^2/\,2\hbar\alpha^2} \qquad \Rightarrow \qquad \psi\,(x) \;=\; e^{-x^2/\,2\alpha^2}$

which is an unnormalized, stationary, Gaussian wave packet.

Postscript: Normalized this is $\dfrac{e^{-x^2/\,2a^2}}{(\pi a^2)^{1/4}}$ as shown earlier.

Only the proportionality condition is used in the reduction, however and as indicated earlier, the condition $<\psi\,|\,\big[\,\mathcal{X},\,\mathcal{P}\,\big]_+\,|\,\psi> \;=\; 0\,,$ though not sufficient, is still necessary.

6–25. Find the uncertainty in position of the normalized Gaussian function $\dfrac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,.$

This problem supports the postscript to problem 6–21. Find $<x>$ and $<x^2>$. Form 3.461.2 from Gradshteyn and Ryzhik,

$$\int_0^\infty x^{2n}\,e^{-px^2}\,dx \;\;=\;\; \frac{(2n-1)!!}{2\,(2p)^n}\,\sqrt{\frac{\pi}{p}}$$

should be useful. Uncertainty is $\triangle x \;=\; \big(\,<x^2>\,-\,<x>^2\,\big)^{1/2}$. Remember odd and even integrand between symmetric limits arguments.

$$<x> \;=\; \int_{-\infty}^{\infty}\psi^*\,(x)\;x\;\psi\,(x)\;dx \;=\; \int_{-\infty}^{\infty}\frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\;(x)\;\frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,dx \;\;=\;\; \frac{1}{\alpha\sqrt{\pi}}\int_{-\infty}^{\infty}x\,e^{-x^2/\,\alpha^2}\,dx \;\;=\;\; 0$$

because the integral of an odd function between symmetric limits is zero.

$$<x^2> \;=\; \int_{-\infty}^{\infty}\psi^*\,(x)\;x^2\;\psi\,(x)\;dx \;=\; \int_{-\infty}^{\infty}\frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\;(x^2)\;\frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,dx \;\;=\;\; \frac{1}{\alpha\sqrt{\pi}}\int_{-\infty}^{\infty}x^2\,e^{-x^2/\,\alpha^2}\,dx$$

$$=\;\; \frac{2}{\alpha\sqrt{\pi}}\int_0^\infty x^2\,e^{-x^2/\,\alpha^2}\,dx \;\;=\;\; \frac{2}{\alpha\sqrt{\pi}}\;\;\frac{(2-1)!!}{2\;\;(2(1/\alpha^2))^1}\;\sqrt{\frac{\pi}{1/\alpha^2}} \;\;=\;\; \frac{2}{\alpha\sqrt{\pi}}\;\frac{\alpha^2}{4}\;\alpha\;\sqrt{\pi} \;\;=\;\; \frac{\alpha^2}{2}$$

using an even function between $-\infty$ and ∞ is twice the integral between zero 0 and ∞.

$$\triangle x \;\;=\;\; \big(\,<x^2>\,-\,<x>^2\,\big)^{1/2} \;\;=\;\; \left(\frac{\alpha^2}{2}-0\right)^{1/2} \;\;=\;\; \frac{\alpha}{\sqrt{2}}\,.$$

Postscript: Uncertainty in position is the square root of one fourth of the denominator of the argument of the exponential for a Gaussian wave function. Uncertainty is $\triangle x = 1/2\sqrt{b}$ for $A\,e^{-bx^2}$, for example. Should complex values be involved, this short cut translates to uncertainty being the square root of one half the denominator of the exponential of the probability density.

6–26. Find the uncertainty in momentum of the normalized Gaussian function $\dfrac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}$.

This problem parallels problem 6–25. Find $< p > \;=\; \int \psi^*(x)\,\left(-i\hbar\,\dfrac{d}{dx}\right)\,\psi(x)\,dx$. Then find the second moment similarly using p^2. Form 3.461.2 from Gradshteyn and Ryzhik used in problem 6–25 is again pertinent. Uncertainty is $\triangle p \;=\; \left(< p^2 > - < p >^2\right)^{1/2}$. Again, integrals of odd/even functions between symmetric limits occur.

$$< p > \;=\; \int_{-\infty}^{\infty} \psi^*(x)\,\left(-i\hbar\,\frac{d}{dx}\right)\,\psi(x)\,dx \;=\; \int_{-\infty}^{\infty} \frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,\left(-i\hbar\,\frac{d}{dx}\right)\,\frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,dx$$

$$= \frac{-i\hbar}{\alpha\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\,2\alpha^2}\,\left(\frac{-2x}{2\alpha^2}\right)\,e^{-x^2/\,2\alpha^2}\,dx \;=\; \frac{i\hbar}{\alpha^3\sqrt{\pi}} \int_{-\infty}^{\infty} x\,e^{-x^2/\,\alpha^2}\,dx \;=\; 0$$

because the integral of an odd function between symmetric limits is zero.

$$\begin{aligned}
< p^2 > \;&=\; \int_{-\infty}^{\infty} \psi^*(x)\,\left(-i\hbar\,\frac{d}{dx}\right)\left(-i\hbar\,\frac{d}{dx}\right)\,\psi(x)\,dx \\
&=\; \int_{-\infty}^{\infty} \frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,\left(-i\hbar\,\frac{d}{dx}\right)\left(-i\hbar\,\frac{d}{dx}\right)\,\frac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,dx \\
&=\; \frac{-\hbar^2}{\alpha\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\,2\alpha^2}\,\left(\frac{d}{dx}\right)\left(\frac{d}{dx}\right)\,e^{-x^2/\,2\alpha^2}\,dx \\
&=\; \frac{-\hbar^2}{\alpha\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\,2\alpha^2}\,\left(\frac{d}{dx}\right)\left(\frac{-2x}{2\alpha^2}\right)\,e^{-x^2/\,2\alpha^2}\,dx \\
&=\; \frac{\hbar^2}{\alpha^3\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\,2\alpha^2}\,\left(\frac{d}{dx}\right)x\;\,e^{-x^2/\,2\alpha^2}\,dx \\
&=\; \frac{\hbar^2}{\alpha^3\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\,2\alpha^2}\,\left(e^{-x^2/\,2\alpha^2} - \frac{x^2}{\alpha^2}\,e^{-x^2/\,2\alpha^2}\right)dx \\
&=\; \frac{\hbar^2}{\alpha^3\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2/\,\alpha^2}\,dx \;-\; \frac{\hbar^2}{\alpha^5\sqrt{\pi}} \int_{-\infty}^{\infty} x^2\,e^{-x^2/\,\alpha^2}\,dx
\end{aligned}$$

The first integral is $\alpha\sqrt{\pi}$ using the result of problem 6–20. The second integral is $\dfrac{\alpha^3\sqrt{\pi}}{2}$ using an intermediate result from problem 6–25 (notice limits on the integrals).

$$< p^2 > \;=\; \frac{\hbar^2}{\alpha^3\sqrt{\pi}}\,\alpha\sqrt{\pi} \;-\; \frac{\hbar^2}{\alpha^5\sqrt{\pi}}\,\frac{\alpha^3\sqrt{\pi}}{2} \;=\; \frac{\hbar^2}{\alpha^2} \;-\; \frac{\hbar^2}{2\alpha^2} \;=\; \frac{\hbar^2}{2\alpha^2}$$

$$\Rightarrow \qquad \triangle p \;=\; \left(< p^2 > - < p >^2\right)^{1/2} \;=\; \left(\frac{\hbar^2}{2\alpha^2} - 0\right)^{1/2} \;=\; \frac{\hbar}{\alpha\sqrt{2}}\,.$$

Postscript: The normalization constants are a necessary evil in the calculations of problems 6–25 and 6–26. Lumping them into an A or B and then translating them back into the constants of the problem at hand when convenient may result in more streamlined calculations. All constants were carried in problems 6–25 and 6–26 to make problem 6–27 most straightforward.

6–27. Show that product of the uncertainties in position and momentum are minimized by the Gaussian wave function.

A short summary is appropriate. A Gaussian function is introduced to be used as an envelope for a wave function, resulting in the concept of a Gaussian wave packet (to be amplified in problem 6–28). The two conditions of problem 6–24 are those for a minimum uncertainty product from the general uncertainty relation. These conditions are shown to require a Gaussian wave function. All that is left is to form the product of the uncertainties calculated in problems 6–25 and 6–26.

The most frequently encountered statement of the Heisenberg uncertainty principle is

$$\triangle x \triangle p \geq \frac{\hbar}{2}.$$

Using the form $\psi(x) = \dfrac{e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}$ results in the product

$$\triangle x \triangle p = \frac{\alpha}{\sqrt{2}} \frac{\hbar}{\alpha\sqrt{2}} = \frac{\hbar}{2}$$

as an <u>equality</u>, and is the minimum of the product of the uncertainties in position and momentum.

6–28. Construct a normalized, traveling, Gaussian wave function.

A general plane wave is $f(x, t) = A e^{i(kx-\omega t)} + B e^{-i(kx+\omega t)}$ where the first term is that portion of the wave traveling in the positive direction and the second is that portion of the plane wave traveling in the negative direction. It is not acceptable as a wave function because it cannot be normalized . . . by itself. Should the plane wave, or some portion of the plane wave, be placed inside an envelope that is already normalized an acceptable wave function results.

Consider only that portion of the plane wave traveling in the positive direction, or $f(x, t) = A e^{i(kx-\omega t)}$. Time as a variable is an unnecessary complication at the moment, so $f(x) = A e^{ikx}$. The product of this function and the Gaussian wave packet is

$$\psi(x) = \frac{e^{ikx}\, e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}$$

which is the desired result realizing that e^{ikx} is of unit magnitude so the normalization constants of the Gaussian wave packet remain $\dfrac{1}{(\pi\alpha^2)^{1/4}}$.

Postscript: It is often convenient to work in terms of wavenumber $k = \dfrac{2\pi}{\lambda}$. At other times it is convenient to work in terms of momentum that is related to wavelength, and thus wavenumber, through the de Broglie relation,

$$\lambda = \frac{h}{p} \quad \Rightarrow \quad p = \frac{h}{\lambda} \quad \Rightarrow \quad p = \frac{h}{2\pi}\,\frac{2\pi}{\lambda} = \hbar\, k \quad \Rightarrow \quad k = \frac{p}{\hbar}. \quad \text{Thus}$$

$$\psi(x) = \frac{e^{ipx/\hbar}\, e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}$$

is an equivalent wave function. The Gaussian wave function is often seen with k_0 or p_0 to indicate that wavenumber or momentum is a constant.

The factor e^{ikx} is often called the **phase** of a Gaussian wave function. It has no affect on probability density, and thus, no affect on probability because

$$\left|\,\psi(x)\,\right|^2 = \left(\frac{e^{ikx}\, e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}\right)^* \left(\frac{e^{ikx}\, e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}\right) = \frac{e^{-ikx}\, e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,\frac{e^{ikx}\, e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}} = \frac{e^{-x^2/\alpha^2}}{(\pi\alpha^2)^{1/2}}$$

6–29. (a) Find the momentum space wave function for $\psi(x) = \dfrac{e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}$.

(b) Interpret this result.

Chapter 5 briefly discusses Fourier transforms. Remember

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} g(k)\, e^{ikx}\, dk\,, \qquad g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx\,,$$

where the function $f(x)$ is the Fourier transform of $g(k)$, and $g(k)$ is the Fourier transform of $f(x)$. The de Broglie relation associates wavelength or wavenumber, and momentum,

$$\lambda = \frac{h}{p} \quad \Rightarrow \quad \frac{2\pi}{k} = \frac{h}{p} \quad \Rightarrow \quad k = \frac{p}{\hbar}\,.$$

Substitute $p/\hbar$ for k in both Fourier transforms. This means the differential $dk = dp/\hbar$ in the integral for $f(x)$. Symmetrize the $1/\hbar$ from this differential by placing a factor $1/\sqrt{\hbar}$ in both integrals, and the result is the quantum mechanical form of the Fourier transforms,

$$f(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \widehat{g}\,(p)\, e^{ipx/\hbar}\, dp, \qquad \widehat{g}\,(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} f(x)\, e^{-ipx/\hbar}\, dx\,.$$

Our usual use of these relations is to transform a wave function in position space to momentum space (or vice versa), so will be applied

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \widehat{\psi}\,(p)\, e^{ipx/\hbar}\, dp, \qquad \widehat{\psi}\,(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \psi(x)\, e^{-ipx/\hbar}\, dx\,.$$

Form 3.323.2 from Gradshteyn and Ryzhik,

$$\int_{-\infty}^{\infty} e^{-a^2x^2 \pm bx}\,dx \;=\; \frac{\sqrt{\pi}}{a}\; e^{b^2/4a^2} \quad \text{should be useful.}$$

(a) $$\widehat{\psi}\,(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi\,(x)\; e^{-ipx/\hbar}\,dx \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \frac{1}{(\pi\alpha^2)^{1/4}}\, e^{-x^2/2\alpha^2}\, e^{-ipx/\hbar}\,dx$$

$$=\; \frac{1}{\sqrt{2\pi\hbar}}\; \frac{1}{(\pi\alpha^2)^{1/4}} \int_{-\infty}^{\infty} e^{-x^2/2\alpha^2 - ipx/\hbar}\,dx\,.$$

Using $a^2 \;=\; \dfrac{1}{2\alpha^2}$, and $b \;=\; \dfrac{ip}{\hbar}$, our integral is

$$\widehat{\psi}\,(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}}\; \frac{1}{(\pi\alpha^2)^{1/4}}\; \sqrt{\pi}\; \sqrt{2\alpha^2}\; \exp\left(\frac{(ip/\hbar)^2}{4/2\alpha^2}\right) \;=\; \left(\frac{\alpha^2}{\pi\hbar^2}\right)^{1/4} e^{-p^2\alpha^2/2\hbar^2}.$$

(b) Notice that $\widehat{\psi}\,(p)$ is also an exponential function with a negative argument that is a constant times the independent variable p squared. In fact, $\widehat{\psi}(p)$ is also a Gaussian wave function.

Postscript: We shall encounter $\psi\,(x) \;=\; \dfrac{e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}$ and $\psi\,(x) \;=\; \dfrac{e^{ikx}\; e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}$ and related momentum space wave functions in the future, particularly in chapter 7 discussing the free particle.

6–30. Using a Gaussian wave packet, find the expectation value of the time rate of change of position in position space assuming that potential energy is a function only of position.

The fact that the Gaussian wave packet is an excellent model is sometimes overlooked in the relatively strenuous mathematics. The Gaussian wave packet is the assumed standard in the absence of additional information. The normalized Gaussian wave packet can be described

$$\psi\,(x) \;=\; \frac{e^{ip_0x/\hbar}e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}, \quad \text{and remember that in one spatial dimension} \quad \mathcal{P} \;=\; -i\hbar\,\frac{d}{dx}\,,$$

so using the result of problem 6–4, $<\dot{\mathcal{X}}> \;=\; \dfrac{<\mathcal{P}>}{m}$, the desired expectation value is

$$<\dot{\mathcal{X}}> \;=\; \frac{<\mathcal{P}>}{m} \;=\; \frac{1}{m}\int_{-\infty}^{\infty} \psi^*(x)\,\left(-i\hbar\,\frac{d}{dx}\right)\psi(x)\,dx\,.$$

This becomes a Gaussian integral and the integral of an odd function between symmetric limits.

Using the result from problem 6–28,

$$
\begin{aligned}
<\dot{\mathcal{X}}> &= \frac{-i\hbar}{m}\int_{-\infty}^{\infty}\frac{e^{-ip_0x/\hbar}e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\left(\frac{d}{dx}\right)\frac{e^{ip_0x/\hbar}e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}\,dx \\
&= \frac{-i\hbar}{m\alpha\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-ip_0x/\hbar}e^{-x^2/\,2\alpha^2}\left(\frac{d}{dx}\right)e^{ip_0x/\hbar}e^{-x^2/\,2\alpha^2}\,dx \\
&= \frac{-i\hbar}{m\alpha\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-ip_0x/\hbar}e^{-x^2/\,2\alpha^2}\left(\frac{ip_0}{\hbar}e^{ip_0x/\hbar}e^{-x^2/\,2\alpha^2} - \frac{x}{\alpha^2}e^{ip_0x/\hbar}e^{-x^2/\,2\alpha^2}\right)dx \\
&= \frac{-i\hbar}{m\alpha\sqrt{\pi}}\frac{ip_0}{\hbar}\int_{-\infty}^{\infty}e^{-x^2/\,\alpha^2}\,dx + \frac{i\hbar}{m\alpha\sqrt{\pi}}\frac{1}{\alpha^2}\int_{-\infty}^{\infty}x\,e^{-x^2/\,\alpha^2}\,dx \\
&= \frac{p_0}{m\alpha\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-x^2/\,\alpha^2}\,dx + \frac{i\hbar}{m\alpha^3\sqrt{\pi}}\int_{-\infty}^{\infty}x\,e^{-x^2/\,\alpha^2}\,dx.
\end{aligned}
$$

The second integrand is the product of an odd and even function so is an odd function. The integral of an odd function evaluated between symmetric limits is zero. The first integral is Gaussian and is $\sqrt{\pi\alpha^2} = \alpha\sqrt{\pi}$. The expectation value then, is

$<\dot{\mathcal{X}}> = \frac{p_0}{m\alpha\sqrt{\pi}}\,\alpha\sqrt{\pi} = \frac{p_0}{m} = \frac{mv_0}{m} = v_0$, which you recognize from introductory physics.

Exercises

6–31. Show $\left[\mathcal{X}, \mathcal{P}\right] = i\hbar$ in momentum space.

See problem 6–3. Problem 6–5 provides appropriate representations. Operate on $\widehat{g}(p)$.

6–32. Show that $\left[\mathcal{P}, \mathcal{X}\right] = -i\hbar$ in both position and momentum space.

Use representations as seen in problem 6–5. The procedures of problem 6–3 and exercise 6–31 are pertinent. Operate on $f(x)$ in position space and $\widehat{g}(p)$ in momentum space.

6–33. Show that $<\mathcal{A}>$ is a real number given that $\mathcal{A}$ is Hermitian.

The basic definition of expectation value is $<\mathcal{A}> = \sum P(\alpha_i)\,\alpha_i$, where α_i are the eigenvalues. The observables and eigenvalue postulates are coupled in that the eigenvalues of a Hermitian operator are real. Then, what are probabilities?

6–34. Show that $<2\,|\,1> = <1\,|\,2>^*$.

This is a straightforward reduction that has been used previously and will be used in problems that follow involving the Schwarz inequality. Let

$$|\,1> = \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \vdots \end{pmatrix} \qquad \text{and} \qquad |\,2> = \begin{pmatrix} a \\ b \\ c \\ \vdots \end{pmatrix}.$$

6–35. Show that $\left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_+^\dagger = \left[\widehat{\mathcal{A}}, \widehat{\mathcal{B}}\right]_+$, if the operators $\mathcal{A}$ and $\mathcal{B}$ are Hermitian.

The anti-commutator is Hermitian if the operators are Hermitian. Stated without proof and used in the derivation of the general uncertainty relation, this exercise addresses that detail. Expand the anti-commutator, remember $\left(\Lambda\,\Omega\right)^\dagger = \Omega^\dagger\,\Lambda^\dagger$, and that the "hatted" operators are Hermitian.

6–36. Show that $\left[\widehat{\mathcal{A}},\, \widehat{\mathcal{B}}\right]_+ \neq \left[\mathcal{A},\, \mathcal{B}\right]_+$ in general.

Follow the derivation of $\left[\widehat{\mathcal{A}},\, \widehat{\mathcal{B}}\right] = \left[\mathcal{A},\, \mathcal{B}\right]$ in problem 6–7.

6–37. Show that $\widehat{\psi}\,(p) = \left(\dfrac{\alpha^2}{\pi\hbar^2}\right)^{1/4} e^{-p^2\alpha^2/2\hbar^2}$ is dimensionally correct.

Probability is $\left|\widehat{\psi}\,(p)\right|^2 dp$ in momentum space and is dimensionless. The differential dp has dimensions of momentum, so probability density $\left|\widehat{\psi}\,(p)\right|^2$ must have the dimensions $\dfrac{1}{\text{momentum}}$, and $\widehat{\psi}\,(p)$ must have the dimensions $\dfrac{1}{\sqrt{\text{momentum}}}$. The argument of an exponential must be dimensionless. Remember that α has dimensions of length.

6–38. Find the uncertainty in position of $\psi\,(x) = \dfrac{e^{-(x-b)^2\,/\,2a^2}}{(\,\pi\,a^2)^{1/4}}$.

The functions $f\,(x) = e^{-bx^2}$ seen in various forms throughout part 3 of this chapter are bell-shaped curves centered at $x = 0$. The given $\psi\,(x)$ is Gaussian function centered at $x = b$. The problems calculating $\triangle x$ and $\triangle p$ should provide direction. Change variables to $y = x - b$. Calculate $<x>$, calculate $<x^2>$, and then calculate $\triangle x = \left(<x^2> - <x>^2\right)^{1/2}$. You should find $<x> = b$, $<x^2> = \dfrac{a^2}{2} + b^2$, and $\triangle x = \dfrac{a}{\sqrt{2}}$. $\displaystyle\int_0^\infty e^{-q^2x^2}\,dx = \frac{\sqrt{\pi}}{2q}$ and the integral used in problem 6–25 may be of use.

Uncertainty (and/or standard deviation if you are doing statistics), is independent of location. The width of the bell shape is independent of the location of the peak. Notice the result is consistent with that of problem 6–25. This problem reinforces the claim of problem 6–21 that the location of the peak of a bell-shaped curve is cosmetic.

6–39. Show that $<\dot{\mathcal{P}}> = -<\dfrac{d\,V\,(x)}{dx}>$ where potential energy is a function of position only.

The second common application of Ehrenfest's theorem is a quantum mechanical equivalent of Newton's second law.

Substitute $\mathcal{P}$ for $\mathcal{A}$ in Ehrenfest's theorem. The commutator

$$\left[\mathcal{H},\, \mathcal{P}\right] = \left[\frac{\mathcal{P}^2}{2m} + \mathcal{V}\,(\mathcal{X}),\, \mathcal{P}\right] = \left[\mathcal{V}\,(\mathcal{X}),\, \mathcal{P}\right],$$

using the fact that the momentum operator commutes with itself and powers of itself. Represent the last expression in position space. Remember to use a $\psi\,(x)$ on which the commutator operates.

6–40. Find the inflection points of (a) $f(x) = \dfrac{1}{\sqrt{2\pi}\ \sigma}\, e^{-x^2/2\sigma^2}$ and

(b) $\psi(x) = \dfrac{e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}$.

(c) Find the inflection points of $\left|\psi(x)\right|^2$ using $\psi(x)$ from part (b)

The normal functions of statistics and the Gaussian wave functions of quantum mechanics may seem quite complicated to those seeing them for the first time. This exercise, as well as many problems early in part 3, attempt to provide insight into why some surrounding conventions exist. You may be surprised to find that the inflection points are at $\pm\sigma$, $\pm\alpha$, and $\pm\alpha/\sqrt{2}$. Might part (a) found the original definition of standard deviation for a normal function?

Remember inflection points are where the concavity of a curve changes. A normal/Gaussian curve is concave downward near the peak, but changes to concave upward at some distance away from the peak. Locate these inflection points by setting the second derivative equal to zero and solving for x. All of the curves in this exercise are centered at $x = 0$. Again, it is just cosmetics to adjust should they be centered at other than the origin.

6–41. What is the uncertainty in position if $\psi(x) = A\, e^{-x^2/2a^2 + x/2b}$?

The form $\psi(x) = A\, e^{-x^2/2a^2}$ may be the most useful form of a Gaussian wave function, but there are others. As before, normalize the wave function, calculate $<x>$, calculate $<x^2>$, and then calculate $\triangle x = \left(<x^2> - <x>^2 \right)^{1/2}$. You may need the basic Gaussian integral (see exercise 6–38), form 3.323.2 from Gradshteyn and Ryzhik (see problem 6–29), and form 3.462.2 from Gradshteyn and Ryzhik,

$$\int_{-\infty}^{\infty} x^n\, e^{-px^2+2qx}dx \;=\; \frac{1}{2^{n-1}p}\,\sqrt{\frac{\pi}{p}}\,\frac{d^{n-1}}{dq^{n-1}}\,qe^{q^2/p}, \quad p > 0\,.$$

Use this integral with $n = 1$ for $<x>$ and with $n = 2$ for $<x^2>$. The $n = 2$ case requires differentiation. If you are not familiar with generation by differentiation, consider

$$\frac{d^{2-1}}{dq^{2-1}}\,qe^{q^2/p} \;=\; \frac{d}{dq}\,qe^{q^2/p} \;=\; e^{q^2/p} \;+\; q\left(\frac{2q}{p}\right)e^{q^2/p} \;=\; \left(1+\frac{2q^2}{p}\right)\,e^{q^2/p},$$

which is an example for the case $n = 2$. The expression $\dfrac{d^0}{dx^0}$ is equivalent to 1 for $n = 1$.

The normalization constant is identical to that given in problem 6–25 and exercise 6–38. You should also find that the uncertainty is the same as the uncertainties in problem 6–25 and exercise 6–38. A portion of the reason for exercises 6–38 and 6–41 is to illustrate that modifications to the basic Gaussian shape are not necessarily relevant, rather the important thing to recognize is that the form is Gaussian.

Chapter 7

The Free Particle

A free particle experiences no forces, or equivalently, the potential energy function is zero. Besides being useful in itself, the free particle is a portion of the solutions to many problems at locations where the potential energy function is zero, though the overall potential energy function is non-zero. It is also a first approximation to a particle immersed in a very weak potential. A zero potential, the free particle, should be among the simplest that quantum mechanics can address.

Wave packets incorporating both a particle and wave nature are used extensively to model free particles. The Gaussian wave packet is dominantly the most popular form though other forms are possible. Time as a variable becomes important in this chapter because the wave packet for a massive particle spreads as time changes, meaning free space is dispersive.

7–1. Find the eigenvalues of a free particle in abstract Hilbert space. Interpret the result.

The free particle is one on which there are no forces, *i.e.*, the free particle is devoid of interactions. No forces means

$$F \;=\; -\frac{d\,V\,(x)}{dx} \;=\; 0 \quad \Rightarrow \quad V\,(x) \;=\; \text{constant.} \quad \text{Choose } V\,(x) \;=\; 0\,,$$

from which the Hamiltonian follows. Remember that every operator commutes with itself and powers of itself, and this will mean that $\big[\mathcal{H},\,\mathcal{P}\,\big] \;=\; 0\,,$ so $\mathcal{H}$ and $\mathcal{P}$ share a common eigenbasis. Use the time-independent Schrodinger equation $\mathcal{H}\,|\,E>\;=\;E_n\,|\,E>\,.$

The classical Hamiltonian for a particle is

$$H \;=\; \frac{p^2}{2m} \;+\; V\,(x) \quad \Rightarrow \quad \mathcal{H} \;=\; \frac{\mathcal{P}^2}{2m} \;+\; \mathcal{V}\,(\mathcal{X})$$

is the quantum mechanical Hamiltonian. The potential energy function for a free particle is chosen

$$V\,(x) \;=\; 0 \quad \Rightarrow \quad \mathcal{V}\,(\mathcal{X}) \;=\; 0 \quad \Rightarrow \quad \mathcal{H} \;=\; \frac{\mathcal{P}^2}{2m}\,.$$

The time-independent Schrodinger equation is

$$\mathcal{H}\,|\,E>\;=\;E_n\,|\,E> \quad \Rightarrow \quad \frac{\mathcal{P}^2}{2m}\,|\,E> \;=\; E_n\,|\,E>\,.$$

This Hamiltonian is a form of a power, proportional to a square, of the momentum operator. Since

$$\big[\mathcal{P}^2,\,\mathcal{P}\,\big] \;=\; 0 \quad \Leftrightarrow \quad \big[\mathcal{H},\,\mathcal{P}\,\big] \;=\; 0\,.$$

This means that $\mathcal{H}$ and $\mathcal{P}$ share a common eigenbasis. Do not attempt to identify the eigenbasis, be concerned only that it exists. The statement that the energy and momentum operators share a common eigenbasis is $|\,E> \;=\; |\,p>\,,$ since the eigenstates of $\mathcal{H}$ are $|\,E>$. Therefore,

$$\frac{\mathcal{P}^2}{2m}\,|\,p> \;=\; E_n\,|\,p>\,.$$

The eigenvalue of the momentum operator acting on a momentum eigenvector is momentum,

$$\mathcal{P}\,|\,p>\;=\;p\,|\,p>\quad\Rightarrow\quad\frac{\mathcal{P}^2}{2m}\,|\,p>\;=\;\frac{p^2}{2m}\,|\,p>\quad\Rightarrow\quad\frac{p^2}{2m}\,|\,p>\;=\;E_n\,|\,p>$$

$$\Rightarrow\quad\frac{p^2}{2m}\;=\;E_n\quad\Rightarrow\quad p\;=\;\pm\sqrt{2mE}\quad\Rightarrow\quad E_+\;=\;\frac{(+p)^2}{2m},\qquad E_-\;=\;\frac{(-p)^2}{2m}$$

are the eigenvalues. The problem is solved without identifying the eigenbasis.

The state vector is a superposition of the eigenstates, *i.e.*,

$$|\,E>\;=\;c_1\,\Big|+\frac{p^2}{2m}>\;+\;c_2\,\Big|-\frac{p^2}{2m}>\;.$$

Both energies or momenta are possible until we measure. When a measurement is made, the free particle is found to be moving to the right with momentum $p\;=\;+\sqrt{2mE}$ or to the left with momentum $p\;=\;-\sqrt{2mE}$. The result of a measurement is consistent with classical mechanics.

7–2. Show that $\psi\,(x,t)\;=\;A\,e^{i(kx-\omega t)}\;+\;B\,e^{-i(kx+\omega t)}$ is a solution to the time-dependent Schrodinger equation for a free particle in one-dimensional position space,

$$-\frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial x^2}\,\psi\,(x,t)\;=\;\;i\hbar\,\frac{\partial}{\partial t}\,\psi\,(x,t)\,,$$

and show that this result is consistent with the result of the previous problem.

This problem asks you to calculate the necessary derivatives of the given wave function. The de Broglie relation, $p\;=\;h/\lambda\,,$ is required to show equivalence with the previous problem. Remember that k is wavenumber, $k\;=\;2\pi/\lambda\,,$ and that $E\;=\;h\nu=\;\hbar\omega\,.$

Abstract Hilbert space offers many advantages, though representations, in this case in position space, are the grounds where most applications are ultimately addressed.

$$\begin{aligned}\frac{\partial}{\partial x}\,\psi\,(x,t)\;&=\;\frac{\partial}{\partial x}\,\Big(A\,e^{i(kx-\omega t)}\;+\;B\,e^{-i(kx+\omega t)}\Big)\\&=\;A\,(ik)\,e^{i(kx-\omega t)}\;+\;B\,(-ik)\,e^{-i(kx+\omega t)},\end{aligned}$$

$$\begin{aligned}\Rightarrow\qquad\frac{\partial^2}{\partial x^2}\,\psi\,(x,t)\;&=\;\frac{\partial}{\partial x}\,\Big(A\,(ik)\,e^{i(kx-\omega t)}\;+\;B\,(-ik)\,e^{-i(kx+\omega t)}\Big)\\&=\;A\,(ik)^2\,e^{i(kx-\omega t)}\;+\;B\,(-ik)^2\,e^{-i(kx+\omega t)}\\&=\;-k^2\Big(A\,e^{i(kx-\omega t)}\;+\;B\,e^{-i(kx+\omega t)}\Big)\;=\;-k^2\,\psi\,(x,t)\,,\quad\text{and}\end{aligned}$$

$$\begin{aligned}\frac{\partial}{\partial t}\,\psi\,(x,t)\;&=\;\frac{\partial}{\partial t}\,\Big(A\,e^{i(kx-\omega t)}\;+\;B\,e^{-i(kx+\omega t)}\Big)\\&=\;A\,(-i\omega)\,e^{i(kx-\omega t)}\;+\;B\,(-i\omega)\,e^{-i(kx+\omega t)}\\&=\;(-i\omega)\Big(A\,e^{i(kx-\omega t)}\;+\;B\,e^{-i(kx+\omega t)}\Big)\;=\;-i\omega\,\psi\,(x,t)\,.\end{aligned}$$

Using these in the time-dependent Schrodinger equation in position space,

$$-\frac{\hbar^2}{2m}\Big(-k^2\,\psi\,(x,t)\Big) \;=\; i\hbar\,\Big(-i\omega\,\psi\,(x,t)\Big) \qquad \Rightarrow \qquad \frac{\hbar^2\,k^2}{2m}\,\psi\,(x,t) \;=\; \hbar\omega\,\psi\,(x,t)\,. \qquad (1)$$

Using the de Broglie relation,

$$p \;=\; \frac{h}{\lambda} \;=\; \frac{h}{2\pi}\frac{2\pi}{\lambda} \;=\; \hbar k \qquad \Rightarrow \qquad \hbar^2k^2 = p^2, \quad \text{and} \quad \hbar\omega \;=\; \frac{h}{2\pi}\,2\pi\nu \;=\; h\nu \;=\; E\,,$$

equation (1) is equivalent to

$$\frac{p^2}{2m}\,\psi\,(x,t) \;=\; E\,\psi\,(x,t) \qquad \Rightarrow \qquad E \;=\; \frac{p^2}{2m} \qquad \Rightarrow \qquad E_+ \;=\; \frac{(+p)^2}{2m}, \quad \text{and} \quad E_- \;=\; \frac{(-p)^2}{2m}\,,$$

which are the eigenvalues. This is consistent with what has previously been shown.

Postscript: The time-dependent Schrodinger equation is a special form of the wave equation. Recognizing this allows assumption of the given wave function which is a known solution.

The $\psi\,(x,t)$ given is a superposition of plane waves. $A\,e^{i(kx-\omega t)}$ is a plane wave moving in the positive x direction and $B\,e^{-i(kx+\omega t)}$ is a plane wave moving in the negative x direction. Unmodified plane waves are not acceptable as wave functions because they cannot be normalized. Combining plane waves with a substantially localized envelope yields an acceptable wave function.

7–3. (a) Show that the classical velocity of a free particle is given by the group velocity.

(b) Show that the classical velocity of a wave within a wave packet is given by the phase velocity.

There are two velocities associated with a wave packet, a **group velocity** which is the speed of the wave packet through space, and a **phase velocity** which is the speed of the wave within the packet. Both velocities are commonly described in terms of angular frequency and wavenumber,

$$v_{\text{group}} \;=\; \frac{d\omega}{dk} \qquad\qquad \text{and} \qquad\qquad v_{\text{phase}} \;=\; \frac{\omega}{k}\,.$$

These can readily be stated in terms of frequency and wavelength. Total energy is kinetic energy for a free particle. Express total energy in terms of momentum, differentiate with respect to momentum, use the de Broglie relation, remember $E \;=\; h\nu \;=\; \hbar\omega\,,$ and caste a form that you can recognize as classical velocity. The speed of a wave in a medium is $v \;=\; \lambda\nu$ for part (b).

(a) A free particle has total energy

$$T \;=\; E \;=\; \frac{1}{2}\,mv^2 \qquad \Rightarrow \qquad E \;=\; \frac{1}{2}\,mv^2 \;=\; \frac{p^2}{2m} \qquad \Rightarrow \qquad \frac{dE}{dp} \;=\; \frac{p}{m}\,.$$

The de Broglie wavelength associated with a particle is

$$\lambda \;=\; \frac{h}{p} \qquad \Rightarrow \qquad p \;=\; \frac{h}{\lambda} \;=\; \frac{hk}{2\pi} \;=\; \hbar k\,.$$

The classical velocity of a particle is

$$v \;=\; \frac{mv}{m} \;=\; \frac{p}{m} \;=\; \frac{dE}{dp} \;=\; \frac{d(\hbar\omega)}{d(\hbar k)} \;=\; \frac{\hbar}{\hbar}\frac{d\omega}{dk} \;=\; \frac{d\omega}{dk}\,.$$

(b) The speed of a wave in a medium is

$$v \;=\; \lambda\nu \;=\; \frac{2\pi}{k}\,\frac{\omega}{2\pi} \;=\; \frac{\omega}{k}\,.$$

Postscript: The relation between ω and k is known as a **dispersion relation**. A dispersion relation is particularly important in fields that use quantum mechanics, such as solid state physics. Graphs are usually plotted ω versus k. A commonly plotted dispersion relation is essentially a graph in the momentum basis since $p = \hbar k$. Further, since energy is proportional to angular frequency, $E = \hbar\omega$, the common graph of a dispersion relation is also proportional to a graph of energy versus momentum.

The solid curve of $\omega = \hbar k^2/2m$ indicates all energies and momenta. The eigenvalues,

$$E_+ \;=\; \frac{(+p)^2}{2m} \quad\text{and}\quad E_- \;=\; \frac{(-p)^2}{2m}\,,$$

are the functional values at $\pm k = \pm p/\hbar$ on the k-axis.

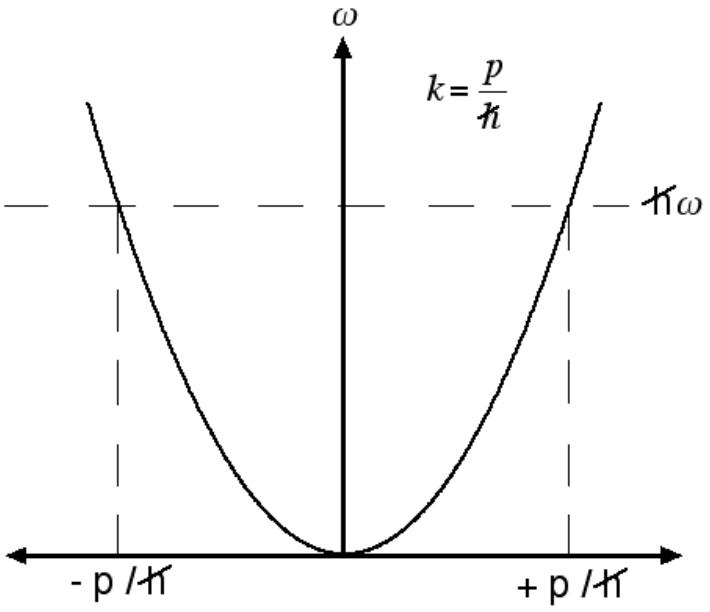


Figure 7–1. Dispersion relation for a free particle.

Notice that the slope at any point is $d\omega/dk$, the group velocity, and the chord from the origin to that point is ω/k, the phase velocity.

7–4. Explain group and phase velocities using sketches of a Gaussian wave packet.

This is an extension and amplification of part 3 of chapter 6.

A plane wave traveling to the right described by $\psi(x) = A e^{ikx}$ may look like figure 7–2.

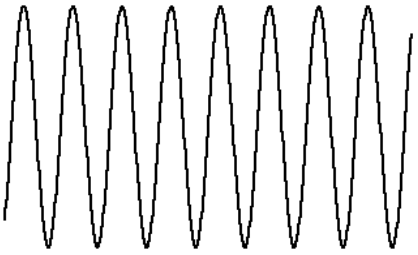


Figure 7–2. Traveling plane wave.

Figure 7–3. A Gaussian curve.

Should a traveling plane wave be multiplied by a Gaussian function $f(x) = e^{-bx^2}$ as depicted in figure 7–3, the positive and negative amplitude of the plane wave is modified so the result is a Gaussian wave packet that may look like figure 7–4. Properly normalized and using

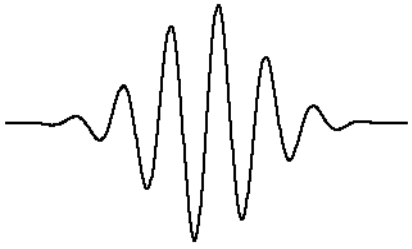


Figure 7–4. A Gaussian wave packet.

conventional notation, a Gaussian wave packet may be described

$$\psi(x) = \frac{1}{(\pi\alpha^2)^{1/4}} e^{ikx} e^{-x^2/2\alpha^2}$$

This has two velocities. The group velocity is that of the entire wave packet through space. The phase velocity is that of the wave within the packet. Figure 7–5 depicts both velocities.

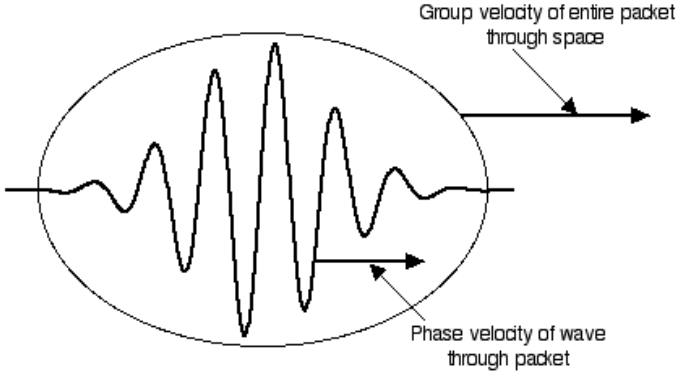


Figure 7–4. Group and phase velocities for a Gaussian wave packet.

Postscript: Remember that the exponential term e^{ikx} in $\psi(x) = \frac{1}{(\pi\alpha^2)^{1/4}} e^{ikx} e^{-x^2/2\alpha^2}$ is called the phase. The exponential term e^{ikx} encodes the wave number, which is related to the wave length and the velocity of the wave through the medium, or in this case, through the wave packet. Thus, the phase velocity is appropriately named.

The phrases Gaussian wave packet and Gaussian wave function are synonymous.

7–5. Find the function in wavenumber space that corresponds to the normalized Gaussian wave function in position space.

That a plane wave solution is limited by a constant wavenumber is its second shortcoming. This problem is a step toward rectifying the limitation of constant wavenumber/momentum. A relation $g(k)$ that models a distribution in momentum, or for all practical purposes equivalently, in wavenumber is the Fourier transform of $f(x) = \frac{1}{(\pi\alpha^2)^{1/4}} e^{-x^2/2\alpha^2}$. Use form 3.323.2 from Gradshteyn and Ryzhik, $\int_{-\infty}^{\infty} e^{-p^2x^2 \pm qx}\, dx = \frac{\sqrt{\pi}}{p} e^{q^2/4p^2}$.

The general Fourier transform is

$$g(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx \qquad \Rightarrow \qquad g(k) = \frac{1}{\sqrt{2\pi}} \frac{1}{(\pi\alpha^2)^{1/4}} \int_{-\infty}^{\infty} e^{-x^2/2\alpha^2 - ikx}\, dx$$

Using form 3.323.2 from Gradshteyn and Ryzhik, $p^2 = 1/2\alpha^2$ and $q = ik$,

$$g(k) = \frac{1}{\sqrt{2\pi}} \frac{1}{(\pi\alpha^2)^{1/4}} \alpha\sqrt{2\pi}\; e^{(ik)^2/4(1/2\alpha^2)} = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-k^2\alpha^2/2}.$$

Postscript: The function $g(k)$ is in wavenumber space. Elements in wavenumber space are proportional to elements momentum space. Working with wavenumber is often preferable to momentum where waves are involved.

The function $g(k)$ models all wavenumber/momenta in a Gaussian distribution. Multiplying the plane wave solution by $g(k)$ provides a Gaussian wave packet.

7–6. Derive the dispersion relation for a free particle of mass m.

Though given in problem 7–3, this is an important piece used in the next problem to arrive at a quantum mechanical Gaussian wave function as a function of time. Total energy is kinetic energy for a free particle. Use this fact and the de Broglie relation to arrive at $\omega(k)$.

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \qquad \Rightarrow \qquad \hbar\omega = \frac{\hbar^2 k^2}{2m} \qquad \Rightarrow \qquad \omega = \omega(k) = \frac{\hbar k^2}{2m}.$$

7–7. Assume that $B = 0$ in the plane wave solution to the Schrodinger equation given earlier. Find the resulting quantum mechanical Gaussian wave function, $\psi(x,t)$.

This problem puts the parts of the last three problems together with the plane wave solution to the Schrodinger equation in an acceptable wave function in position space. The plane wave solution is

$$\psi(x,t) = A\,e^{i(kx-\omega t)} + B\,e^{-i(kx+\omega t)} \quad \text{and} \quad B = 0 \qquad \Rightarrow \qquad \psi(x,t) = A\,e^{i(kx-\omega t)}\,.$$

$B = 0$ is assumed to simplify the development. Multiply by the Gaussian distribution in wavenumber space, $g(k)$. Use the dispersion relation in place of ω in $e^{i(kx-\omega t)}$ to complete this product wave function in terms of wavenumber. Integrate this product over all wavenumbers to establish the functional relation in position space. Use the integral given in problem 7–5. Reduce to

$$\psi(x,t) = \frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar}{m\alpha^2}t\right)^{-1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2+\frac{i\hbar}{m}t\right)}\right].$$

$$\begin{aligned}
\psi(x,t) &= \int_{-\infty}^{\infty} g(k)\left(A\,e^{i(kx-\omega t)}\right)dk = A\int_{-\infty}^{\infty} g(k)\,e^{i(kx-\hbar\,k^2\,t/\,2m)}\,dk \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-k^2\,\alpha^2/\,2}\;e^{ikx-i\hbar\,k^2\,t/\,2m}\,dk \\
&= \frac{1}{\sqrt{2\pi}}\left(\frac{\alpha^2}{\pi}\right)^{1/4}\int_{-\infty}^{\infty}\exp\left[-\left(\frac{\alpha^2}{2}+\frac{i\hbar\,t}{2m}\right)k^2+ix\,k\right]dk
\end{aligned}$$

and use the same integral as in problem 7–5 with $p^2 = \left(\frac{\alpha^2}{2}+\frac{i\hbar\,t}{2m}\right)$, and $q = ix$,

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\left(\frac{\alpha^2}{\pi}\right)^{1/4}\left(\frac{\pi}{\frac{\alpha^2}{2}+\frac{i\hbar}{2m}t}\right)^{1/2}\exp\left[\frac{(ix)^2}{4\left(\frac{\alpha^2}{2}+\frac{i\hbar}{2m}t\right)}\right] \\
&= \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\pi}\right)^{1/4}\alpha^{1/2}\sqrt{2\pi}\left(\frac{1}{\alpha^2+\frac{i\hbar}{m}t}\right)^{1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2+\frac{i\hbar}{m}t\right)}\right] \\
&= \frac{1}{\pi^{1/4}}\frac{1}{\alpha^{1/2}}\left(\frac{\alpha^2}{\alpha^2+\frac{i\hbar}{m}t}\right)^{1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2+\frac{i\hbar}{m}t\right)}\right] \\
&= \frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar}{m\alpha^2}t\right)^{-1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2+\frac{i\hbar}{m}t\right)}\right].
\end{aligned}$$

Postscript: The factor $1/\sqrt{2\pi}$ appears in the second line as part of the Fourier transform completing the process of normalization. The Gaussian wave function derived above is normalized.

Problem 7–7 is for a wave packet centered at $k = 0$. For a wave packet centered at $k = k_0$,

$$\psi(x,t) = \frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\exp\left[ik_0\left(x-\frac{\hbar k_0 t}{2m}\right)\right]\exp\left[\frac{-\left(x-\hbar k_0 t/m\right)^2}{2\alpha^2+2i\hbar t/m}\right].$$

The details, while not overwhelming, are distracting, and are consigned to Appendix C.

7–8. (a) Find the probability density associated with the Gaussian wave function of problem 7–7.

(b) Use this result to interpret the uncertainty in position as a function of time.

Uncertainty is the square root of one quarter of the denominator of the argument of the exponential factor of a normalized Gaussian wave function. This is problematic for the wave function of problem 7–7 since the argument of the exponential factor contains an imaginary number. Uncertainty in position or momentum, like probability, are intrinsically real quantities. Thus, the strategy is to calculate probability density and read the uncertainty from that. Symbolically,

$$\psi(x) = A\,e^{-x^2/2\alpha^2} \quad \Rightarrow \quad \triangle x = \frac{\alpha}{\sqrt{2}}$$

where A is a normalization constant, but if the argument of the exponential has complex values

$$\psi(x) = Ae^{-x^2/2\alpha^2+ikx} \quad \Rightarrow \quad \left|\psi(x)\right|^2 = \left|A\right|^2 e^{-x^2/\alpha^2} \quad \Rightarrow \quad \triangle x = \frac{\alpha}{\sqrt{2}}$$

or uncertainty in position is the square root of one half of the denominator of the argument of the exponential when read from a Gaussian probability density.

Probability density is $|\psi(x,t)|^2 = \psi^*(x,t)\,\psi(x,t)$. For part (a), you should find that

$$|\psi(x,t)|^2 = \frac{1}{\alpha\sqrt{\pi}}\left(1+\frac{\hbar^2}{m^2\alpha^4}t^2\right)^{-1/2}\exp\left[-\frac{x^2}{\alpha^2+\dfrac{\hbar^2}{m^2\alpha^2}t^2}\right].$$

A straightforward application of the last equation in the previous paragraph yields

$$\triangle x(t) = \frac{\alpha}{\sqrt{2}}\left(1+\frac{\hbar^2}{m^2\alpha^4}t^2\right)^{1/2}.$$

What does it mean that uncertainty is a function of time?

(a) $|\,\psi\,(x,t)\,|^{\,2} \;=\; \psi^{*}\,(x,t)\;\psi\,(x,t)$

$$= \frac{1}{(\pi\alpha^2)^{1/4}}\left(1-\frac{i\hbar}{m\alpha^2}t\right)^{-1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2-\dfrac{i\hbar}{m}t\right)}\right]\frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar}{m\alpha^2}t\right)^{-1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2+\dfrac{i\hbar}{m}t\right)}\right]$$

$$= \frac{1}{\alpha\sqrt{\pi}}\left(1+\frac{\hbar^2}{m^2\alpha^4}t^2\right)^{-1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2-\dfrac{i\hbar}{m}t\right)}-\frac{x^2}{2\left(\alpha^2+\dfrac{i\hbar}{m}t\right)}\right]$$

and the remaining task is to simplify the argument of the exponential. Factoring and multiplying each rational expression by its complex conjugate, the argument of the exponential is

$$\left[-\frac{x^2}{2}\left(\frac{\alpha^2+\dfrac{i\hbar}{m}t}{\alpha^4+\dfrac{\hbar^2}{m^2}t^2}+\frac{\alpha^2-\dfrac{i\hbar}{m}t}{\alpha^4+\dfrac{\hbar^2}{m^2}t^2}\right)\right] \;=\; \left[-\frac{x^2}{2}\left(\frac{\alpha^2+\dfrac{i\hbar}{\not m}t+\alpha^2-\dfrac{i\hbar}{\not m}t}{\alpha^4+\dfrac{\hbar^2}{m^2}t^2}\right)\right]$$

$$= \left[-\frac{x^2}{2}\left(\frac{2\alpha^2}{\alpha^4+\dfrac{\hbar^2}{m^2}t^2}\right)\right] \;=\; \left[-\frac{x^2}{\alpha^2+\dfrac{\hbar^2}{m^2\alpha^2}t^2}\right]$$

$$\Rightarrow \qquad |\,\psi(x,t)\,|^{\,2} \;=\; \frac{1}{\alpha\sqrt{\pi}}\left(1+\frac{\hbar^2}{m^2\alpha^4}t^2\right)^{-1/2}\exp\left[-\frac{x^2}{\alpha^2+\dfrac{\hbar^2}{m^2\alpha^2}t^2}\right].$$

(b) $\quad \left|\,\psi\,(x)\,\right|^2 \;=\; \left|\,A\,\right|^2 e^{-x^2/\,\alpha^2} \qquad \Rightarrow \qquad \triangle x \;=\; \dfrac{\alpha}{\sqrt{2}}\,, \quad$ therefore,

$$\triangle x \;=\; \triangle x\,(t) \;=\; \frac{1}{\sqrt{2}}\left(\alpha^2+\frac{\hbar^2}{m^2\alpha^2}t^2\right)^{1/2} \;=\; \frac{\alpha}{\sqrt{2}}\left(1+\frac{\hbar^2}{m^2\alpha^4}t^2\right)^{1/2}.$$

The uncertainty in position is a function of time. This means that the Gaussian wave packet "spreads" and "flattens" with time. The uncertainty resultingly grows as time advances ... or as time is retarded. There is a minimum uncertainty in position at time $t = 0$. This is the meaning of the phrase "free space is dispersive." Figure 7–6 is in terms of probability density. The area

Figure 7–6. Wave packet spreads with time.

under both curves for all times must be 1 to satisfy the probability postulate. As t gets larger, the t^2 term necessarily gets larger, and $\triangle x\,(t)$ gets larger, and flattening of the Gaussian curve is necessary to preserve the area. The same is true if t is retarded.

Postscript: The distribution in wavenumber/momentum is not time dependent. The average momentum and the uncertainty in momentum are constants for a free particle.

7–9. Show that the uncertainty in momentum of a Gaussian wave function is independent of time.

The wave packet does not "spread" in momentum space as time advances. Use a Fourier transform to change the wave function of problem 7–7 from position space into momentum space, and use this result to form the probability density in momentum space. The uncertainty in momentum follows from the probability density. The Fourier transform yields

$$\widehat{\psi}\,(p,t) \;=\; \sqrt{\frac{\alpha}{\hbar\,\sqrt{\pi}}}\;\exp\left[-p^2\left(\frac{\alpha^2}{2\hbar^2}+\frac{it}{2\hbar m}\right)\right]$$

You need form 3.323.2 from Gradshteyn and Ryzhik which we write

$$\int_{-\infty}^{\infty} e^{-b^2x^2\pm qx}\,dx \;=\; \frac{\sqrt{\pi}}{b}\,e^{q^2/\,4b^2},$$

to prevent confusion between constants and momentum. You should find that

$$|\,\widehat{\psi}\,(p,t)\,|^{\,2} \;=\; \frac{\alpha}{\hbar\sqrt{\pi}}\,e^{-p^2\alpha^2/\,\hbar^2}$$

which is independent of time. The uncertainty in momentum is therefore also independent of time.

$$\begin{aligned}\widehat{\psi}\,(p,t) \;&=\; \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi\,(x,t)\,e^{-ipx/\hbar}\,dx\\ &=\; \frac{1}{\sqrt{2\pi\hbar}}\,\frac{1}{(\alpha^2\pi)^{1/4}}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\int_{-\infty}^{\infty}\exp\left[-\left(\frac{1}{2\alpha^2+2i\hbar t/m}\right)x^2-\frac{ip}{\hbar}\,x\right]\,dx\end{aligned}$$

Here $b^2 \;=\; \dfrac{1}{2\alpha^2+2i\hbar t/m}$ and $q \;=\; \dfrac{ip}{\hbar}$ for use in the integral, so

$$\begin{aligned}\widehat{\psi}\,(p,t) \;&=\; \frac{1}{\sqrt{2\pi\hbar}}\,\frac{1}{(\alpha^2\pi)^{1/4}}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\sqrt{\pi}\,\left(2\alpha^2+\frac{2i\hbar t}{m}\right)^{1/2}\exp\left[\frac{1}{4}\,\left(\frac{ip}{\hbar}\right)^2\left(2\alpha^2+\frac{2i\hbar t}{m}\right)\right]\\ &=\; \frac{1}{\sqrt{2\pi\hbar}}\,\frac{\alpha}{(\alpha^2\pi)^{1/4}}\left(\alpha^2+\frac{i\hbar t}{m}\right)^{-1/2}\sqrt{2\pi}\,\left(\alpha^2+\frac{i\hbar t}{m}\right)^{1/2}\exp\left[-\frac{p^2}{4\hbar^2}\left(2\alpha^2+\frac{2i\hbar t}{m}\right)\right]\\ &=\; \sqrt{\frac{\alpha}{\hbar\,\sqrt{\pi}}}\;\exp\left[-p^2\left(\frac{\alpha^2}{2\hbar^2}+\frac{it}{2\hbar m}\right)\right]\,.\end{aligned}$$

The associated probability density is

$$|\,\widehat{\psi}\,(p,t)\,|^{\,2} \;=\; \left(\sqrt{\frac{\alpha}{\hbar\,\sqrt{\pi}}}\,\right)^{2}\exp\left[-p^{2}\left(\frac{\alpha^{2}}{2\hbar^{2}}-\frac{it}{2\hbar m}\right)\right]\exp\left[-p^{2}\left(\frac{\alpha^{2}}{2\hbar^{2}}+\frac{it}{2\hbar m}\right)\right]$$
$$=\;\frac{\alpha}{\hbar\sqrt{\pi}}\,e^{-p^{2}\alpha^{2}/\hbar^{2}}.$$

This is a Gaussian probability density in momentum space. Uncertainty in momentum is the square root of one half of the denominator of the argument of the exponential when read from a Gaussian probability density, or

$$\triangle p \;=\; \frac{\hbar}{\alpha\sqrt{2}}\,.$$

Postscript: The wave packet does not "spread" in momentum as time advances. The average momentum and the uncertainty in momentum are constants for a free particle.

7–10. Does the wave packet of a photon spread as time advances?

The time-dependent wave functions in both position and momentum space contain explicit factors of m which becomes problematic for particles with zero mass.

The developments leading to the spreading of a wave packet as time advances are dependent on $E \;=\; \frac{1}{2}\,mv^{2}$ which does not apply to the photon. In general,

$$E^{2} \;=\; (pc)^{2} \;+\; (m_{0}c^{2})^{2} \qquad \Rightarrow \qquad E \;=\; pc$$

for a photon, thus the group velocity is the same as the phase velocity. The phase velocity is

$$c \;=\; \lambda\nu \;=\; \frac{\lambda}{2\pi}\,2\pi\nu \;=\; \frac{\omega}{k}$$

and the group velocity is obtained

$$E \;=\; pc \qquad \Rightarrow \qquad \frac{dE}{dp} \;=\; c \;=\; \frac{\omega}{k}$$

from precisely the same argument. Spreading of the wave packet is not anticipated when the group velocity is the same as the phase velocity. Incidentally, one explanation of the refraction of light when passing through a prism is the group velocity of the photons is less than the phase velocity in the refractive medium resulting in dispersion.

The spreading of the wave packet in position space applies only to particles with mass $m \;\neq\; 0\,.$

Exercises

7–11. (a) What are the possible outcomes of a measurement of momentum of a free particle? Calculate the probability of each possible outcome.

(b) Explain why you can assume the orthonormality of eigenstates for parts (a) and (c).

(c) Assume $<E\,|\,\mathcal{P}\,|\,E> \;=\; <p\,|\,\mathcal{P}\,|\,p>$ to use $<E\,|\,\mathcal{P}\,|\,E>$ to find the expectation value of momentum for a free particle.

(d) Explain why you can assume that $<E\,|\,\mathcal{P}\,|\,E> \;=\; <p\,|\,\mathcal{P}\,|\,p>$.

(e) Use $<\mathcal{A}> \;=\; \sum P(\alpha_i)\,\alpha_i$ to verify your result from part (c).

This problem amplifies problem 7–1. The state vector postulate says that

$$|\,E> \;=\; c_1\,|\,+p^2/2m> \;+\; c_2\,|\,-p^2/2m>\;.$$

The eigenvalue postulate describes possibilities. Using the probability postulate,

$$P(\alpha) \;\propto\; \left|<\alpha\,|\,\psi>\right|^2 \quad \text{or} \quad P(\alpha) \;=\; \frac{\left|<\alpha\,|\,\psi>\right|^2}{<\psi\,|\,\psi>}, \quad \text{given that } |\,\alpha> \text{ are normalized.}$$

You should find $P(+p) \;=\; \dfrac{|\,c_1\,|^2}{|\,c_1\,|^2 + |\,c_2\,|^2}$ and $P(-p) \;=\; \dfrac{|\,c_2\,|^2}{|\,c_1\,|^2 + |\,c_2\,|^2}$ for part (a). Refer to the observables postulate for part (b). Remember that $\mathcal{H}$ and $\mathcal{P}$ commute for part (d). You should find that the expectation value is $<\mathcal{P}> \;=\; |\,c_1\,|^2\,(+p) \;+\; |\,c_2\,|^2\,(-p)$.

7–12. Solve the Schrodinger equation for a free particle in momentum space.

This problem is largely an exercise in representation. For a free particle,

$$V(x) \;=\; 0 \quad \Rightarrow \quad \mathcal{V}(\mathcal{X}) \;=\; 0\,,$$

so the Hamiltonian is $\mathcal{P}^2/2m$. In momentum space, $\mathcal{P} \;\rightarrow\; p$. Use this to form the Hamiltonian, then use your Hamiltonian in the Schrodinger equation. Act on both sides of the resulting Schrodinger equation with $<p\,|$ to arrive at a momentum space representation. You should find

$$\frac{p^2}{2m}\,\widehat{\psi}\,(p,t) \;=\; i\hbar\,\frac{\partial}{\partial t}\,\widehat{\psi}\,(p,t)\,.$$

Recognize that the solution is $\widehat{\psi}\,(p,t) \;=\; A\,e^{-iEt/\hbar}$. Substitute this into the Schrodinger equation and do the requisite differentiation to demonstrate that it is a solution. Find eigenvalues similarly to the method used to find eigenvalues in position space in problem 7–2.

7–13. Show that Gaussian wave function

$$\psi(x,t) \;=\; \frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar}{m\alpha^2}t\right)^{-1/2}\exp\left[-\frac{x^2}{2\left(\alpha^2+\frac{i\hbar}{m}t\right)}\right] \quad \text{is normalized.}$$

Stated earlier without proof, the time-dependent Gaussian wave function of problem 7–7 is, in fact, normalized. Integrate $|\,\psi(x,t)\,|^2$, the probability density, over all space. You may want to start with the result of problem 7–8 (a). $|\,\psi(x,t)\,|^2$ is Gaussian in x which is the parameter over which you want to integrate. Remember $\displaystyle\int_0^\infty e^{-q^2x^2}\,dx \;=\; \frac{\sqrt{\pi}}{2q}$.

7–14. A particle in free space is described by the wave function

$$\psi(x) \;=\; \frac{1}{(\pi\alpha^2)^{1/4}}\,e^{ikx}\,e^{-x^2/\,2\alpha^2}\,.$$

Find the probability that the particle is located between

(a) 0 and $\alpha/2$,

(b) 0 and α, and

(c) $-\alpha$ and $\alpha/2$.

Integrate $|\,\psi(x,t)\,|^2$ between the designated limits. The phases are $e^{-ikx}\,e^{ikx} \;=\; e^0 \;=\; 1$ so complex arguments vanish. Form 3.321.2 from Gradshteyn and Ryzhik is

$$\int_0^u e^{-q^2x^2}dx \;=\; \frac{\sqrt{\pi}}{2q}\,\mathrm{erf}\,(qu)\,, \qquad q \;>\; 0\,.$$

The $\mathrm{erf}\,(x)$ is the error function related to the Gaussian curve/normal function. Values are readily available on line or in tables. The abbreviated table

x	0	0.5	0.7071	1.0	1.4142	1.5	2.0	2.1213
$\mathrm{erf}\,(x)$	0.0000	0.5205	0.6827	0.8427	0.9545	0.9661	0.9953	0.9973

is adequate for both this and the next exercise. Part (c) requires you to realize a Gaussian wave packet is symmetric and combine the probabilities from parts (a) and (b).

7–15. Use the wave function given in exercise 7–14. Find

(a) $P\left(-\alpha/\sqrt{2} \;<\; x \;<\; \alpha/\sqrt{2}\,\right)$,

(b) $P\left(-2\alpha/\sqrt{2} \;<\; x \;<\; 2\alpha/\sqrt{2}\,\right)$, and

(c) $P\left(-3\alpha/\sqrt{2} \;<\; x \;<\; 3\alpha/\sqrt{2}\,\right)$.

The symmetric intervals allow you to use the integral of the last problem and then multiply by 2. Remember that standard deviation is related to the parameter α as $\sigma = \dfrac{\alpha}{\sqrt{2}}$, thus this exercise is equivalent to finding the area under the Gaussian/normal curve for one, two, and three standard deviations from the mean. The probabilities are usually given as percentages in introductory statistics courses, and are 68%, 95%, and 99% respectively. This correspondence is frequently called the "empirical rule" to avoid integration in Statistics I for which calculus is not a prerequisite. There is nothing empirical about it. This exercise is intended to strengthen the link between introductory statistics and the probabilistic interpretation of quantum mechanics. Notice that the answer to part (c) would correctly round to 100% to the nearest percent, but that would exclude the area under the curve from three standard deviations to infinity on both sides, thus, the "empirical rule" deliberately rounds incorrectly to 99% to save a half percent for each wing.

7–16. For the Gaussian wave packet of problem 7–7.

(a) Find the $t = 0$ product of $\triangle x$ and $\triangle p$,

(b) the $t > 0$ product of $\triangle x$ and $\triangle p$, and

(c) compare and interpret these two results.

These are straightforward applications of the results of part (b) of problem 7–8 and problem 7–9. The product of $\triangle x$ and $\triangle p$ is a minimum at $t = 0$, and larger at all other times.

7–17. Show that the uncertainty in position for the Gaussian wave packet centered at $k = k_0$ is identical to that for the Gaussian wave packet centered at $k = 0$.

Problem 7–8 develops probability density for a Gaussian wave packet centered at $k = 0$ to obtain $\triangle x$. The postscript to problem 7–7 indicates for a Gaussian wave packet centered at $k = k_0$

$$\psi(x,t) = \frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\exp\left[ik_0\left(x-\frac{\hbar k_0 t}{2m}\right)\right]\exp\left[\frac{-\left(x-\hbar k_0 t/m\right)^2}{2\alpha^2+2i\hbar t/m}\right].$$

One method of solution is to follow the processes of problem 7–8, rather see Appendix C first.

That wavenumber does not affect uncertainty in position is interesting but not entirely unexpected. A reduction is completed in Appendix C to allow the reader to invest their time and energy in more significant phenomena. Those with a specific interest in mathematical physics may appreciate Appendix C. Others should spend a few moments scanning the details and be familiar with the fact indicated in the statement of this exercise.

Chapter 8

The Infinite Square Well

Any wave function limited to an interval such as $-a < x < a$ can be interpreted physically as being between infinitely thick, infinitely high potential energy "walls." Intervals were introduced in chapter 4 so that methods of calculating probabilities, expectation values, and uncertainties for continuous systems could be addressed; wave functions that are not square integrable over all space generally are square integrable on an interval. This chapter introduces energy quantization for a continuous system, quantum numbers, the meaning of a linear combination of continuous eigenfunctions, and some common methods of treating boundary value problems.

An electron in an atom is an example of a particle confined to a limited region. It demonstrates energy quantization while confined. The limited region can be considered to be a "box" with indistinct "soft walls" formed by electrical forces. The first step toward describing such a realistic system is to examine a one dimensional box with the simplest possible geometry and infinite "hard walls." This bit of unrealism makes the mathematics most tractable yet reveals the same quantum mechanical phenomena of any bound particle, in particular, energy quantization. Any particle trapped in any potential energy well exhibits energy quantization.

The "particle in a box" is an informal name for a square well. It is a nickname that sometimes masks phenomena of physical interest and seemingly becomes an end in itself. It is rather the second step (the free particle being the first step) in treating increasingly realistic potential energy functions describing increasingly sophisticated boundary conditions. It may be useful to picture an electron in a highly unusual atom or a proton in a highly unusual nucleus as you work through this precursor to and idealization of more realistic systems. An electron trapped in an atom is a particle in an electrostatic "box."

8–1. Derive the eigenenergies of a particle in an infinite square well.

The potential energy function is

$$V(x) = \infty, \quad x \leq -a \text{ and } x \geq a,$$
$$V(x) = 0, \qquad -a < x < a,$$

for an infinite square well. Figure 8–1 depicts an energy versus position sketch. The potential energy function goes from zero in the region of confinement to infinity vertically and horizontally at each edge. All space is divided into three regions. A consequence of the walls being of infinite height and thickness is that the probability of finding the particle in regions 1 or 3 is zero, thus the wave function is zero in regions 1 and 3. A solution to the time-independent Schrodinger equation is

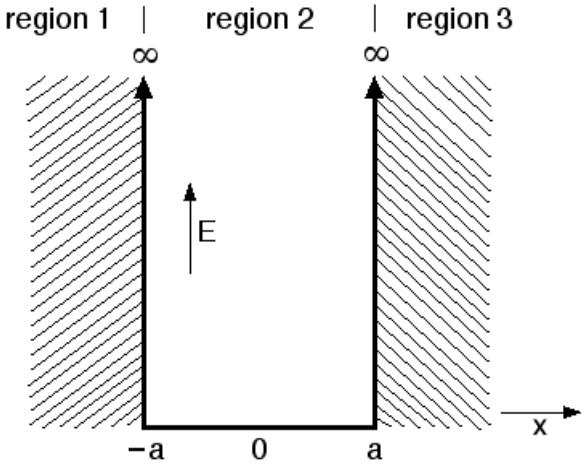


Figure 8–1. Infinite square well potential.

$$\psi(x) \;=\; \begin{cases} 0 & x \le -a\,, \\ Ae^{-ikx} \;+\; Be^{ikx} & -a < x < a\,, \\ 0 & x \ge a\,, \end{cases}$$

where $k = \lambda/2\pi$ is the wave number, and λ is the de Broglie wavelength. The eigenvalues are

$$E \;=\; \frac{1}{2}\,mv^2 \;=\; \frac{p^2}{2m} \quad\Rightarrow\quad E \;=\; \frac{\hbar^2 k^2}{2m}\,,$$

the same as a free particle within the "box." The eigenenergies are then expressed in terms of the parameters of the given potential using the condition of continuity of the wave function.

Continuity of the wave function at the left boundary means $\psi(-a) = 0\,,$ or

$$A\,e^{-ik(-a)} \;+\; B\,e^{ik(-a)} \;=\; 0 \quad\Rightarrow\quad A\,e^{ika} \;+\; B\,e^{-ika} \;=\; 0$$

$$\Rightarrow\quad A\cos(ka) \;+\; A\,i\sin(ka) \;+\; B\cos(ka) \;-\; B\,i\sin(ka) \;=\; 0\,, \tag{1}$$

and at the right boundary $\psi(a) = 0\,,$ so $A\,e^{-ika} \;+\; B\,e^{ika} \;=\; 0$

$$\Rightarrow\quad A\cos(ka) \;-\; A\,i\sin(ka) \;+\; B\cos(ka) \;+\; B\,i\sin(ka) \;=\; 0\,. \tag{2}$$

Adding equations (1) and (2),

$$2A\cos(ka) \;+\; 2B\cos(ka) \;=\; 0 \quad\Rightarrow\quad 2\,(A+B)\cos(ka) \;=\; 0 \quad\Rightarrow\quad \cos(ka) \;=\; 0$$

$$\Rightarrow\quad ka \;=\; \frac{n\pi}{2},\;\; n = 1,\,3,\,5,\ldots \quad\Rightarrow\quad k \;=\; \frac{n\pi}{2a}\,,\;\; n = 1,\,3,\,5,\ldots \tag{3}$$

Subtracting equations (1) and (2),

$$2A\,i\sin(ka) \;-\; 2B\,i\sin(ka) \;=\; 0 \quad\Rightarrow\quad 2i\,(A-B)\sin(ka) \;=\; 0 \quad\Rightarrow\quad \sin(ka) \;=\; 0$$

$$\Rightarrow\quad ka = \frac{n\pi}{2},\;\; n = 2,\,4,\,6,\ldots \quad\Rightarrow\quad k = \frac{n\pi}{2a},\;\; n = 2,\,4,\,6, \tag{4}$$

Equations (3) and (4) can be summarized in one relation,

$$\Rightarrow\quad k \;=\; \frac{n\pi}{2a},\;\; n = 1,\,2,\,3,\,4,\ldots \quad\text{so}$$

$$E \;=\; \frac{p^2}{2m} \;=\; \frac{\hbar^2 k^2}{2m} \;=\; \frac{\hbar^2}{2m}\left(\frac{n\pi}{2a}\right)^2 \quad\Rightarrow\quad E_n \;=\; n^2\,\frac{\pi^2\hbar^2}{8ma^2}\,.$$

Notice that the only variable is the quantum number, and that it varies as $n^2\,.$

Postscript: The confined particle, though it is free within the region of confinement, can possess only allowed energies that depend upon the geometry of the region of confinement. Allowed energies are discrete and are pictured only at discrete heights above the floor of the potential. Energies of a confined particle are **quantized**. The eigenenergies, or energy eigenvalues, are subscripted because they depend on the index n called the **quantum number**. A quantum number is simply an integer index. Since n can be any positive integer, there are an infinite number of eigenenergies for a particle in an infinite square well.

A free particle can have any energy, or be at any height above the floor of the potential. Confinement is not a consideration for a free particle so this type of energy quantization was not encountered in chapter 7. Confinement, or forced localization, is the physical condition that results in energy quantization regardless of whether the walls of the "box" are of infinite height and infinite extent, or are of finite height that diminish with r as does an electrostatic potential. The idealizations of infinitely high and infinitely thick walls with perfectly square corners is a limiting case for which the mathematics is most tractable. The physics is that any potential well will have bound states that are quantized.

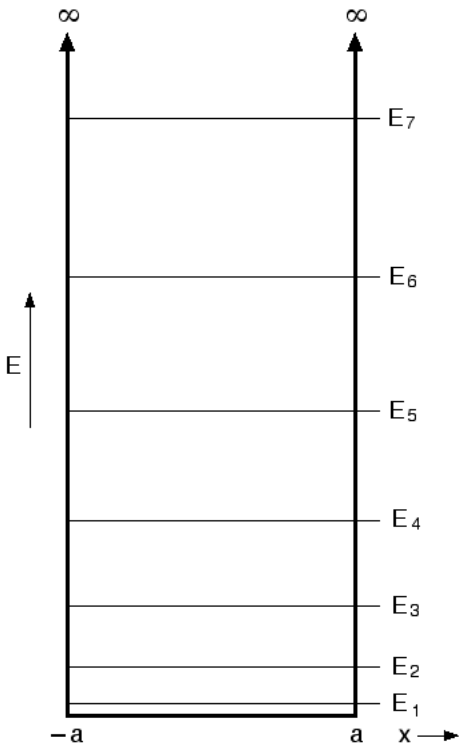


Figure 8–2. Energy levels in an infinite square well.

8–2. Find the normalized eigenfunctions for a particle confined to an infinite square well.

Eigenfunctions are also found using continuity of the wave function at the boundaries, $\psi(\pm a) = 0$.

Using the wavenumber in terms of quantum number at the right boundary,

$$A\,e^{-ika} = -B\,e^{ika} \quad \Rightarrow \quad A = -B\,e^{i2ka} = -B\,e^{i2\,(n\pi/2a)\,a} = -B\,e^{in\pi}\,.$$

Now $e^{in\pi} = \cos(n\pi) + i\sin(n\pi) = \begin{cases} -1 & n \text{ odd} \\ 1 & n \text{ even} \end{cases} \quad \Rightarrow \quad A = \begin{cases} B & n \text{ odd} \\ -B & n \text{ even.} \end{cases}$

The result is the same at the left boundary. The wave function within the well for odd n is

$$\psi(x) = A\,e^{-ikx} + B\,e^{ikx} = A\,e^{-ikx} + A\,e^{ikx} = A\Big(e^{-ikx} + e^{ikx}\Big)$$

$$= A\Big[\cos(kx) - i\sin(kx) + \cos(kx) + i\sin(kx)\Big] = 2A\cos(kx)$$

$$\Rightarrow \quad \psi_n(x) = C\cos\left(\frac{n\pi}{2a}\,x\right), \quad n \text{ odd}, \tag{1}$$

where $C = 2A$ is the "updated" normalization constant. For even n,

$$\psi(x) = A\,e^{-ikx} + B\,e^{ikx} = A\,e^{-ikx} - A\,e^{ikx} = A\left(e^{-ikx} - e^{ikx}\right)$$

$$= A\Big[\cos(kx) - i\sin(kx) - \cos(kx) - i\sin(kx)\Big] = -2A\,i\sin(kx)$$

$$\Rightarrow \quad \psi_n(x) \;=\; D\sin\left(\frac{n\pi}{2a}\,x\right), \quad n \text{ even} \tag{2}$$

where $D = -2Ai$ is the "conglomerate" normalization constant. The normalization condition is

$$<\psi(x)\,|\,\psi(x)> \;=\; 1 \quad \Rightarrow \quad \int_{-\infty}^{\infty}\psi^*(x)\,\psi(x)\,dx \;=\; \int_{-a}^{a}\psi^*(x)\,\psi(x)\,dx \;=\; 1\,.$$

For odd n this is

$$\begin{aligned}
1 \;&=\; \int_{-a}^{a} C^*\cos\left(\frac{n\pi}{2a}\,x\right)^* C\cos\left(\frac{n\pi}{2a}\,x\right)\,dx \;=\; C^*C\int_{-a}^{a}\cos^2\left(\frac{n\pi}{2a}\,x\right)\,dx \\
&=\; |\,C\,|^{\,2}\left[\frac{1}{2}\,x \;+\; \frac{2a}{4n\pi}\sin\left(\frac{n\pi}{a}\,x\right)\right]_{-a}^{a} \\
&=\; |\,C\,|^{\,2}\left[\frac{1}{2}\,a \;-\; \frac{1}{2}\,(-a) \;+\; \frac{a}{2n\pi}\left(\sin\left(\frac{n\pi}{a}\,a\right) \;-\; \sin\left(\frac{n\pi}{a}\,(-a)\right)\right)\right] \\
&=\; |\,C\,|^{\,2}\left[a \;+\; \frac{a}{2n\pi}\left(\sin(n\pi) \;+\; \sin(n\pi)\right)\right] \;=\; |\,C\,|^{\,2}\left[a \;+\; \frac{a}{n\pi}\sin(n\pi)\right].
\end{aligned}$$

But $\sin(n\pi) = 0$ for all integral n, so $a\,|\,C\,|^{\,2} = 1 \quad \Rightarrow \quad C \;=\; \dfrac{1}{\sqrt{a}}$. A similar calculation for even n yields $D \;=\; \dfrac{1}{\sqrt{a}}$. Using these results in equations (1) and (2), we have

$$\psi_n(x) \;=\; \frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}\,x\right), \quad n = 1,3,5,\ldots, \quad \text{and} \quad \psi_n(x) \;=\; \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}\,x\right), \quad n = 2,4,6,\ldots$$

Postscript: The derivations of problems 8–1 and 8–2 are based on the width of the infinite square well being $2a$ with the origin in the center. Other conventions exist. Since the width of the well appears in the eigenenergies, the normalization constants, and the arguments of the trigonometric functions, the exact form of the eigenenergies and eigenfunctions is dependent on the convention used. An infinite square well of width a with the origin at the center has

$$E_n \;=\; n^2\,\frac{\pi^2\hbar^2}{2ma^2} \qquad \text{and} \qquad \psi_n(x) \;=\; \begin{cases} \sqrt{\dfrac{2}{a}}\cos\left(\dfrac{n\pi}{a}\,x\right), & n \text{ odd}\,, \\ \sqrt{\dfrac{2}{a}}\sin\left(\dfrac{n\pi}{a}\,x\right), & n \text{ even}\,. \end{cases}$$

An infinite square well of width a with the origin at the left edge has

$$E_n \;=\; n^2\,\frac{\pi^2\hbar^2}{2ma^2} \qquad \text{and} \qquad \psi_n(x) \;=\; \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}\,x\right).$$

All three conventions provide the same numerical values for the eigenenergies and identical graphs of the eigenfunctions. See problems 8–3 and 8–4, for example.

Notice that $n = 1$ is the lowest energy state, or the **ground state**, of the eigenenergies for the infinite square well. A system of zero energy is non-physical so $n = 0$, which would describe zero energy for a particle in an infinite square well, is not allowed and quantum numbers start at

$n = 1$. In contrast, the simple harmonic oscillator (SHO) addressed in chapter 10 uses $n = 0$ for the ground state. The eigenenergies of the SHO are non-zero when $n = 0$, so $n = 0$ suitably describes the ground state energy of the SHO.

The infinite square well gets its name from the perfectly square corners and the "walls" of infinite thickness and height. Should the walls be of less than infinite thickness **tunneling** is anticipated (chapter 9). Should the walls be less than infinite height it would be a **finite square well** and the number of bound states is limited (chapter 11).

8–3. (a) What is the ground state energy of an electron in a one–dimensional infinite square well of "radius" one half Angstrom?

(b) Find the eigenenergies of the first three excited states.

A "one–dimensional radius" of 1/2 Angstrom means use $a = 0.5$ Å in the result of problem 8–1. It is often convenient to describe the energy of excited states in terms of the ground state energy. If E_g is the ground state energy, $n^2 E_g$ describes all eigenenergies of an infinite square well.

(a) $$E_1 = E_g = (1)^2 \frac{\pi^2 \hbar^2}{8ma^2} = \frac{\pi^2 h^2}{(2\pi)^2 8ma^2} = \frac{h^2 c^2}{(4)\, 8mc^2 a^2}$$

$$= \frac{(1.24 \times 10^4\, eV \cdot \text{Å})^2}{32 \left(0.511 \times 10^6 \frac{eV}{c^2} \right) c^2 (0.5\,\text{Å})^2} = \frac{1.54 \times 10^8\, eV^2 \cdot \text{Å}^2}{4.09 \times 10^6\, eV \cdot \text{Å}^2} = 37.65\ eV\,.$$

(b) $$E_2 = 2^2 E_g = 4\left(37.65\, eV\right) = 150.60\ eV\,,$$

$$E_3 = 3^2 E_g = 9\left(37.65\, eV\right) = 338.85\ eV\,,$$

$$E_4 = 4^2 E_g = 16\left(37.65\, eV\right) = 602.40\ eV\,.$$

Postscript: The diameter of a small atom is on the order of one Angstrom.

Converting quantities from CGS or MKS units is inconvenient by comparison to using constants such as $hc = 1.24 \times 10^4\, eV \cdot \text{Å}$ and the electron mass $= 0.511\ MeV/c^2$.

8–4. Given an infinite square well of width $2a$, graph the first four eigenenergies on an energy versus position plot and superimpose the first four eigenfunctions on corresponding eigenenergies on the same plot. Plot the probability densities of the first four eigenfunctions in the same manner.

Examine the two graphs below.

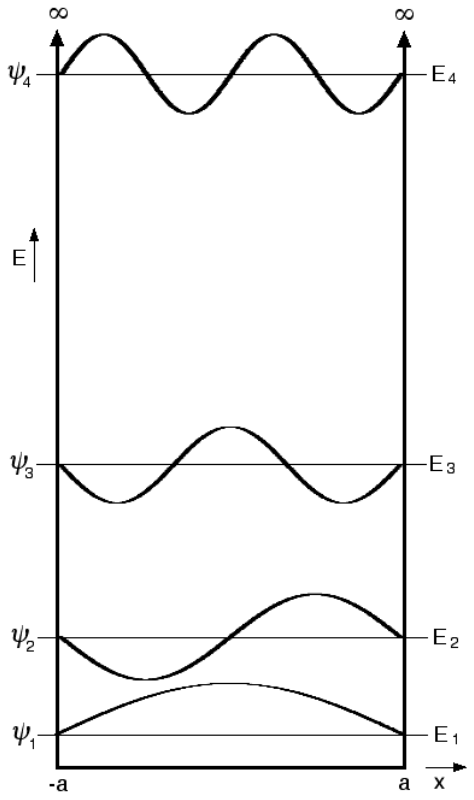


Figure 8–3. Wave functions for the infinite square well.

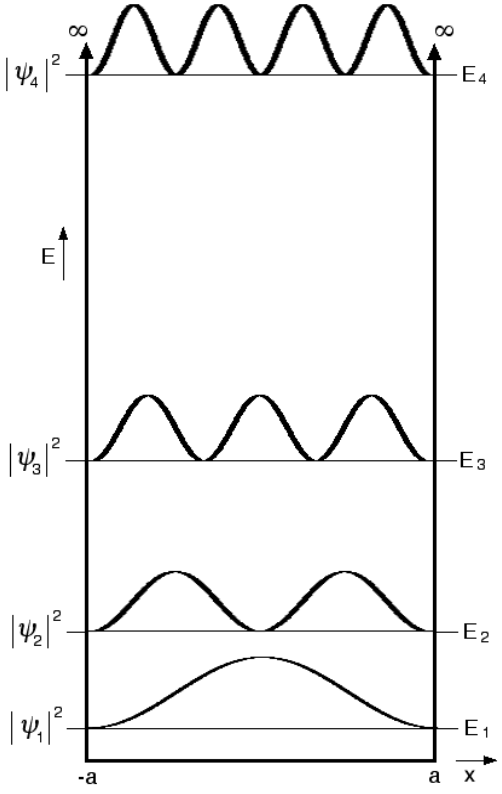


Figure 8–4. Probabilities densities for the infinite square well.

Postscript: It is conventional to graph energy versus position for the wave functions. The vertical is amplitude for the eigenfunctions. The eigenfunctions all have an amplitude of zero at the boundaries. They should, therefore, all be located on the horizontal axis that denotes zero amplitude. They are, however, conventionally located at the level of the corresponding eigenenergies where each horizontal line represents zero amplitude for that eigenfunction. Energy is usually scaled $E_1 = E_g$, $E_2 = 4\,E_g$, $E_3 = 9\,E_g$, $E_4 = 16\,E_g$, etc., but the vertical scale for amplitudes of the eigenfunctions is often qualitative, as it is in figure 8–3.

Probability density is also conventionally placed at the level of the corresponding eigenenergy where the vertical is probability density amplitude using an arbitrary scale. Notice that probability density is non-negative. The pertinent non-classical feature is that there are regions of maximal and minimal, including zero, probability. Remember that probability is $|\,\psi(x)\,|^2\,dx$ so probability density is $|\,\psi(x)\,|^2$ with dimensions of 1/length for $\psi(x)$ with dimensions of $1/\sqrt{\text{length}}$.

8–5. Find the probabilities of locating a particle in its ground state in an infinite square well of width $2a$ between $\pm a/10$ at the center and an interval of equal length at the right edge.

This is an application of the probability postulate in position space. Integrate probability density for a particle in its ground state between $\pm a/10$, then integrate probability density between $8a/10$ and a, and compare the numerical results. Classically, these probabilities would be identical.

$$\text{Using} \quad \psi_1(x) \;=\; \frac{1}{\sqrt{a}} \cos\left(\frac{\pi}{2a}\, x\right) \quad \text{in} \quad P(x_1 < x < x_2) \;=\; \int_{x_1}^{x_2} \psi^*(x)\, \psi(x)\, dx\,,$$

$$\begin{aligned} P(-a/10 < x < a/10) \;&=\; \int_{-a/10}^{a/10} \left(\frac{1}{\sqrt{a}}\right)^* \cos^*\left(\frac{\pi}{2a}\, x\right) \left(\frac{1}{\sqrt{a}}\right) \cos\left(\frac{\pi}{2a}\, x\right) dx \\ &=\; \frac{1}{a} \int_{-a/10}^{a/10} \cos^2\left(\frac{\pi}{2a}\, x\right)\, dx \;=\; \frac{1}{a}\left[\, \frac{1}{2}\, x \;+\; \frac{2a}{4\pi} \sin\left(\frac{\pi}{a}\, x\right) \right]_{-a/10}^{a/10} \\ &=\; \frac{1}{a}\left[\, \frac{1}{2}\left(\frac{a}{10} \;-\; -\frac{a}{10}\right) \;+\; \frac{a}{2\pi}\left(\sin\left(\frac{\pi}{a}\frac{a}{10}\right) \;-\; \sin\left(\frac{\pi}{a}\frac{-a}{10}\right)\right)\right] \\ &=\; \frac{1}{a}\left[\, \frac{a}{10} \;+\; \frac{a}{2\pi}\, 2\sin\left(\frac{\pi}{10}\right)\right] \;=\; \frac{1}{10} \;+\; \frac{1}{\pi} \sin\left(\frac{\pi}{10}\right) \;\approx\; 0.198\,. \end{aligned}$$

For an interval of equal length at the right edge of the well,

$$\begin{aligned} P(8a/10 < x < a) \;&=\; \frac{1}{a} \int_{8a/10}^{a} \cos^2\left(\frac{\pi}{2a}\, x\right)\, dx \;=\; \frac{1}{a}\left[\, \frac{1}{2}\, x \;+\; \frac{2a}{4\pi} \sin\left(\frac{\pi}{a} x\right) \right]_{4a/5}^{a} \\ &=\; \frac{1}{a}\left[\, \frac{1}{2}\left(a \;-\; \frac{4a}{5}\right) \;+\; \frac{a}{2\pi}\left(\sin\left(\frac{\pi}{a}\, a\right) \;-\; \sin\left(\frac{\pi}{a}\frac{4a}{5}\right)\right)\right] \\ &=\; \frac{1}{a}\left[\, \frac{a}{10} \;-\; \frac{a}{2\pi} \sin\left(\frac{4\pi}{5}\right)\right] \;=\; \frac{1}{10} \;-\; \frac{1}{2\pi} \sin\left(\frac{4\pi}{5}\right) \;\approx\; 0.00645\,. \end{aligned}$$

The probability of finding the particle near the center is approximately 30 times greater than the probability of finding the particle near the edge when comparing intervals of length $a/5$.

8–6. Calculate the momentum space wave functions, $\widehat{\psi}_n(p)$, for an infinite square well of width $2a$. Write the eigenfunctions for $\widehat{\psi}_n(p)$ for $n = 1,\ 2,\ 3,$ and 4.

The momentum space wave functions are obtained from the position space wave functions using

$$\widehat{\psi}(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-ipx/\hbar}\, \psi(x)\, dx\,. \qquad \text{Do the integral for odd } n \text{ which is}$$

$$\widehat{\psi}_n(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int_{-a}^{a} e^{-ipx/\hbar}\, \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi x}{2a}\right) dx \qquad \text{and then for even } n\,, \text{ where}$$

the wave function will include a sine. The limits of the integral reflect the fact that all eigenfunctions are zero outside the potential well. Recall angle sum formulas from trigonometry and the expressions for cosine and sine in terms of complex exponentials. You should get

$$\widehat{\psi}_n(p) \;=\; \frac{1}{\sqrt{2\pi\hbar a}}\,\frac{(-1)^{\frac{n+1}{2}}}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{2a}\right)^2}\,\frac{n\pi}{a}\,\cos\left(\frac{p}{\hbar}\,a\right) \qquad \text{for n odd.}$$

Also, $\sin(n\pi/2) = (-1)^{\frac{n-1}{2}}$ for odd n. $\widehat{\psi}_n(p)$ for even n is similar though not the same.

Calculating the Fourier transforms of the position space wave functions starting with odd n,

$$\widehat{\psi}_n(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}}\int_{-a}^{a} e^{-ipx/\hbar}\frac{1}{\sqrt{a}}\,\cos\left(\frac{n\pi x}{2a}\right)dx \qquad \text{Let } c = p/\hbar \text{ and } b = n\pi/2a\,. \text{ Then}$$

$$\sqrt{2\pi\hbar a}\;\widehat{\psi}_n(p) \;=\; \int_{-a}^{a} e^{-icx}\cos(bx)\,dx \;=\; \int_{-a}^{a} e^{-icx}\left(\frac{e^{ibx}\;+\;e^{-ibx}}{2}\right)dx\,,$$

$$\begin{aligned}
\Rightarrow\quad 2\sqrt{2\pi\hbar a}\;\widehat{\psi}_n(p) \;&=\; \int_{-a}^{a}\left(e^{-i(c-b)x}\;+\;e^{-i(c+b)x}\right)dx \\
&=\; \left[\frac{1}{-i(c-b)}\,e^{-i(c-b)x}\;+\;\frac{1}{-i(c+b)}\,e^{-i(c+b)x}\right]_{-a}^{a} \\
&=\; \frac{i}{c^2-b^2}\left[(c+b)\,e^{-i(c-b)x}\;+\;(c-b)\,e^{-i(c+b)x}\right]_{-a}^{a} \\
&=\; \frac{i}{c^2-b^2}\left[(c+b)\left(e^{-i(c-b)a}-e^{i(c-b)a}\right)\;+\;(c-b)\left(e^{-i(c+b)a}-e^{i(c+b)a}\right)\right] \\
&=\; \frac{i}{c^2-b^2}\left[(c+b)(-2i)\sin\Big((c-b)\,a\Big)\;+\;(c-b)(-2i)\sin\Big((c+b)\,a\Big)\right] \\
&=\; \frac{2}{c^2-b^2}\left[(c+b)\Big(\sin(ca)\,\cos(ba)\;-\;\cos(ca)\,\sin(ba)\Big)\right] \\
&\qquad +\;\frac{2}{c^2-b^2}\left[(c-b)\Big(\sin(ca)\,\cos(ba)\;+\;\cos(ca)\,\sin(ba)\Big)\right] \\
&=\; \frac{4}{c^2-b^2}\Big[\,c\sin(ca)\,\cos(ba)\;-\;b\cos(ca)\,\sin(ba)\,\Big] \\
&=\; \frac{4}{c^2-b^2}\left[c\sin(ca)\,\cancel{\cos\left(\frac{n\pi}{2}\right)}\;-\;\frac{n\pi}{2a}\,\cos(ca)\,\sin\left(\frac{n\pi}{2}\right)\right].
\end{aligned}$$

$\cos\left(\frac{n\pi}{2}\right) = 0$ for odd n so is struck, $\sin\left(\frac{n\pi}{2}\right) = (-1)^{\frac{n-1}{2}}$ so $-\sin\left(\frac{n\pi}{2}\right) = (-1)^{\frac{n+1}{2}}$,

$$\Rightarrow\qquad 2\sqrt{2\pi\hbar a}\;\widehat{\psi}_n(p) \;=\; \frac{(-1)^{\frac{n+1}{2}}}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{2a}\right)^2}\,\frac{2n\pi}{a}\,\cos\left(\frac{p}{\hbar}\,a\right)$$

$$\Rightarrow\qquad \widehat{\psi}_n(p) \;=\; \frac{1}{\sqrt{2\pi\hbar a}}\,\frac{(-1)^{\frac{n+1}{2}}}{\left(\frac{p}{\hbar}\right)^2-\left(\frac{n\pi}{2a}\right)^2}\,\frac{n\pi}{a}\,\cos\left(\frac{p}{\hbar}\,a\right) \qquad \text{for odd } n\,.$$

For even n,

$$\widehat{\psi}_n(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}}\int_{-a}^{a} e^{-ipx/\hbar}\frac{1}{\sqrt{a}}\sin\left(\frac{n\pi x}{2a}\right)dx\,.\quad \text{Again let } c = p/\hbar \text{ and } b = n\pi/2a\,.\ \text{Then}$$

$$\sqrt{2\pi\hbar a}\;\widehat{\psi}_n(p) \;=\; \int_{-a}^{a} e^{-icx}\sin(bx)\,dx \;=\; \int_{-a}^{a} e^{-icx}\left(\frac{e^{ibx} \;-\; e^{-ibx}}{2i}\right)dx\,,$$

$$\Rightarrow \qquad 2i\sqrt{2\pi\hbar a}\;\widehat{\psi}_n(p) \;=\; \int_{-a}^{a}\left(e^{-i(c-b)x} \;-\; e^{-i(c+b)x}\right)dx\,.$$

This is the same integral just evaluated, except for the minus sign in front of the second exponential term. Using essentially the same procedure,

$$\begin{aligned} 2i\sqrt{2\pi\hbar a}\;\widehat{\psi}_n(p) \;&=\; \frac{4b}{c^2-b^2}\Big[\,\sin(ca)\,\cos(ba) \;-\; \cos(ca)\,\sin(ba)\,\Big] \\ &=\; \frac{2n\pi/a}{c^2-b^2}\left[\sin(ca)\,\cos\left(\frac{n\pi}{2}\right) \;-\; \cos(ca)\,\cancel{\sin\left(\frac{n\pi}{2}\right)}\right] \end{aligned}$$

The $\sin\left(\frac{n\pi}{2}\right) = 0$ for all even n, and $\cos\left(\frac{n\pi}{2}\right) = (-1)^{\frac{n}{2}}$, so

$$2i\sqrt{2\pi\hbar a}\;\widehat{\psi}_n(p) \;=\; \frac{(-1)^{\frac{n}{2}}}{\left(\frac{p}{\hbar}\right)^2 - \left(\frac{n\pi}{2a}\right)^2}\frac{2n\pi}{a}\;\sin\left(\frac{p}{\hbar}\,a\right)$$

$$\Rightarrow \qquad \widehat{\psi}_n(p) \;=\; \frac{i}{\sqrt{2\pi\hbar a}}\;\frac{(-1)^{\frac{n+2}{2}}}{\left(\frac{p}{\hbar}\right)^2 - \left(\frac{n\pi}{2a}\right)^2}\;\frac{n\pi}{a}\;\sin\left(\frac{p}{\hbar}\,a\right) \qquad \text{for even } n\,.$$

The factor of i in the numerator on the right accounts for the exponent of -1 being $(n+2)/2$ instead of $n/2$. The first four momentum space wave functions then are

$$\widehat{\psi}_1(p) \;=\; \frac{1}{\sqrt{2\pi\hbar a}}\;\frac{-1}{\left(\frac{p}{\hbar}\right)^2 - \left(\frac{\pi}{2a}\right)^2}\;\frac{\pi}{a}\;\cos\left(\frac{p}{\hbar}\,a\right),$$

$$\widehat{\psi}_2(p) \;=\; \frac{i}{\sqrt{2\pi\hbar a}}\;\frac{1}{\left(\frac{p}{\hbar}\right)^2 - \left(\frac{\pi}{a}\right)^2}\;\frac{2\pi}{a}\;\sin\left(\frac{p}{\hbar}\,a\right),$$

$$\widehat{\psi}_3(p) \;=\; \frac{1}{\sqrt{2\pi\hbar a}}\;\frac{1}{\left(\frac{p}{\hbar}\right)^2 - \left(\frac{3\pi}{2a}\right)^2}\;\frac{3\pi}{a}\;\cos\left(\frac{p}{\hbar}\,a\right),$$

$$\widehat{\psi}_4(p) \;=\; \frac{i}{\sqrt{2\pi\hbar a}}\;\frac{-1}{\left(\frac{p}{\hbar}\right)^2 - \left(\frac{2\pi}{a}\right)^2}\;\frac{4\pi}{a}\;\sin\left(\frac{p}{\hbar}\,a\right).$$

8–7. Draw sketches of the $n = 1$, $n = 2$, and $n =$ many wave functions in position space, energy space, and momentum space.

Examine the sketches below.

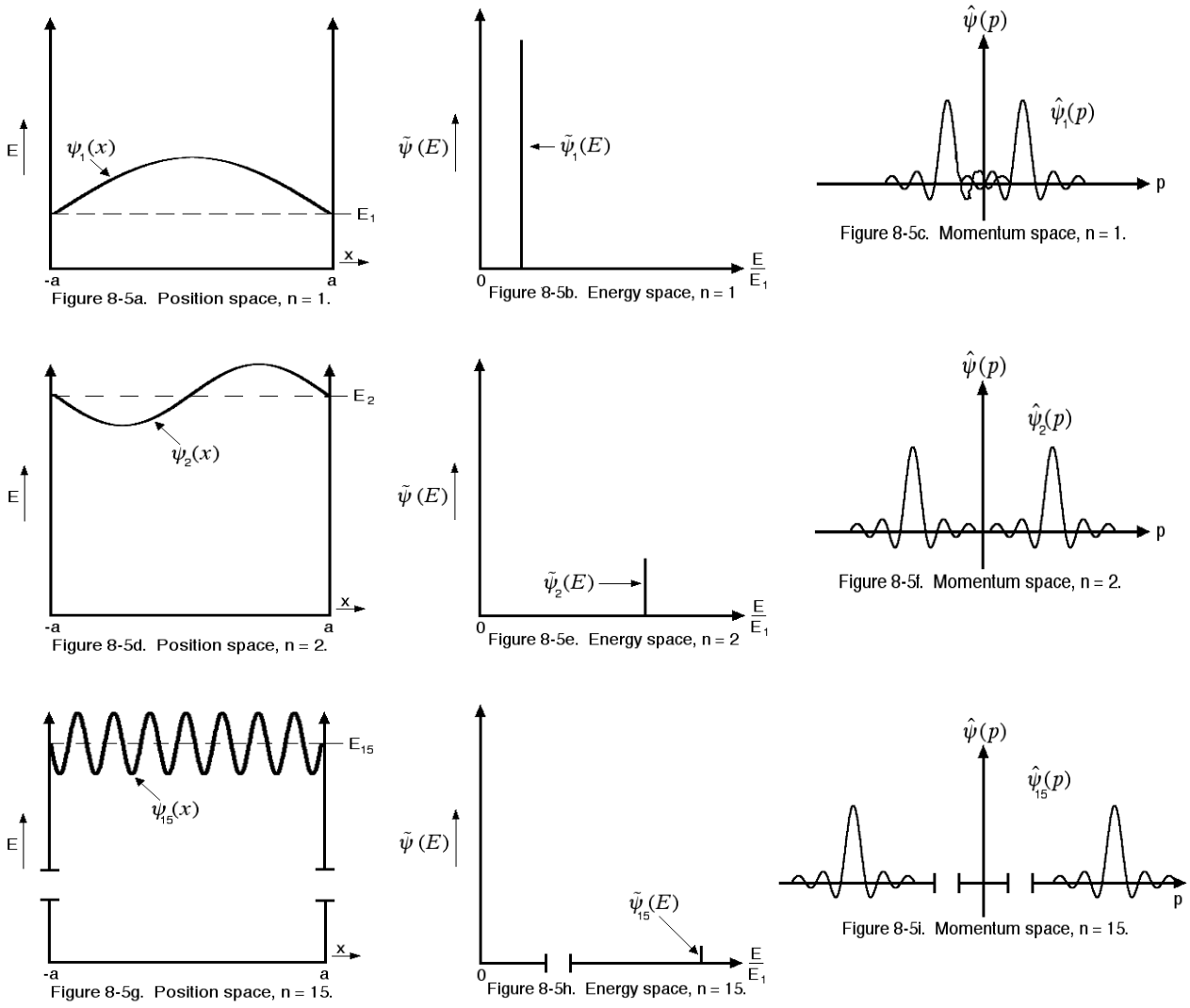


Figure 8-5a. Position space, n = 1.
Figure 8-5b. Energy space, n = 1
Figure 8-5c. Momentum space, n = 1.
Figure 8-5d. Position space, n = 2.
Figure 8-5e. Energy space, n = 2
Figure 8-5f. Momentum space, n = 2.
Figure 8-5g. Position space, n = 15.
Figure 8-5h. Energy space, n = 15.
Figure 8-5i. Momentum space, n = 15.

Figure 8–5. Sketches for $n = 1$, $n = 2$, and $n = 15$ in position, energy, and momentum space.

Postscript: The energy eigenfunctions, $\widetilde{\psi}(E)$, are the eigenvalues of energy so are discontinuous spikes for quantized energies. In momentum space, $\widehat{\psi}(p)$ versus momentum or wavenumber, the wave functions are sinc functions. Energy is related to momentum, $E = p^2/2m = \hbar^2 k^2/2m$, so energy proportional to the square of the wavenumber is related to the horizontal axes of the momentum space graphs. The spikes in energy space are "spread" in momentum space at the wave number that corresponds to the eigenenergy. Remember that the relation between position space and momentum space wave functions is that one is the Fourier transform of the other.

8–8. Given $\Psi(x) = \sum_n c_n \psi_n(x)$, show that $c_n = \int \psi_n^*(x)\,\Psi(x)\,dx$.

Here is a derivation of the procedure used to calculate Fourier coefficients in a quantum mechanical context which should also highlight some of the utility of the Dirac notation. Remember the techniques of inserting and resolving the identity, and forming position space functions by operating from the left with $<x|$. One thing to recall is $<x|E_n> = \psi_n(x)$; the inner product of the continuum of position space with the energy eigenkets are the energy eigenfunctions in position space. These eigenfunctions have the independent variable of position and eigenvalues that are energy. For the infinite square well, they are the normalized sines and cosines of problem 8–2.

$$
\begin{aligned}
|\psi> &= \mathcal{I}\,|\psi> &&= \sum_n |E_n><E_n|\psi> \\
\Rightarrow \quad <x|\psi> &= <x|\sum_n |E_n><E_n|\psi> &&= \sum_n <x|E_n><E_n|\psi> \\
\Rightarrow \quad \Psi(x) &= \sum_n \psi_n(x) <E_n|\psi>
\end{aligned}
$$

where the identity is inserted and resolved in the first line and we prepare to represent the expression in the second line. The third line is the partial position space representation. Inserting and resolving the identity again preparing to represent the right side entirely in position space,

$$
\begin{aligned}
\Psi(x) &= \sum_n \psi_n(x) <E_n|\mathcal{I}|\psi> = \sum_n \psi_n(x) <E_n|\Big(\sum |x><x|\Big)|\psi> \\
&= \sum_n \psi_n(x) \sum <E_n|x><x|\psi> = \sum_n \psi_n(x) \sum \Big(<E_n|x>\Big)\Big(<x|\psi>\Big)
\end{aligned}
$$

where we have simply rearranged and regrouped. Representing the terms in parentheses,

$$\Psi(x) \longrightarrow \sum_n \psi_n(x) \int \Big(\psi_n^*(x)\Big)\Big(\Psi(x)\Big)\,dx$$

in the limit that the distance between $|x>$'s approaches zero. Comparing the last line with the given $\Psi(x) = \sum_n \psi_n\, c_n(x)$, $\Rightarrow$ $c_n = \int \psi_n^*(x)\,\Psi(x)\,dx$.

Postscript: Notice that the derivation is independent of potential.

"In the limit that the distance between $|x>$'s approaches zero" is simply another way to say that x is treated as a continuous variable.

8–9. Calculate the uncertainty in position for a particle in an infinite square well of width $2a$.

Find (a) $< x >$, (b) $< x^2 >$, and (c) $\triangle x$ for all n. The limits of integration for an expectation value for position become $-a$ and a because the wave function is zero outside those bounds. There are two integrations for each expectation value, one for n_{odd} and one for n_{even}. Realize $\sin(n\pi) = 0$ and $\cos(n\pi) = \pm 1$ for all n. Having found the expectation values, uncertainty is $\triangle x = \left(< x^2 > - < x >^2\right)^{1/2}$. What is reasonable for $< x >$? Will it surprise you if the "average" is near the center of the box? The second moment, $< x^2 >$, reflects the magnitude of position. Expect this to be a non-zero quantity.

(a) When n is odd,

$$< x >_{\text{n odd}} = \int_{-a}^{+a} \left[\sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right)\right]^* x \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right) dx = \frac{1}{a}\int_{-a}^{+a} x \cos^2\left(\frac{n\pi x}{2a}\right) dx$$

$$= \frac{1}{a}\left[\frac{x^2}{4} + \frac{x \sin\left(\frac{n\pi x}{a}\right)}{\frac{2n\pi}{a}} + \frac{\cos\left(\frac{n\pi x}{a}\right)}{\frac{4n^2\pi^2}{a^2}}\right]_{-a}^{+a}.$$

The first and the third terms inside the brackets are zero, because they are even functions evaluated between symmetric limits (after integration; do not confuse this evaluation with that of an even integrand between symmetric limits), so

$$< x >_{\text{n odd}} = \frac{1}{a}\left[\frac{x \sin\left(\frac{n\pi x}{a}\right)}{\frac{2n\pi}{a}}\right]_{-a}^{+a} = \frac{a \sin(n\pi)}{2n\pi} - \frac{-a \sin(-n\pi)}{2n\pi} = \frac{a}{2n\pi}\left[\sin(n\pi) - \sin(n\pi)\right] = 0.$$

For even n,

$$< x >_{\text{n even}} = \int_{-a}^{+a} \left[\sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right)\right]^* x \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right) dx = \frac{1}{a}\int_{-a}^{+a} x \sin^2\left(\frac{n\pi x}{2a}\right) dx$$

$$= \frac{1}{a}\left[\frac{x^2}{4} - \frac{x \sin\left(\frac{n\pi x}{a}\right)}{\frac{2n\pi}{a}} - \frac{\cos\left(\frac{n\pi x}{a}\right)}{\frac{4n^2\pi^2}{a^2}}\right]_{-a}^{+a}.$$

Again, the first and third terms inside the brackets are even functions evaluated between symmetric limits so they are zero, and

$$< x >_{\text{n even}} = \frac{1}{a}\left[-\frac{x \sin\left(\frac{n\pi x}{a}\right)}{\frac{2n\pi}{a}}\right]_{-a}^{+a} = -\frac{1}{a}\left[\frac{a \sin(n\pi)}{\frac{2n\pi}{a}} - \frac{-a \sin(-n\pi)}{\frac{2n\pi}{a}}\right] = -\frac{1}{a}\Big[0 - 0\Big] = 0$$

$$\Rightarrow \quad < x > = 0 \quad \text{for all } n,$$

or notice that both integrals are odd functions evaluated between symmetric limits so are zero.

(b) The expectation value of position squared for odd quantum number is

$$<x^2>_{\text{n odd}} \;=\; \int_{-a}^{+a} \left[\sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right)\right]^* x^2 \sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right) dx \;=\; \frac{1}{a}\int_{-a}^{+a} x^2\,\cos^2\left(\frac{n\pi x}{2a}\right) dx$$

$$= \frac{1}{a}\left[\frac{x^3}{6} + \left(\frac{x^2}{4\left(\frac{n\pi}{2a}\right)} - \frac{1}{8\left(\frac{n\pi}{2a}\right)^3}\right)\sin\left(\frac{n\pi x}{a}\right) + \frac{x\,\cos\left(\frac{n\pi x}{a}\right)}{4\left(\frac{n\pi}{2a}\right)^2}\right]_{-a}^{+a}.$$

The middle term is zero because $\sin(n\pi) = 0$ for all n at both a and $-a$,

$$\Rightarrow \quad <x^2>_{\text{n odd}} \;=\; \frac{1}{a}\left[\frac{a^3}{6} - \frac{(-a)^3}{6} + \frac{a\,\cos(n\pi)}{4\left(\frac{n^2\pi^2}{4a^2}\right)} - \frac{-a\,\cos(-n\pi)}{4\left(\frac{n^2\pi^2}{4a^2}\right)}\right].$$

Both the cosine terms are -1 for all odd n, so

$$<x^2>_{\text{n odd}} \;=\; \frac{1}{a}\left[\frac{a^3}{3} - \frac{2a^3}{n^2\pi^2}\right] \;=\; \frac{a^2}{3} - \frac{2a^2}{n^2\pi^2}.$$

For even n, the calculation is very similar except the integration is over sine squared,

$$<x^2>_{\text{n even}} \;=\; \frac{1}{a}\int_{-a}^{+a} x^2\,\sin^2\left(\frac{n\pi x}{2a}\right) dx$$

$$= \frac{1}{a}\left[\frac{x^3}{6} - \left(\frac{x^2}{4\left(\frac{n\pi}{2a}\right)} - \frac{1}{8\left(\frac{n\pi}{2a}\right)^3}\right)\sin\left(\frac{n\pi x}{a}\right) - \frac{x\,\cos\left(\frac{n\pi x}{a}\right)}{4\left(\frac{n\pi}{2a}\right)^2}\right]_{-a}^{+a}.$$

Again, the middle term vanishes at $x = \pm a$, and the cosine terms are $+1$ for all even n, so

$$<x^2>_{\text{n even}} \;=\; \frac{1}{a}\left[\frac{a^3}{3} - \frac{2a^3}{n^2\pi^2}\right] \;=\; \frac{a^2}{3} - \frac{2a^2}{n^2\pi^2}.$$

This is the same as the n odd case, so we conclude

$$<x^2> \;=\; \frac{a^2}{3} - \frac{2a^2}{n^2\pi^2}.$$

(c) $\qquad \triangle x \;=\; \left(<x^2> - <x>^2\right)^{1/2} \;=\; \left(\frac{a^2}{3} - \frac{2a^2}{n^2\pi^2}\right)^{1/2}$ for all n.

8–10. Calculate the uncertainty in momentum for a particle in an infinite square well of width $2a$.

Find (a) $<p>$, (b) $<p^2>$, and (c) $\triangle p$ for all n. These could be calculated in momentum space using the $\widehat{\psi}_n(p)$ from problem 8–6, but that path leads to involved integrals with limits of $\pm\infty$. The position space calculation using the P_{op} representation in position space, i.e.,

$$<p> \;=\; \int_{-\infty}^{+\infty} \psi^*(x)\; P_{op}\,\psi(x)\,dx \qquad \text{where} \qquad P_{op} \;=\; -i\hbar\nabla \;=\; -i\hbar\,\frac{d}{dx} \qquad \text{in one dimension}$$

where the limits of integration are $\pm a$ is preferable. Find $<p^2>$ similarly using

$$P_{op}^2 \;=\; (-i\hbar\nabla)\,(-i\hbar\nabla) \;=\; \left(-i\hbar\,\frac{d}{dx}\right)\left(-i\hbar\,\frac{d}{dx}\right) \;=\; -\hbar^2\frac{d^2}{dx^2}\,.$$

Nothing prejudices momentum to the left or right so expect $<p> \;=\; 0$. The magnitude of the momentum is non-zero, so will be reflected by non-zero expectation values in the second moment.

$$\text{(a)}\quad <p>_{\text{n odd}} \;=\; \int_{-\infty}^{\infty}\left[\sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right)\right]^*\left(-i\hbar\frac{d}{dx}\right)\left[\sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right)\right]dx$$

$$= \;\frac{-i\hbar}{a}\int_{-a}^{a}\cos\left(\frac{n\pi x}{2a}\right)\frac{d}{dx}\cos\left(\frac{n\pi x}{2a}\right)dx \;=\; \frac{in\pi\hbar}{2a^2}\int_{-a}^{a}\cos\left(\frac{n\pi x}{2a}\right)\sin\left(\frac{n\pi x}{2a}\right)dx$$

$$= \;\frac{in\pi\hbar}{2a^2}\left[\frac{2a}{2n\pi}\sin^2\left(\frac{n\pi x}{2a}\right)\right]_{-a}^{a} \;=\; \frac{i\hbar}{2a}\left[\sin^2\left(\frac{n\pi}{2}\right) \;-\; \sin^2\left(\frac{-n\pi}{2}\right)\right].$$

Since $\sin\left(\dfrac{\pm n\pi}{2}\right) = \pm 1$ for odd n, $\sin^2\left(\dfrac{\pm n\pi}{2}\right) = 1$, so $<p>_{\text{n odd}} \;=\; \dfrac{i\hbar}{2a}\,[\,1-1\,] \;=\; 0$.

$$<p>_{\text{n even}} \;=\; \int_{-\infty}^{\infty}\left[\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)\right]^*\left(-i\hbar\frac{d}{dx}\right)\left[\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)\right]dx$$

$$= \;\frac{-i\hbar}{a}\int_{-a}^{a}\sin\left(\frac{n\pi x}{2a}\right)\frac{d}{dx}\sin\left(\frac{n\pi x}{2a}\right)dx \;=\; -\frac{in\pi\hbar}{2a^2}\int_{-a}^{a}\sin\left(\frac{n\pi x}{2a}\right)\cos\left(\frac{n\pi x}{2a}\right)dx$$

$$= \;-\frac{in\pi\hbar}{2a^2}\left[\frac{2a}{2n\pi}\sin^2\left(\frac{n\pi x}{2a}\right)\right]_{-a}^{a} \;=\; -\frac{i\hbar}{2a}\left[\sin^2\left(\frac{n\pi}{2}\right) \;-\; \sin^2\left(\frac{-n\pi}{2}\right)\right].$$

$\sin\left(\dfrac{n\pi}{2}\right) = 0$ for all even n so both sine terms are zero,

$$\Rightarrow \quad <p>_{\text{n even}} \;=\; -\frac{i\hbar}{2a}\,[\,0-0\,] \;=\; 0 \quad \Rightarrow \quad <p> \;=\; 0 \quad \text{for all } n\,.$$

Alternatively, both integrals are odd functions evaluated between symmetric limits so are zero.

$$\text{(b)}\quad <p^2>_{\text{n odd}} \;=\; \int_{-\infty}^{\infty}\left[\sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right)\right]^*\left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right)\left[\sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right)\right]dx$$

$$= \;-\frac{\hbar^2}{a}\int_{-a}^{a}\cos\left(\frac{n\pi x}{2a}\right)\frac{d^2}{dx^2}\cos\left(\frac{n\pi x}{2a}\right)dx \;=\; \frac{\hbar^2}{a}\left(\frac{n\pi}{2a}\right)^2\int_{-a}^{a}\cos^2\left(\frac{n\pi x}{2a}\right)dx$$

$$= \;\frac{n^2\pi^2\hbar^2}{4a^3}\left[\frac{x}{2} \;+\; \frac{2a}{4n\pi}\sin\left(\frac{n\pi x}{a}\right)\right]_{-a}^{a} \;=\; \frac{n^2\pi^2\hbar^2}{4a^3}\left[\frac{a}{2} \;-\; \frac{-a}{2} \;+\; \frac{2a}{4n\pi}\left(\sin(n\pi) - \sin(-n\pi)\right)\right]$$

Both sine terms are zero so $<p^2>_{\text{n odd}} = \dfrac{n^2\pi^2\hbar^2}{4a^2}$.

$$
\begin{aligned}
<p^2>_{\text{n even}} &= -\frac{\hbar^2}{a}\int_{-a}^{a}\sin\left(\frac{n\pi x}{2a}\right)\frac{d^2}{dx^2}\sin\left(\frac{n\pi x}{2a}\right)dx = \frac{\hbar^2}{a}\left(\frac{n\pi}{2a}\right)^2\int_{-a}^{a}\sin^2\left(\frac{n\pi x}{2a}\right)dx \\
&= \frac{n^2\pi^2\hbar^2}{4a^3}\left[\frac{x}{2} - \frac{2a}{4n\pi}\sin\left(\frac{n\pi x}{a}\right)\right]_{-a}^{a} \\
&= \frac{n^2\pi^2\hbar^2}{4a^3}\left[\frac{a}{2} - \frac{-a}{2} - \frac{2a}{4n\pi}\left(\sin(n\pi)+\sin(-n\pi)\right)\right] = \frac{n^2\pi^2\hbar^2}{4a^2} \\
\Rightarrow \quad <p^2> &= \frac{n^2\pi^2\hbar^2}{4a^2} \quad \text{for all } n\,.
\end{aligned}
$$

(c) $\triangle p = \left(<p^2> - <p>^2\right)^{1/2} = \left(<p^2> - 0\right)^{1/2} = \left(<p^2>\right)^{1/2} \quad \Rightarrow \quad \triangle p = \dfrac{n\pi\hbar}{2a}$ for all n.

8–11. Normalize the wavefunction

$$\Psi(x) = N(a^2 - x^2)$$

describing a particle confined in an infinite square well of width $2a$.

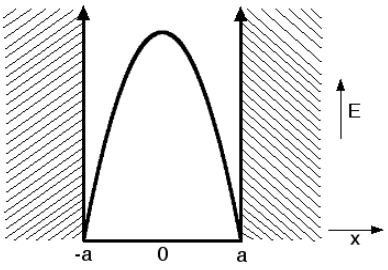


Figure 8–6. $\Psi(x) = N(a^2 - x^2)$ in an infinite square well potential.

Problems 8–11 and 8–12 are intended to emphasize that wave functions are generally linear combinations of the eigenfunctions. A particle in an infinite square well can be in its ground state, any excited state, or any linear combination of its ground state and its excited states. Symbolically,

$$\Psi(x) = c_1\psi_1(x) + c_2\psi_2(x) + c_3\psi_3(x) + \cdots = \sum_{n=1}^{\infty} c_n\psi_n(x)\,,$$

where the c_n are constants that describe the relative contributions of each eigenfunction. The relative magnitudes of the c_n are fixed by normalization. Limited only by the constraint of normalization, the c_n can be anything, meaning the linear combination $\Psi(x)$ can be any shape.

The components of $\Psi(x)$ must be orthogonal, otherwise, eigenfunctions would contain portions of other eigenfunctions, and the c_n would not be unique. Without unique c_n, the expansion $\Psi(x) = \sum c_n\psi_n(x)$ is not unique, and thus, it is not useful. Sines and cosines were shown to be orthogonal on an interval in chapter 5. The eigenfunctions of a particle are sines and cosines within an infinite square well so are orthogonal, and thus, can be made orthonormal.

This problem starts with a position space statement of the normalization condition.

$$1 \;=\; \int_{-\infty}^{\infty} N^*\,(a^2-x^2)^*\;N\,(a^2-x^2)\,dx \;=\; |\,N\,|^{\,2}\int_{-a}^{a}(a^2-x^2)^2\,dx$$

$$=\; |\,N\,|^{\,2}\int_{-a}^{a}(a^4-2a^2x^2+x^4)\,dx \;=\; |\,N\,|^{\,2}\left(a^4\int_{-a}^{a}dx \;-\; 2a^2\int_{-a}^{a}x^2\,dx \;+\; \int_{-a}^{a}x^4\,dx\right)$$

$$=\; |\,N\,|^{\,2}\left[\,a^4x \;-\; 2a^2\,\frac{x^3}{3} \;+\; \frac{x^5}{5}\,\right]_{-a}^{a}$$

$$=\; |\,N\,|^{\,2}\left[\,a^4\,(a--a) \;-\; \frac{2a^2}{3}\,(a^3-(-a)^3) \;+\; \frac{1}{5}\,(a^5-(-a)^5)\,\right]$$

$$=\; |\,N\,|^{\,2}\left[\,2a^5-\frac{4a^5}{3}+\frac{2a^5}{5}\,\right] \;=\; |\,N\,|^{\,2}a^5\left[\,\frac{2}{3}+\frac{2}{5}\,\right] \;=\; |\,N\,|^{\,2}a^5\left[\,\frac{10}{15}+\frac{6}{15}\,\right] \;=\; |\,N\,|^{\,2}a^5\,\frac{16}{15}$$

$$\Rightarrow \quad N^2 \;=\; \frac{15}{16a^5} \quad\Rightarrow\quad N \;=\; \frac{1}{4a^2}\sqrt{\frac{15}{a}} \quad\Rightarrow\quad \Psi\,(x) \;=\; \frac{1}{4a^2}\sqrt{\frac{15}{a}}\left(a^2-x^2\right).$$

8–12. Expand the system described in problem 8–11 into its component eigenfunctions.

For the infinite square well,

$$\Psi\,(x) \;=\; \sum_{n=1}^{\infty} c_n\,\psi_n\,(x) \quad \text{means} \quad \Psi\,(x) \;=\; \sum_{n\ \text{odd}}^{\infty} b_n\sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right) \;+\; \sum_{n\ \text{even}}^{\infty} d_n\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right),$$

where the c_n are written as b_n and d_n just to aid identification. The wave function is an even function because $\Psi\,(-x)=\Psi\,(x)$. Only even eigenfunctions, therefore, can contribute so $d_n=0$ for all even n. (Do not confuse even/odd quantum numbers with even/odd functions. Cosines are even functions, and for the infinite square well, they correspond to the odd quantum numbers. Sines are odd functions, but correspond to even quantum numbers for our infinite square well). Odd eigenfunctions cannot contribute to an even $\Psi\,(x)$, otherwise $\Psi\,(x)$ would have at least one odd component and would be neither an even nor an odd function. The wave function reduces to

$$\Psi\,(x) \;=\; \sum_{\text{n odd}}^{\infty} b_n\sqrt{\frac{1}{a}}\cos\left(\frac{n\pi x}{2a}\right).$$

The b_n are then found using procedures similar to finding Fourier coefficients.

$$b_n \;=\; \int_{-a}^{a} \psi_n^*(x)\,\Psi(x)\,dx \;=\; \int_{-a}^{a} \sqrt{\frac{1}{a}}\,\cos\Big(\frac{n\pi x}{2a}\Big)\;\frac{1}{4}\sqrt{\frac{15}{a^5}}\,(a^2-x^2)\,dx$$

$$= \;\frac{\sqrt{15}}{4a^3}\int_{-a}^{a}\cos\Big(\frac{n\pi x}{2a}\Big)\,(a^2-x^2)\,dx \;=\; \frac{\sqrt{15}}{4a}\int_{-a}^{a}\cos\Big(\frac{n\pi x}{2a}\Big)\,dx - \frac{\sqrt{15}}{4a^3}\int_{-a}^{a} x^2\cos\Big(\frac{n\pi x}{2a}\Big)\,dx$$

$$= \;\frac{\sqrt{15}}{4a}\left(\frac{2a}{n\pi}\right)\sin\Big(\frac{n\pi x}{2a}\Big)\Big|_{-a}^{a}$$
$$-\frac{\sqrt{15}}{4a^3}\left[\frac{2x\,\cos\Big(\frac{n\pi x}{2a}\Big)}{\Big(\frac{n\pi}{2a}\Big)^2} \;+\; \frac{x^2}{\Big(\frac{n\pi}{2a}\Big)}\sin\Big(\frac{n\pi x}{2a}\Big) \;-\; \frac{2}{\Big(\frac{n\pi}{2a}\Big)^3}\sin\Big(\frac{n\pi x}{2a}\Big)\right]_{-a}^{a}$$

$$= \;\frac{\sqrt{15}}{2n\pi}\sin\Big(\frac{n\pi x}{2a}\Big)\Big|_{-a}^{a} - \;\frac{\sqrt{15}}{4a^3}\left[\frac{8a^2x}{n^2\pi^2}\cos\Big(\frac{n\pi x}{2a}\Big) + \frac{2ax^2}{n\pi}\sin\Big(\frac{n\pi x}{2a}\Big) \;-\; \frac{16a^3}{n^3\pi^3}\sin\Big(\frac{n\pi x}{2a}\Big)\right]_{-a}^{a}$$

$$= \;\frac{\sqrt{15}}{2n\pi}\left[\sin\Big(\frac{n\pi}{2}\Big) \;-\; \sin\Big(-\frac{n\pi}{2}\Big)\right] \;-\; \frac{\sqrt{15}}{4a^3}\left[\frac{8a^2a}{n^2\pi^2}\cos\Big(\frac{n\pi}{2}\Big) \;-\; \frac{8a^2(-a)}{n^2\pi^2}\cos\Big(-\frac{n\pi}{2}\Big)\right.$$

$$\left. +\;\frac{2a\,a^2}{n\pi}\sin\Big(\frac{n\pi}{2}\Big) \;-\; \frac{2a\,(-a)^2}{n\pi}\sin\Big(-\frac{n\pi}{2}\Big) \;-\; \frac{16a^3}{n^3\pi^3}\Big(\sin\Big(\frac{n\pi}{2}\Big) \;-\; \sin\Big(-\frac{n\pi}{2}\Big)\Big)\right]$$

$$= \;\frac{\sqrt{15}}{n\pi}\sin\Big(\frac{n\pi}{2}\Big) \;-\; \frac{\sqrt{15}}{4a^3}\left[\frac{16a^3}{n^2\pi^2}\cos\Big(\frac{n\pi}{2}\Big) \;+\; \frac{4a^3}{n\pi}\sin\Big(\frac{n\pi}{2}\Big) \;-\; \frac{32a^3}{n^3\pi^3}\sin\Big(\frac{n\pi}{2}\Big)\right].$$

Remembering that the quantum number n is odd only,

$$\cos\Big(\frac{n\pi}{2}\Big) \;=\; 0 \quad \text{for all } n, \qquad \text{and} \qquad \sin\Big(\frac{n\pi}{2}\Big) \;=\; (-1)^{\frac{n-1}{2}}.$$

Using these in the last expression yields

$$b_n \;=\; (-1)^{\frac{n-1}{2}}\frac{\sqrt{15}}{n\pi} \;-\; \sqrt{15}\left[(-1)^{\frac{n-1}{2}}\frac{1}{n\pi} \;-\; (-1)^{\frac{n-1}{2}}\frac{8}{n^3\pi^3}\right]$$
$$= \;(-1)^{\frac{n-1}{2}}\frac{\cancel{\sqrt{15}}}{\cancel{n\pi}} \;-\; (-1)^{\frac{n-1}{2}}\frac{\cancel{\sqrt{15}}}{\cancel{n\pi}} \;+\; (-1)^{\frac{n-1}{2}}\frac{8\sqrt{15}}{n^3\pi^3} \;=\; (-1)^{\frac{n-1}{2}}\frac{8\sqrt{15}}{n^3\pi^3}\,.$$

Then the expansion in terms of component eigenfunctions is

$$\Psi(x) \;=\; \sum_{\text{n odd}}^{\infty}(-1)^{\frac{n-1}{2}}\frac{8\sqrt{15}}{n^3\pi^3}\sqrt{\frac{1}{a}}\cos\Big(\frac{n\pi x}{2a}\Big) \;=\; \frac{8}{\pi^3}\sqrt{\frac{15}{a}}\sum_{\text{n odd}}^{\infty}\frac{(-1)^{\frac{n-1}{2}}}{n^3}\cos\Big(\frac{n\pi x}{2a}\Big).$$

8–13. Find the time-dependent wave function for the system described in problems 8–11 and 8–12.

Time evolution for the case $\mathcal{H} \neq \mathcal{H}(t)$ was introduced using small matrix operators by first expanding $|\psi(t)>$ in the eigenstates of $\mathcal{H}$, and then using the fact that the eigenstates of $\mathcal{H}$ obey $i\hbar \dfrac{d}{dt}|E_n> = E_n|E_n>$ with the simple time dependence $|E_n(t)> = e^{-iE_n t/\hbar}|E_n>$. When the general wave function is a linear combination of eigenfunctions, the time-dependent wave function is the sum of the time evolved eigenfunctions, or

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

The Hamiltonian of the infinite square well is $\mathcal{H} = p^2/2m$ inside the well and zero elsewhere. This Hamiltonian is time independent so these procedures apply to the infinite square well.

The eigenenergies of the infinite square well are given in problem 8–1, so the exponential terms are

$$e^{-iE_n t/\hbar} = \exp\left[-i\left(n^2\frac{\pi^2\hbar^2}{8ma^2}\right)\frac{t}{\hbar}\right] = \exp\left(-i\,\frac{\pi^2 n^2 \hbar}{8ma^2}\,t\right).$$

Merging this with the normalized eigenstates calculated in problems 8–11 and 8–12,

$$\Psi(x,t) = \frac{8}{\pi^3}\sqrt{\frac{15}{a}}\sum_{\text{n odd}}^{\infty}\frac{(-1)^{\frac{n-1}{2}}}{n^3}\cos\left(\frac{n\pi x}{2a}\right)\exp\left(-i\,\frac{\pi^2 n^2\hbar}{8ma^2}\,t\right).$$

8–14. Find the eigenenergies of a two-dimensional infinite square well of width $2a$ on each side.

This problem extends the discussion to higher dimension. It also introduces the method of **separation of variables** for partial differential equations (PDE). This method is used in future chapters and it is often among the first techniques selected to try to solve a PDE. A variables separable PDE has a solution of the form $f(x,y) = g(x)\,h(y)$, meaning that the solution in two dimensions is the product of two one-dimensional solutions. The strategy is to assume the existence of such a solution, and if such a solution is found, the assumption was valid.

In two dimensions, wave functions in position space are $\psi = \psi(x,y)$. The time-independent form of the Schrodinger equation within a two-dimensional infinite square well is

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y) = E\,\psi(x,y)$$

where the potential energy function is excluded because it is defined to be zero in the region of confinement. The wave function is zero elsewhere so other regions are not considered. Assume a solution of the form $\psi(x,y) = f(x)\,g(y)$. The Schrodinger equation becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) f(x)\,g(y) = E\,f(x)\,g(y)$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\left(g(y)\frac{\partial^2}{\partial x^2}f(x) + f(x)\frac{\partial^2}{\partial y^2}g(y)\right) = E f(x) g(y)$$

$$\Rightarrow \quad \frac{1}{f(x)g(y)}\left(g(y)\frac{d^2}{dx^2}f(x) + f(x)\frac{d^2}{dy^2}g(y)\right) = -\frac{2mE}{\hbar^2}$$

$$\Rightarrow \quad \frac{1}{f(x)}\frac{d^2}{dx^2}f(x) + \frac{1}{g(y)}\frac{d^2}{dy^2}g(y) = -\frac{2mE}{\hbar^2}\,.$$

The first term is dependent only on x and the second term is dependent only on y. Their sum is constant because the right side of the equation is constant. Except for trivial cases, this can occur only if the first term is equal to a constant and the second term is equal to another constant, or

$$\frac{1}{f(x)}\frac{d^2}{dx^2}f(x) = C_1\,, \qquad \text{and} \qquad \frac{1}{g(y)}\frac{d^2}{dy^2}g(y) = C_2\,.$$

The constants C_1 and C_2 must sum to $-2mE/\hbar^2$. We choose the **separation constants**

$$\frac{1}{f(x)}\frac{d^2}{dx^2}f(x) = -\frac{2mE_x}{\hbar^2}\,, \qquad \text{and} \qquad \frac{1}{g(y)}\frac{d^2}{dy^2}g(y) = -\frac{2mE_y}{\hbar^2}\,, \tag{1}$$

$$\Rightarrow \quad \frac{d^2}{dx^2}f(x) = -\frac{2mE_x}{\hbar^2}f(x)\,, \qquad \text{and} \qquad \frac{d^2}{dy^2}g(y) = -\frac{2mE_y}{\hbar^2}g(y)\,.$$

Both have the same form as the Schrodinger equation for the infinite square well in one dimension,

$$\frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x)\,,$$

so necessarily both equations have the same solution. Therefore, the component eigenvalues are

$$E_x = n_x^2\frac{\pi^2\hbar^2}{8ma^2} \qquad \text{and} \qquad E_y = n_y^2\frac{\pi^2\hbar^2}{8ma^2}\,.$$

Total energy is the sum of the energies in the two degrees of freedom, so

$$E_{n_x,n_y} = E_x + E_y = \frac{\pi^2\hbar^2}{8ma^2}\left(n_x^2 + n_y^2\right)\,.$$

Postscript: Do not confuse the method of separation of variables used for partial differential equations with the variables separable method used for ordinary differential equations (ODE). Separating the variables of a PDE is an effort to reduce the PDE to two or more ODE's. If the PDE can be separated, methods appropriate to ODE's may then be used to solve the ODE's individually, and the product of these individual solutions is the solution to the PDE.

That $\psi(x,y) = f(x)g(y)$ is an assumption. A solution of this form was found for the two-dimensional infinite square well so the assumption proved to be valid. If such a solution cannot be found in attempting to solve a PDE, then the assumption $\psi(x,y) = f(x)g(y)$ is invalid and other means must be used to obtain a solution.

The selection of separation constants, as in equation (1), is an art. Realize that we are guided by the literature in our selections.

Notice that there are two quantum numbers, n_x and n_y, for the two-dimensional problem. In general, there will be as many quantum numbers as there are degrees of freedom in the problem. For a three dimensional system, for instance, there will be three quantum numbers.

Probability for $\psi(x,y)$ is $|\psi(x,y)|^2\,dx\,dy$, probability density is $|\psi(x,y)|^2$, $\psi(x,y)$ has the dimensions $1/\text{length}$, and probability density has dimensions of $1/\text{length}^2$.

8–15. Find the sets of quantum numbers for a two-dimensional infinite square well that yield the lowest 12 eigenenergies. Identify the eigenenergies from this list that demonstrate degeneracy.

This problem demonstrates degeneracy in a pseudo-physical system. It is generally conventional to express eigenenergies in terms of ground state energy. The ground state energy of the one–dimensional infinite square well, which we denote E_0 here (notice that $E_{\text{ground}} = 2E_0$ in this system), is convenient for this two-dimensional system since component eigenenergies are integral multiples of E_0. Ground state energy is the lowest possible energy where zero energy is disallowed because a physical system cannot exist at zero energy. Zero is disallowed as a component quantum number in a multi-dimensional infinite square well because it would result in an overall zero wave function, meaning the system does not exist.

---

n_x	n_y	E	#	n_x	n_y	E	#
1	1	$2E_0$	1	3	3	$18E_0$	7
2	1	$5E_0$	2	4	2	$20E_0$	8
1	2	$5E_0$	2	2	4	$20E_0$	8
2	2	$8E_0$	3	4	3	$25E_0$	9
3	1	$10E_0$	4	3	4	$25E_0$	9
1	3	$10E_0$	4	5	1	$26E_0$	10
3	2	$13E_0$	5	1	5	$26E_0$	10
2	3	$13E_0$	5	5	2	$29E_0$	11
4	1	$17E_0$	6	2	5	$29E_0$	11
1	4	$17E_0$	6	4	4	$32E_0$	12

Degeneracy is seen at $5E_0$, $10E_0$, $13E_0$, $17E_0$, $20E_0$, $25E_0$, $26E_0$, and $29E_0$ in this list.

Postscript: Notice that component quantum number 4 is encountered in the energy sequence before component quantum number 3 is exhausted, and component quantum number 5 is encountered before component quantum number 4 is exhausted. This is a feature seen in realistic systems.

If a component quantum number of zero was allowed, for instance if $n_y = 0$, then

$$\psi_{n_x=1,\,n_y=0} \;=\; \frac{1}{\sqrt{a}}\cos\left(\frac{\pi x}{2a}\right)\frac{1}{\sqrt{a}}\sin(0) \;=\; 0\,.$$

A zero wave function is a system that does not exist so zero is disallowed as a component quantum number for a multi-dimensional infinite square well.

Exercises

8–16. Calculate the energies of the first five energy levels of an electron trapped in a one-dimensional infinite square well of width 2 Angstroms.

Using $m_e = 0.511\ MeV/c^2$ and $hc = 1.24 \times 10^4\ \text{eV} \cdot \text{Å}$ makes this calculation simpler than using MKS or CGS units. Well width is $2a = 2\,\text{Å} \quad \Rightarrow \quad a = 1\,\text{Å}$. See problems 8–1 and 8–3.

8–17. (a) Write down the fifth and sixth position space eigenfunctions for an electron in an infinite square well of width 2 Angstroms.

(b) Sketch these eigenfunctions indicating what happens outside of the well.

(c) Sketch the probability densities corresponding to these eigenfunctions.

Sketch means show qualitatively the features of each $\psi_n(x)$ and $\left|\psi_n(x)\right|^2$. Since the walls are impermeable, the wave function must be zero outside the well. See problems 8–2 and 8–4.

8–18. (a) Compare the probability of locating a particle in its first excited state in a one-dimensional infinite square well of width $2a$ between $\pm a/10$ at the center of the well and an interval of equal length at the right edge.

(b) Compare your probabilities to those for the same intervals from problem 8–5 (ground state).

(c) Explain why the probability of finding the particle in its first excited state near the center of the well is significantly less than for its ground state.

The first excited state means $n = 2$ for the infinite square well. Use the appropriate eigenfunction from problem 8–2 and the techniques from problem 8–5. Examine figure 8–4 to explain what may initially appear to be a numerical discrepancy between the two intervals of equal length.

8–19. Compare the probability of locating a particle in an infinite square well of width $2a$ between $\pm a/10$ at the center of the well and an interval of equal length at the right edge given

$$\Psi(x) = \frac{1}{4a^2}\sqrt{\frac{15}{a}}\left(a^2 - x^2\right).$$

Compare your center of the well probability with the center of the well result from problem 8–5.

The given state function is the normalized result of problem 8–11. The overall wave function may be an eigenfunction, but it will more generally be a superposition of eigenfunctions. The overall wave function, as various amounts of different eigenfunctions contribute, can assume any shape including this parabolic example. Use the techniques of problem 8–5.

8–20. Show that the product of the uncertainties of position and momentum in a one-dimensional infinite square well of width $2a$ obey the Heisenberg uncertainty principle.

Problems 8–9 and 8–10 provide the uncertainties. Work with $(\triangle x)^2$ and $(\triangle p)^2$. Their product is $(\triangle x \triangle p)^2$. Simplify your expression, take a square root of both sides to obtain the product $\triangle x \triangle p$. Show that this product is greater than $\hbar/2$ for the ground state, and then notice that all excited states must have $\triangle x \triangle p$ larger than this to arrive at your conclusion.

8–21. Calculate the uncertainty in energy for a particle in a one-dimensional infinite square well of width $2a$. Explain the result.

Use E_{op} in position space and procedures closely resembling problem 8–10. Calculate

(a) $<E>$, (b) $<E^2>$, and (c) ΔE for all n in one spatial dimension.

$$E_{op} \;=\; \frac{P_{op}^2}{2m} \;=\; \frac{1}{2m}\,(-i\hbar\nabla)\,(-i\hbar\nabla) \;\rightarrow\; -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

in one spatial dimension. The n odd and n even integrals for $<E>$ are the same as those used to calculate $<p^2>$ in problem 8–10 divided by $2m$. For $<E^2>$,

$$E_{op}^2 \;=\; E_{op}\,E_{op} \;=\; \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right) \;=\; \frac{\hbar^4}{4m^2}\frac{d^4}{dx^4}$$

Sines and cosines duplicate themselves when they are differentiated four times so this is not overly arduous. The E_n are eigenvalues (see problem 8–1). What do you anticipate for the uncertainty of an energy eigenvalue?

Exercises 8–22 through 8–31 all refer to an infinite square well of width $2a$, where the wave function is in a superposition of eigenstates such that the state is a triangular wave centered in the well , i.e.

$$\begin{aligned} \Psi\,(x,0) \;&=\; N\left(1-\frac{|\,x\,|}{a}\right) \quad \text{for } |\,x\,| \;\leq\; a \\ &=\; 0 \qquad\qquad\quad \text{for } |\,x\,| \;>\; a \end{aligned}$$

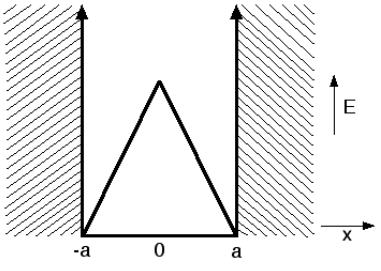


Figure 8–7. Triangular wave function in an infinite square well potential.

8–22. Calculate the normalization constant N.

The normalization condition for a continuous system in one variable for the given wave function is

$$1 \;=\; \int_{-a}^{a} \left[N \left(1 - \frac{|\,x\,|}{a} \right) \right]^{*} \left[N \left(1 - \frac{|\,x\,|}{a} \right) \right] dx \;=\; |\,N\,|^{\,2} \int_{-a}^{a} \left(1 - \frac{|\,x\,|}{a} \right)^{2} dx$$

where the limits of integration indicate the wave function is zero outside the well. Express this without the absolute value to clarify the integration. Treat it as a sum of two integrals describing regions on both sides of zero,

$$1 \;=\; |\,N\,|^{\,2} \int_{-a}^{0} \left(1 + \frac{x}{a} \right)^{2} dx \;+\; |\,N\,|^{\,2} \int_{0}^{a} \left(1 - \frac{x}{a} \right)^{2} dx.$$

These integrals are straightforward. You may recognize that the integrals have the same magnitude, so you can evaluate one integral and multiply it by 2 to get the same result. See problem 8–11.

8–23. Expand the initial state function $\Psi\,(x,0)$ in terms of the position space eigenfunctions, and use the time dependence of the $\psi_n\,(x)$'s to write down the full time dependent $\Psi\,(x,t)$.

You have done time evolution calculations for discrete systems. The difference for continuous systems is that instead of two or three eigenstates there are an infinite number of eigenstates. Per problem 8–8, determining which eigenstates contribute what amount is an exercise in calculating Fourier coefficients. Integration is the challenging part of this problem. Here

$$\psi\,(x,0) \;=\; \sum_{\text{n odd}}^{\infty} b_n \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a} \right) \;+\; \sum_{\text{n even}}^{\infty} d_n \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a} \right)$$

This $\Psi\,(x,0)$ is an even function. Cosines are even functions and sines are odd functions. Odd functions, sine terms, will not contribute so all $d_n = 0$. You only have to find the b_n's, and

$$b_n \;=\; \int_{-a}^{a} \psi_n^{*}\,(x)\,\Psi\,(x,0)\,dx \;=\; \int_{-a}^{a} \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a} \right) \sqrt{\frac{3}{2a}} \left[1 - \frac{|\,x\,|}{a} \right] dx\,.$$

Remember that cosines correspond to the odd quantum numbers. To add time dependence

$$\Psi\,(x,t) \;=\; \sum_{\text{n odd}}^{\infty} b_n\,\psi_n\,(x)\,e^{-iE_n t/\hbar}$$

where the E_n's are those for an infinite square well of width $2a$, per problem 8–1.

$$\Psi\,(x,t) \;=\; 8\sqrt{\frac{3}{2a}} \sum_{\text{n odd}}^{\infty} \frac{1}{n^2\pi^2} \cos\left(\frac{n\pi x}{2a} \right) \exp\left(-\frac{i\pi^2\hbar n^2}{8ma^2}\,t \right)$$

for this system. Problems 8–12 and 8–13 may also be illustrative.

8–24. (a) Calculate the uncertainty in position for the particle in the state given as $\Psi(x,0)$.

(b) Sketch the probability density versus x at $t = 0$.

(c) Indicate values of $<x>$ and $\triangle x$ on the sketch.

$\Psi(x,0)$ is potentially a superposition of infinite eigenstates, as are all continuous wave functions. A continuous wave function contains all information about the "weighting" of the eigenstates.

Take advantage of the fact that $\Psi(x,0)$ is an even function, and use odd/even function arguments. For instance, the requested expectation value is

$$\begin{aligned} <x> &= \int_{-\infty}^{\infty} \Psi^*(x)\, x\, \Psi(x)\, dx \\ &= \int_{-a}^{a} \sqrt{\frac{3}{2a}} \left(1 - \frac{|x|}{a}\right) x \sqrt{\frac{3}{2a}} \left(1 - \frac{|x|}{a}\right) dx\,. \end{aligned}$$

The integrand is a product of an even function, $\Psi^*(x,0)$, and an odd function, x, and another even function $\Psi(x,0)$. This composite function is odd. An odd function integrated between symmetric limits is zero. Expect results for the second moment and the uncertainty that differ from the analogous calculations in problem 8–9 because this exercise addresses differently weighted eigenstates. The second moment is likely easiest calculated as

$$<x^2> = \int_{-a}^{0} \sqrt{\frac{3}{2a}} \left(1 + \frac{x}{a}\right) x^2 \sqrt{\frac{3}{2a}} \left(1 + \frac{x}{a}\right) dx + \int_{0}^{a} \sqrt{\frac{3}{2a}} \left(1 - \frac{x}{a}\right) x^2 \sqrt{\frac{3}{2a}} \left(1 - \frac{x}{a}\right) dx\,.$$

8–25. (a) Find the initial state momentum wave function $\widehat{\Psi}(p,0)$.

(b) Sketch $\widehat{\Psi}(p,0)$ versus p.

You need the "quantum mechanical" Fourier transform of chapter 5,

$$\widehat{\psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-ipx/\hbar}\, \psi(x,0)\, dx\,.$$

The calculation is similar to problem 8–6, though the given $\Psi(x,0)$ is independent of quantum number. Break the integral into two parts from $-a$ to zero, and from zero to a, clearing the absolute value in the process. Each of the parts is straightforward. You should get

$$\widehat{\Psi}(p,0) = \frac{\hbar^2}{ap^2} \sqrt{\frac{3}{\pi\hbar a}} \left[1 - \cos\left(\frac{p}{\hbar}a\right)\right],$$

which is the function you want to sketch.

8–26. Calculate the uncertainty in momentum for the particle in the state given as $\Psi(x,0)$, then show this system is consistent with the Heisenberg uncertainty principle.

Use the P_{op} sandwich in position space to find $<p>$ like problem 8–10. The calculation for $<p^2>$ is done below because it uses the theta function discussed in chapter 4. Attempt to understand the use of the theta function and the fact that the theta function can be useful at discontinuities. If we attempt a P_{op}^2 sandwich,

$$\begin{aligned}
<p^2> &= \int_{-\infty}^{\infty} \psi^*(x)\left(-i\hbar\frac{d}{dx}\right)\left(-i\hbar\frac{d}{dx}\right)\psi(x)\,dx \\
&= -\hbar^2\int_{-a}^{a}\left(\sqrt{\frac{3}{2a}}\right)^*\left(1-\frac{|x|}{a}\right)^*\frac{d^2}{dx^2}\sqrt{\frac{3}{2a}}\left(1-\frac{|x|}{a}\right)dx \\
&= -\hbar^2\frac{3}{2a}\int_{-a}^{0}\left(1+\frac{x}{a}\right)\frac{d^2}{dx^2}\left(1+\frac{x}{a}\right)dx \;-\; \hbar^2\frac{3}{2a}\int_{0}^{a}\left(1-\frac{x}{a}\right)\frac{d^2}{dx^2}\left(1-\frac{x}{a}\right)dx \\
&= -\frac{3\hbar^2}{2a}\left\{\int_{-a}^{0}\left(1+\frac{x}{a}\right)\frac{d}{dx}\left(\frac{1}{a}\right)dx \;+\; \int_{0}^{a}\left(1-\frac{x}{a}\right)\frac{d}{dx}\left(-\frac{1}{a}\right)dx\right\} \\
&= -\frac{3\hbar^2}{2a}\left\{\int_{-a}^{0}\left(1+\frac{x}{a}\right)(0)\,dx \;+\; \int_{0}^{a}\left(1-\frac{x}{a}\right)(0)\,dx\right\} \\
&= -\frac{3\hbar^2}{2a}\left\{\int_{-a}^{0}(0)\,dx \;+\; \int_{0}^{a}(0)\,dx\right\}
\end{aligned}$$

which is not very satisfying. This allows us to ascertain only that $<p^2> \;=\;$ constant.

Consider the theta function, which is the integral of a delta function. Said another way, the delta function is the derivative of the theta function. The theta function is

$$\Theta(x-x') \;=\; \begin{cases} 1, & x-x' \;>\; 0 \\ 0, & x-x' \;<\; 0 \end{cases}. \qquad \text{Now} \qquad \int_{-\infty}^{\infty}\delta(x-x')\,dx \;=\; 1\,. \quad \text{The integral}$$

$$\int_{-\infty}^{x}\delta(x-x')\,dx \;=\; \begin{cases} 1, & -\infty \;<\; x' \;<\; x \\ 0, & x' \;>\; x \end{cases} \quad \Rightarrow \quad \int_{-\infty}^{x}\delta(x-x')\,dx \;=\; \begin{cases} 1, & x-x' \;>\; 0 \\ 0, & x-x' \;<\; 0 \end{cases} \quad \text{so}$$

$$\int_{-\infty}^{x}\delta(x-x')\,dx \;=\; \Theta(x-x') \quad \Rightarrow \quad \delta(x-x') \;=\; \frac{d}{dx}\Theta(x-x')$$

We will use the form $\displaystyle\int_{-\infty}^{x}\delta(x)\,dx \;=\; \Theta(x) \quad \Rightarrow \quad \delta(x) \;=\; \frac{d}{dx}\Theta(x)$

Our integral is $\displaystyle <p^2> \;=\; -\hbar^2\int_{-a}^{a}\left(\sqrt{\frac{3}{2a}}\right)^*\left(1-\frac{|x|}{a}\right)^*\frac{d^2}{dx^2}\sqrt{\frac{3}{2a}}\left(1-\frac{|x|}{a}\right)dx$

$$= -\frac{3\hbar^2}{2a}\int_{-a}^{a}\left(1-\frac{|x|}{a}\right)\frac{d}{dx}\left[\frac{d}{dx}\left(1-\frac{|x|}{a}\right)\right]dx$$

Consider just the expression in the square brackets.

$$\frac{d}{dx}\left(1-\frac{|x|}{a}\right) \;=\; \frac{1}{a}\Big(1-2\,\Theta(x)\Big).$$

If you do not see this immediately, take the derivative on the left and apply the definition of the theta function for the cases $x > 0$ and $x < 0$ on the right. Replace the expression in square brackets by the right side of the last equation, or

$$\begin{aligned} <p^2> &= -\frac{3\hbar^2}{2a}\int_{-a}^{a}\left(1-\frac{|\,x\,|}{a}\right)\frac{d}{dx}\left[\frac{1}{a}\Big(1-2\,\Theta\,(x)\Big)\right]dx \\ &= -\frac{3\hbar^2}{2a^2}\int_{-a}^{a}\left(1-\frac{|\,x\,|}{a}\right)\frac{d}{dx}\Big[\,1-2\,\Theta\,(x)\Big]\,dx \\ &= \frac{3\hbar^2}{a^2}\int_{-a}^{a}\left(1-\frac{|\,x\,|}{a}\right)\delta\,(x)\,dx \;=\; \frac{3\hbar^2}{a^2}\left[\,1-\frac{|\,x\,|}{a}\,\right]_{x\,=\,0} \;=\; \frac{3\hbar^2}{a^2}\,. \end{aligned}$$

This calculation uses a theta function to caste an integral into a form containing a delta function so that the integral is then readily evaluated. Theta and delta functions can be useful at discontinuities. The "tent" wave function is continuous, but its first derivative is discontinuous by a constant amount which is why the second derivative is zero. Another approach not involving theta functions is to find $<E>$, then $<p^2> \;=\; 2m\,<E>$, (exercise 8–29). It is straightforward to now find $\triangle p$. You have $\triangle x$ from exercise 8–24.

8–27. Write a general time–dependent wave function in momentum space as a summation of the momentum space eigenfunctions.

Exercises 8–27 and 8–28 are not coupled to the "tent" wave function, rather they are general results located here as precursors to exercise 8–29.

You can decompose a wave function into its component eigenstates in momentum space just as is done in position space. This exercise is answered below, in preparation for exercise 8–28, so simply examine the argument below. Similar to problem 8–8,

$$\begin{aligned} |\,\psi> \;&=\; \mathcal{I}\,|\,\psi> \;=\; \sum_n |\,E_n><E_n\,|\,\psi> \\ \Rightarrow\quad <p\,|\,\psi> \;&=\; <p\,|\sum_n |\,E_n><E_n\,|\,\psi> \;=\; \sum_n <p\,|\,E_n><E_n\,|\,\psi> \\ \Rightarrow\quad \widehat{\Psi}\,(p) \;&=\; \sum_n \widehat{\psi}_n\,(p)\,<E_n\,|\,\psi> \;=\; \sum_n \widehat{\psi}_n\,(p)\,<E_n\,|\,\mathcal{I}\,|\,\psi> \\ &=\; \sum_n \widehat{\psi}_n\,(p)\,<E_n\,|\,\Big(\sum |\,p><p\,|\,\Big)\,|\,\psi> \;=\; \sum_n \widehat{\psi}_n\,(p)\sum <E_n\,|\,p><p\,|\,\psi> \\ &=\; \sum_n \widehat{\psi}_n\,(p)\sum \Big(\,<E_n\,|\,p>\,\Big)\Big(\,<p\,|\,\psi>\,\Big) \end{aligned}$$

$$\Rightarrow\quad \widehat{\Psi}\,(p) \;\rightarrow\; \sum_n \widehat{\psi}_n\,(p)\int \Big(\widehat{\psi}_n^{\,*}\,(p)\Big)\Big(\widehat{\Psi}\,(p)\Big)\,dp$$

$$\Rightarrow\quad \widehat{\Psi}\,(p) \;=\; \sum_n \beta_n\,\widehat{\psi}_n\,(p) \qquad \text{where} \qquad \beta_n \;=\; \int \widehat{\psi}_n^{\,*}\,(p)\;\widehat{\Psi}\,(p)\,dp \qquad \text{and}$$

$$\widehat{\Psi}\,(p,t) \;=\; \sum_n \beta_n\,\widehat{\psi}_n\,(p)\;e^{-iE_nt/\hbar}$$

which is a general time–dependent wave function in momentum space as a summation of the momentum space eigenfunctions.

8–28. Express a general time–dependent wave function in energy space, $\widetilde{\Psi}(E,t)$, in terms of the energy space eigenfunctions, $\widetilde{\psi}_n(E)$'s.

Can you use Dirac notation including insertion and resolution of the identity well enough to find

$$\widetilde{\Psi}(E,t) \;=\; \sum_{\text{n odd}} b_n\, \widetilde{\psi}_n(E)\, e^{-iE_n t/\hbar} \;?$$

Follow problem 8–8 and exercise 8–27. Here $<E\,|\,E_n> \;=\; \widetilde{\psi}_n(E)$.

8–29. (a) Confirm $<p^2> \;=\; \dfrac{3\hbar^2}{a^2}$ for the tent wave function $\Psi(x,0)$.

(b) Write an initial state wave function $\widetilde{\Psi}(E,0)$.

(c) Qualitatively sketch $\widetilde{\Psi}(E,0)$ versus E.

Expectation value is

$$<\psi\,|\,\Omega\,|\,\psi> \;=\; <\Omega> \;=\; \sum_{i=1}^{\infty} P(\omega_i)\,\omega_i$$

$$\Rightarrow \quad <E> \;=\; \sum_{n=1}^{\infty} P(E_n)\,E_n \;=\; \sum_{n=1}^{\infty} |\,<E_n\,|\,\Psi>\,|^2\,E_n \tag{1}$$

using the probability postulate. From problem 8–8

$$\Psi(x) \;=\; \sum_{n=1}^{\infty} \psi_n(x)\;<E_n\,|\,\psi> \quad \Rightarrow \quad \Psi(x) \;=\; \sum_{n=1}^{\infty} \psi_n(x)\,b_n\,.$$

$$\Rightarrow \quad \sum_{n=1}^{\infty} \psi_n(x)\;<E_n\,|\,\psi> \;=\; \sum_{n=1}^{\infty} \psi_n(x)\,b_n \quad \Rightarrow \quad <E_n\,|\,\psi> \;=\; b_n\,,$$

so that equation (1) can be written $<E> \;=\; \sum_{n=1}^{\infty} |\,b_n\,|^2\,E_n$. In exercise 8–23 you calculated $b_n \;=\; \dfrac{8}{n^2\pi^2}\sqrt{\dfrac{3}{2}}$ for the tent wavefunction. The E_n are calculated in problem 8–1. Consider only odd n. Form 1.3.1.5.11 in *Handbook of Mathematical Formulas and Integrals* by Jeffrey is

$$\sum_{\text{n odd}}^{\infty} \frac{1}{n^2} \;=\; \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2} \;=\; \frac{\pi^2}{8}\,,$$

which enables a solution for $<E>$, and then $<p^2> \;=\; 2m\;<E>$

The initial state wave function $\widetilde{\Psi}(E,0)$ is a two or three line problem using the delta function arguments of chapter 4. You should find

$$\widetilde{\Psi}(E,t) \;=\; \sum_{\text{n odd}}^{\infty} 8\,\sqrt{\frac{3}{2}}\;\frac{1}{n^2\pi^2}\;\delta(E-E_n)\,.$$

The sketch will be a series of spikes; delta functions "finitized" by the coefficients of each eigenenergy. Exaggerate the heights after $\widetilde{\psi}_1(E)$, to simulate the envelope of $1/n^2$.

8–30. (a) If the energy of the system is measured at time t, what results can be found

(b) and with what probabilities will these results be found?

(c) Describe the shapes of the wave functions $\Psi(x,t)$ and $\widetilde{\Psi}(E,t)$ before an energy measurement, then sketch them after measuring E_3 at $t = 0$.

This exercise illustrates the meaning of some of the postulates as they apply to a continuous system. For part (a), the possible results of a measurement of energy are the energy eigenvalues per the eigenvalue postulate. See problem 8–1. Examine the equations in the discussion of the last exercise if it is not readily apparent how to do part (b). You should find a relationship involving the coefficients b_n that enables a one line solution to part (b). Immediately before you measure the energy, the wave function is $\Psi(x,0)$. Immediately after you measure the energy, the wave function is $\psi_3(x,t)$ per the eigenvector postulate. That is what you should sketch in part (c). Remember that neither $\widetilde{\Psi}(E,t)$ nor $\widetilde{\psi}_3(E)$ is continuous.

8–31. (a) Show that the probability of finding a system in its jth eigenstate is $P(j) = |c_j|^2$, where c_j is the expansion coefficient of the jth eigenstate.

(b) What are the probabilities of finding the particle given to be in the state $\Psi(x,0)$ in its ground state and in each of its first two excited states?

(c) What is the probability of finding the particle given to be in the state $\Psi(x,0)$ in any excited state greater than the second excited state?

This problem should reinforce both probability calculations for a continuous system and some common terminology. For any continuous system, the probability of finding the particle in any eigenstate is the magnitude squared of the expansion coefficient of that eigenstate. Symbolically,

$$\Psi(x) = \sum c_n \psi_n(x) \quad \Rightarrow \quad P(n) = |c_n|^2 .$$

The c_n's are known as **probability amplitudes** or simply **amplitudes** because of this fact.

Part (a) is a small extension of the discussion for exercise 8–29. You can obtain numerical values for part (b) because you have the expansion coefficients from exercise 8–30. Deciphering which coefficients to use requires that you know the ground state is the lowest possible energy state. It will correspond to the lowest possible quantum number, in this case, $n = 1$. The next lowest energy or next possible quantum number corresponds to the first excited state meaning $n = 3$ for the given "tent function" system. The second excited state has $n = 5$. Add the probabilities you obtained for the first three possible states for part (c). The complement is the probability of finding the particle in any higher excited state. The probability of finding most systems in any excited state is often very small, which your part (c) calculations will illustrate for this system.

Postscript: This exercise ends the "tent" wave function sequence.

8–32. Given a particle in an infinite square well where the wave function is

$$\Psi(x) \;=\; \begin{cases} x+a & -a \,<\, x \,<\, a \\ 0 & \text{elsewhere} \end{cases}$$

(a) graph this wave function, then

(b) normalize the wave function,

(c) expand the wave function in terms of its eigenfunctions,

(d) calculate the time dependent wave function,

(e) calculate the probability of finding the particle in the ground state,

(f) calculate the probability of finding the particle in the third excited state.

The wave function is neither even nor odd so both cosine and sine terms need to be considered. The time dependent wave function is

$$\Psi(x,t) \;=\; \frac{2}{\pi}\sqrt{\frac{3}{2a}}\left(\sum_{n\ \text{odd}}^{\infty}\frac{(-1)^{\frac{n-1}{2}}}{n}\cos\left(\frac{n\pi x}{2a}\right) \;+\; \sum_{n\ \text{even}}^{\infty}\frac{(-1)^{\frac{n-2}{2}}}{n}\sin\left(\frac{n\pi x}{2a}\right)\right)\exp\left(-i\,\frac{\pi^2 n^2\hbar}{8ma^2}\,t\right)$$

which includes the answers to parts (c) and (d). This is the linear combination

$$\Psi(x) \;=\; \sum_{\text{n=1}}^{\infty} c_n\,\psi_n(x) \;=\; c_1\,\psi_1(x) \;+\; c_2\,\psi_2(x) \;+\; c_3\,\psi_3(x) \;+\; \cdots$$

for the given wave function.

The last two parts ask for probabilities. For normalized wave/eigenfunctions

$$P(n) \;=\; \left|<\psi_n\,|\,\Psi>\right|^2 \;=\; \left|\int_{-a}^{a}\psi_n^*(x)\,\Psi(x)\,dx\right|^2 \;=\; \left|\int_{-a}^{a}\frac{1}{\sqrt{a}}\cos\left(\frac{3\cdot\pi}{2a}\,x\right)\cdot\Psi(x)\,dx\right|^2$$

for the second excited state for this continuous system. Recalling the orthonormality of the eigenfunctions (chapter 5 for sines and cosines),

$$P(3) \;=\; \left|\int_{-a}^{a}\frac{1}{\sqrt{a}}\cos\left(\frac{3\cdot\pi}{2a}\,x\right)\cdot\frac{2}{\pi}\sqrt{\frac{3}{2a}}\,\frac{1}{3}\cos\left(\frac{3\cdot\pi}{2a}\,x\right)\,dx\right|^2 = \left|\frac{2}{3\pi}\sqrt{\frac{3}{2}}\cdot\frac{1}{a}\int_{-a}^{a}\cos^2\left(\frac{3\pi}{2a}\,x\right)\,dx\right|^2$$

where the integral is a for all n per problem 8–2, thus

$$P(n=3) \;=\; \left|\frac{2}{3\pi}\sqrt{\frac{3}{2}}\cdot\frac{1}{a}\cdot a\right|^2 \;=\; \left|\frac{2}{3\pi}\sqrt{\frac{3}{2}}\right|^2 \;=\; \frac{2}{3\pi^2} \;\approx\; 0.0675$$

is the probability of finding the particle in its second excited state. The probabilities of finding the particle in any given eigenstate are just the squares of the expansion coefficients/probability amplitudes from which the parameter a cancels for all n.

8–33. What are the eigenfunctions for a particle in a two-dimensional infinite square well of width $2a$ on each side?

The solutions to a variables separable partial differential equation in two dimensions are the products of the two one-dimensional solutions, or $\psi(x,y) = f(x)\,g(y) = \psi_{n_x}(x)\,\psi_{n_y}(y)$ in this case. This exercise requires no calculation. The one-dimensional solutions are found in problem 8–2. Simply write the four possible products. Eigenenergies are given in problem 8–14.

8–34. What are the eigenenergies and eigenfunctions of a particle in a rectangular two-dimensional infinite square well of length $2a$ and width $2b$?

Similar to the previous exercise. Simply replace a with b in eigenenergies and eigenfunctions for the y dimension. Add the two component energies to obtain eigenenergies, and the eigenfunctions are the four possible products.

8–35. (a) Find the eigenenergies of a cubic infinite square well of width $2a$ on each side.

(b) Find the sets of quantum numbers that yield the lowest seven eigenenergies.

(c) Identify the eigenenergies from part (b) that demonstrate degeneracy.

(d) What are the ground state and first excited state eigenfunctions for this potential?

This exercise is practice in solving a PDE using a variables separable approach. You should find

$$E_{n_x,n_y,n_z} = E_x + E_y + E_z = \frac{\pi^2\hbar^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right).$$

This result can be generalized from problem 8–14, however, the PDE's that we will soon encounter are not nearly so straightforward. Follow problem 8–15 to obtain eigenenergies using

$$E_0 = n_i^2\,\frac{\pi^2\hbar^2}{8ma^2},$$

meaning any one of the three component eigenenergies. The ground state is at $3E_0$ using this convention. It takes 20 sets of quantum numbers to delineate the lowest seven eigenenergies. Notice that degeneracy is more prevalent in the three-dimensional system than the two-dimensional case.

Degeneracy is the circumstance where different eigenstates have the same energy so that eigenstates cannot be uniquely determined without additional information. It is a requirement for realistic systems to uniquely identify the eigenstates for all energies including degenerate energies. This is done using a **Complete Set of Commuting Observables** (CSCO), for which techniques are addressed in chapters 12 and 13 for continuous systems. For the moment, realize that a continuous system that can be addressed in two spatial dimensions has two quantum numbers, and a continuous system that can be addressed in a three spatial dimensions has three quantum numbers. Should an additional degree of freedom be encountered, like spin (chapter 14), four quantum numbers are necessary. Any system with more than one degree of freedom has the potential to be degenerate.

Chapter 9

Scattering in One Dimension

The free state where $V(x) = 0$ is likely the simplest potential. The infinite square well with impenetrable walls so $\Psi(x) = 0$ at the boundaries and $V(x) = 0$ within the well is likely next simplest. Potential energy functions that are piecewise constant are likely next simplest.

A potential that is piecewise constant is discontinuous at one or more points. The potential is zero in one region and is non-zero in other regions without a transition region. A discontinuity in a potential is not completely realistic though piecewise constant potentials do illustrate some realistic physical concepts and can be used to model realistic systems.

A discontinuous change in potential is generally more mathematically tractable than a continuous change. These problems are usually addressed in position space. The strategy is to divide space into regions at the locations where the potential changes and then obtain a solution for each region. The points at which the potential changes are boundaries. The wave function and its first derivative must be the same on both sides of a boundary, so equating these provides a system of equations that yields descriptive information. Remember that the time independent Schrodinger equation in position space is simply a convenient form of the Schrodinger postulate.

A particle is in either a **free state** (chapter 7), a **bound state** (chapters 8, 10, and parts of 11, 12, and 13), or a **scattering state**. The bound state is described by a potential that holds a particle for a non-zero time period. The scattering state can be described as an interaction of a free particle with a potential that results in a free particle. If a free particle interacts with the potential and does not become bound, the particle is in a scattering state. The electron can escape from a hydrogen atom and enter a free state, but it cannot escape without the influence of an external photon. Scattering concerns the situation where there is no external influence.

There are some new quantum mechanical behaviors introduced in this chapter. A particle has a non-zero probability to appear on the other side of a potential barrier that it does not classically have the energy to surmount. This is known as **barrier penetration** or **tunneling**. A particle has a non-zero probability to be reflected at any boundary regardless of energy, meaning that a particle possessing enough energy to surmount a potential barrier can be reflected.

9–1. Find the reflection and transmission coefficients for a particle of energy $E > V_0$ incident from the left on the vertical step potential

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \quad \text{region 1}, \\ V_0 & \text{if } x > 0 \quad \text{region 2}. \end{cases}$$

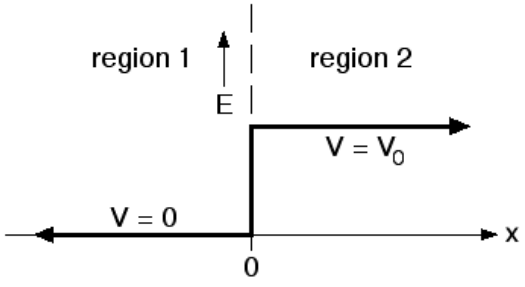


Figure 9–1. Vertical step potential.

The particle is free in region 1. Notice that region 2 extends to infinity. This is an approximation to a finite potential that is very steep and of significant width. If the step is not actually vertical, it is difficult to match boundary conditions, and if the step is not of infinite extent, "tunneling" (problem 9–3) is possible.

A particle incident from the left will either be reflected or transmitted. The **reflection coefficient**, denoted R, is classically defined as the ratio of intensity reflected to intensity incident. The classical **transmission coefficient**, denoted T, is the ratio of intensity transmitted to intensity incident. Quantum mechanically, intensity is analogous to probability density. Quantum mechanical transmission and reflection coefficients are based on probability density flux (problem 9–2). The reflection and transmission coefficients sum to 1 both classically and quantum mechanically.

The two physical boundary conditions applicable to this and many other boundary value problems are **the wave function and its first derivative are continuous.**

A general solution to the Schrodinger equation for a particle approaching from the left is

$$\psi_1(x) = A e^{ik_1 x} + B e^{-ik_1 x}, \quad x < 0,$$

$$\psi_2(x) = C e^{ik_2 x}, \quad x > 0,$$

where the subscripts on the wave functions and wavenumbers indicate regions 1 or 2, and

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad \text{and} \qquad k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}.$$

The k_i are real because $E > V_0$. In region 1, the term $A e^{ik_1 x}$ is the incident wave and $B e^{-ik_1 x}$ describes the reflected wave. $C e^{ik_2 x}$ models the transmitted wave in region 2. A term like $D e^{-ik_2 x}$, modeling a particle moving to the left in region 2, is not physically meaningful for a particle given to be incident from the left. Equivalently, $D = 0$ for the same reason. Applying the boundary condition that the wave function is continuous at $x = 0$,

$$\psi_1(0) = \psi_2(0) \quad \Rightarrow \quad A e^0 + B e^0 = C e^0 \quad \Rightarrow \quad A + B = C.$$

The derivative of the wave function is

$$\psi_1'(x) = A ik_1 e^{ik_1 x} - B ik_1 e^{-ik_1 x}, \quad x < 0,$$

$$\psi_2'(x) = C ik_2 e^{ik_2 x}, \quad x > 0,$$

so continuity of the first derivative at $x = 0$ means

$$\psi_1'(0) = \psi_2'(0) \quad \Rightarrow \quad A ik_1 e^{ik_1(0)} - B ik_1 e^{-ik_1(0)} = C ik_2 e^{ik_2(0)} \quad \Rightarrow \quad k_1(A-B) = k_2 C.$$

We now have two equations in the three unknowns A, B, and C. Eliminating C,

$$k_1(A-B) = k_2(A+B) \quad \Rightarrow \quad (k_1-k_2)A = (k_1+k_2)B \quad \Rightarrow \quad B = \left(\frac{k_1-k_2}{k_1+k_2}\right)A.$$

From this relation we can calculate the reflection coefficient. The incident probability density is

$$\left|A e^{ik_1 x}\right|^2 = \left(A e^{ik_1 x}\right)^* \left(A e^{ik_1 x}\right) = \left(A^* e^{-ik_1 x}\right)\left(A e^{ik_1 x}\right) = A^* A e^0 = \left|A\right|^2,$$

or the intensity of the incident wave is the square of the norm of the coefficient of the incident wave. Similarly, the intensity of the reflected wave is $\left|B\right|^2$, and the intensity of the transmitted wave is $\left|C\right|^2$. In this specific problem the reflection coefficient is

$$R = \frac{\left|B\right|^2}{\left|A\right|^2} = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 \left|A\right|^2 \Big/ \left|A\right|^2 = \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 \quad \text{and}$$

$$R+T \;=\; 1 \quad \Rightarrow \quad T \;=\; 1-R \;=\; 1-\left(\frac{k_1-k_2}{k_1+k_2}\right)^2 \;=\; \left(\frac{k_1+k_2}{k_1+k_2}\right)^2-\left(\frac{k_1-k_2}{k_1+k_2}\right)^2 \;=\; \frac{4k_1k_2}{\left(k_1+k_2\right)^2}\,.$$

Postscript: Classically, $R = 0$ and $T = 1$ if $E > V_0$. Figure 9–2 illustrates the quantum mechanical analogy. What does it mean that $R > 0$ when $E > V_0$? For a single particle, it means that a portion of the wave function is transmitted and a portion of the wave function is reflected. The probability postulate says that you can calculate the probabilities for finding the particle in region 1 or 2 from the probability amplitudes, but can do no better. If you look, you will find the particle in either region 1 or region 2 per the eigenvalue postulate, and the measurement will leave the state vector in the eigenstate corresponding to the location that you measured per the eigenvector postulate. The probability of finding the particle in the other region is then zero.

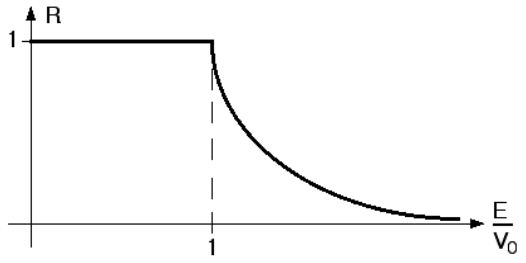


Figure 9–2. Reflection when $E > V_0$.

Notice that the particle will have longer wavelength and thus less momentum in region 2 since the energy relative to the "floor" of the potential is less in region 2 than region 1.

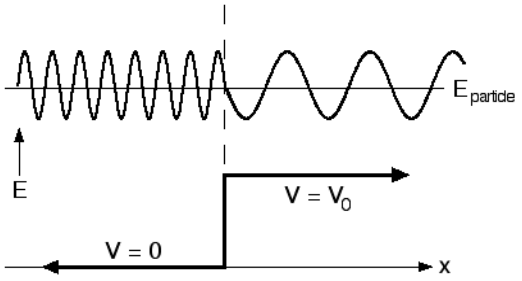


Figure 9–3. Longer wavelength over potential step.

The classical trajectory of a particle is continuous and a change in trajectory (the first derivative) must be continuous. Quantum mechanically, refined arguments are necessary. The validity of these two boundary conditions can be demonstrated for a Gaussian wave function. Will a wave packet that is quantized in wavenumber scatter from a potential with precisely the same reflection and transmission coefficients as a Gaussian wave function? Yes, for a wave packet quantized in wavenumber that is still smooth compared to the scale of the potential variations, though this is a non-trivial calculation that is beyond our scope. The point is that the boundary conditions of continuity of the wave function and its first derivative are justified quantum mechanically.

9–2. (a) Calculate the amplitude C of the transmitted portion of the wave function in terms of the coefficient A for the vertical step potential of problem 9–1.

(b) Show that the ratio $|\,C\,|^2/|\,A\,|^2$ is $\neq T$ from problem 9–1.

(c) Rectify the discrepancy between part (b) and the result of problem 9–1.

Parts (a) and (b) are intended to demonstrate a counterintuitive fact that is explained in part (c). Use intermediate results from problem 9–1 to solve for C in terms of A. Form the ratio $|\,C\,|^2/|\,A\,|^2$ which is not the same as T from problem 9–1. Part (c) requires that you know that flux is velocity times intensity. Since the particle has a different height above the floor of the potential in regions 1 and 2, it has not only a different wavenumber but a different velocity. These velocities are related to the de Broglie relation. The ratio $v_2\,|\,C\,|^2/v_1\,|\,A\,|^2$ is the transmission coefficient found in problem 9–1.

(a) Using intermediate results from problem 9–1, the amplitude of the transmitted portion is

$$C \;=\; A \;+\; B \;=A \;+\; \left(\frac{k_1-k_2}{k_1+k_2}\right)A \;=\; \left(\frac{k_1+k_2}{k_1+k_2}\right)A \;+\; \left(\frac{k_1-k_2}{k_1+k_2}\right)A \;=\; \left(\frac{2k_1}{k_1+k_2}\right)A\,.$$

(b) The ratio of the squares of the magnitudes is not the transmission coefficient of problem 9–1,

$$\frac{\big|\,C\,\big|^2}{\big|\,A\,\big|^2} \;=\; \left(\frac{2k_1}{k_1+k_2}\right)^2 |\,A\,|^2\Big/\,|\,A\,|^2 \;=\; \frac{4k_1^2}{\big(k_1+k_2\big)^2} \;\neq\; \frac{4k_1k_2}{\big(k_1+k_2\big)^2}\,.$$

(c) Energy relative to the floor of the potential, and thus velocity, changes as the particle crosses the step. Flux is intensity times velocity. Probability density flux, probability density times velocity, is appropriate for a quantum mechanical description. Since $v_i \;=\; \dfrac{p_i}{m} \;=\; \dfrac{\hbar k_i}{m}$,

$$T \;=\; \frac{v_2\,\big|\,C\,\big|^2}{v_1\,\big|\,A\,\big|^2} \;=\; \frac{\hbar k_2/m\,\big|\,C\,\big|^2}{\hbar k_1/m\,\big|\,A\,\big|^2} \;=\; \frac{k_2\,\big|\,C\,\big|^2}{k_1\,\big|\,A\,\big|^2} \;=\; k_2\left(\frac{2k_1}{k_1+k_2}\right)^2 |\,A\,|^2\Big/k_1\,|\,A\,|^2 \;=\; \frac{4k_1k_2}{\big(k_1+k_2\big)^2}\,,$$

which is consistent with the problem 9–1.

Postscript: A reflected wave is the same height above the floor of the potential as the incident wave so the reflected wave has the same energy, velocity, and wavenumber as the incident wave. The velocities cancel in region 1 so are not considered in calculating the reflection coefficient, *i.e.*,

$$R \;=\; \frac{v_1\,\big|\,B\,\big|^2}{v_1\,\big|\,A\,\big|^2} \;=\; \frac{\big|\,B\,\big|^2}{\big|\,A\,\big|^2}\,.$$

9–3. Determine the transmission coefficient for a particle with $E < V_0$ incident from the left on the rectangular barrier

$$V(x) = \begin{cases} V_0 & \text{for } -a < x < a, \\ 0 & \text{for } |x| > a. \end{cases}$$

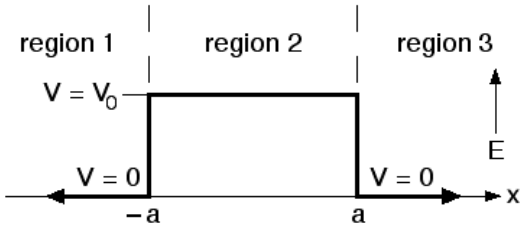


Figure 9–4. Rectangular barrier potential.

If the energy of the particle is less than the height of the step, and the " potential plateau" is of finite length, the particle incident from the left can appear on the right side of a barrier. This is a non–classical phenomena known as **barrier penetration** or **tunneling**. Classically, if a ball is rolled up a ramp of height h with kinetic energy K, the ball will roll back down the ramp if $K < mgh$. A quantum mechanical "ball" has a non–zero probability that the ball would appear on the other side of the ramp even when $K < mgh$.

After zero is one boundary, so the next simplest geometry is two boundaries, and thus three regions. The strategy is to require continuity of the wave function and its first derivative at all boundaries and solve for the transmission coefficients in terms of the ratios of the squares of the appropriate wave function coefficients.

(a) Divide "all space" into three regions at the boundaries of the potential $\pm a$. The wave functions consist of a linear combination of waves in both directions in each of the three regions:

$$\begin{aligned} \psi_1(x) &= A e^{ikx} + B e^{-ikx} \qquad \text{for} \quad x < -a, \\ \psi_2(x) &= C e^{\kappa x} + D e^{-\kappa x} \qquad \text{for} \quad -a < x < a, \\ \psi_3(x) &= F e^{ikx} + G e^{-ikx} \qquad \text{for} \quad x > a, \end{aligned}$$

where $k = \sqrt{2mE}\,/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}\,/\hbar$. Notice that κ is defined so that it is real for $E < V_0$. This is a technique that leads to minor simplifications. Conclude that $G = 0$ because it is not physically meaningful for a particle incident from the left.

(b) Apply the boundary condition that the wave function must be continuous at the boundaries. This yields two equations. Differentiate the wave function and then apply the boundary condition that the first derivative of the wave function must be continuous at boundaries. This yields two more equations. Eliminating B from the two equations for the left boundary, you should find

$$2A e^{-ika} = \left(1 - \frac{i\kappa}{k}\right) C e^{-\kappa a} + \left(1 + \frac{i\kappa}{k}\right) D e^{\kappa x}.$$

Using the two equations at the right boundary to solve for two of the unknown coefficients in terms of the coefficient F, you should find

$$C e^{\kappa a} = \frac{1}{2}\left(1 + \frac{ik}{\kappa}\right) F e^{ika} \qquad \text{and} \qquad D e^{-\kappa a} = \frac{1}{2}\left(1 - \frac{ik}{\kappa}\right) F e^{ika}.$$

(c) Use the last two equations to eliminate the coefficients C and D from the first equation so

$$A e^{-ika} = F e^{ika}\left[\cosh(2\kappa a) + \frac{i(\kappa^2 - k^2)}{2k\kappa}\sinh(2\kappa a)\right].$$

$$\text{Remember that} \qquad \sinh(x) \;=\; \frac{e^x - e^{-x}}{2} \qquad \text{and} \qquad \cosh(x) \;=\; \frac{e^x + e^{-x}}{2}\,.$$

(d) The transmission coefficient is the ratio of probability density of that portion of the wave function which "goes through" the barrier, represented by $|F|^2$, to the incident probability density, represented by $|A|^2$. The reciprocal of this ratio, $|A|^2/|F|^2$, is

$$T^{-1} \;=\; 1 \;+\; \frac{V_0^2}{4E(V_0 - E)}\sinh^2\left(\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\right),$$

which is a more conventional expression than T that still indicates $T \neq 0$ when $E < V_0$.

(a) For the region $x > a$, $\psi(x) \;=\; F e^{ikx} \;+\; G e^{-ikx}$, and $G = 0$ because it is the coefficient of an oppositely directed incident wave that cannot be physical. So the wave function is

$$\psi(x) \;=\; \begin{cases} A e^{ikx} \;+\; B e^{-ikx}, & \text{for} \quad x < -a\,, \\ C e^{\kappa x} \;+\; D e^{-\kappa x}, & \text{for} \;\; -a < x < a\,, \\ F e^{ikx}, & \text{for} \quad x > a\,, \end{cases}$$

where $k \;=\; \sqrt{2mE}\,/\,\hbar$ and $\kappa \;=\; \sqrt{2m(V_0 - E)}\,/\,\hbar$.

(b) There are three regions so there are two boundaries. Continuity at the boundaries requires

$$A e^{-ika} \;+\; B e^{ika} \;=\; C e^{-\kappa a} \;+\; D e^{\kappa a}, \quad x = -a\,, \;\text{ and} \tag{1}$$

$$C e^{\kappa a} \;+\; D e^{-\kappa a} \;=\; F e^{ika}, \quad x = a\,, \tag{2}$$

so there are two equations in five unknowns. The derivative of $\psi(x)$ is

$$\psi'(x) \;=\; \begin{cases} A\,ik\,e^{ikx} \;-\; B\,ik\,e^{-ikx}, & \text{for} \quad x < -a\,, \\ C\,\kappa\,e^{\kappa x} \;-\; D\,\kappa\,e^{-\kappa x}, & \text{for} \;\; -a < x < a\,, \\ F\,ik\,e^{ikx}, & \text{for} \quad x > a\,. \end{cases}$$

Applying the boundary condition of continuity of the first derivative at $x = -a$,

$$A\,ik\,e^{-ika} \;-\; B\,ik\,e^{ika} \;=\; C\,\kappa\,e^{-\kappa a} \;-\; D\,\kappa\,e^{\kappa a}, \;\text{ and at } \; x = a\,, \tag{3}$$

$$C\,\kappa\,e^{\kappa a} \;-\; D\,\kappa\,e^{-\kappa a} \;=\; F\,ik\,e^{ika}. \tag{4}$$

We have four equations in five unknowns. Multiply equation (1) by ik and solve for the term with the coefficient B,

$$B\,ik\,e^{ika} \;=\; C\,ik\,e^{-\kappa a} \;+\; D\,ik\,e^{\kappa a} \;-\; A\,ik\,e^{-ika}\,.$$

Substituting this into equation (3) for $B\,ik\,e^{ika}$,

$$A\,ik\,e^{-ika} \;-\; C\,ik\,e^{-\kappa a} \;-\; D\,ik\,e^{\kappa a} \;+\; A\,ik\,e^{-ika} \;=\; C\,\kappa\,e^{-\kappa a} \;-\; D\,\kappa\,e^{\kappa a}$$

$$\begin{aligned} \Rightarrow \quad 2A\,ik\,e^{-ika} \;&=\; C\,ik\,e^{-\kappa a} \;+\; C\,\kappa\,e^{-\kappa a} \;+\; D\,ik\,e^{\kappa a} \;-\; D\,\kappa\,e^{\kappa a} \\ &=\; C\,(ik \;+\; \kappa)\,e^{-\kappa a} \;+\; D\,(ik - \kappa)\,e^{\kappa a} \end{aligned}$$

$$\Rightarrow \quad 2A\,e^{-ika} \;=\; \left(1 - \frac{i\kappa}{k}\right) C\,e^{-\kappa a} \;+\; \left(1 + \frac{i\kappa}{k}\right) D\,e^{\kappa a}. \tag{5}$$

Multiplying equation (2) by κ and solving for the term with the coefficient D,

$$D\,\kappa\,e^{-\kappa a} \;=\; F\,\kappa\,e^{ika} \;-\; C\,\kappa\,e^{\kappa a}$$

Substituting the right side into equation (4) for $D\,\kappa\,e^{-\kappa a}$,

$$C\,\kappa\,e^{\kappa a} \;-\; F\,\kappa\,e^{ika} \;+\; C\,\kappa\,e^{\kappa a} \;=\; F\,ik\,e^{ika}$$

$$\Rightarrow \quad 2C\,\kappa\,e^{\kappa a} \;=\; F\,\kappa\,e^{ika} \;+\; F\,ik\,e^{ika} \;=\; F\,(\kappa + ik)\,e^{ika}$$

$$\Rightarrow \quad C\,e^{\kappa a} \;= \frac{1}{2}\left(1 + \frac{ik}{\kappa}\right) F\,e^{ika}. \tag{6}$$

Multiplying equation (2) by κ and solving for the term with the coefficient C,

$$C\,\kappa\,e^{\kappa a} \;=\; F\,\kappa\,e^{ika} \;-\; D\,\kappa\,e^{-\kappa a}$$

Substituting the right side into equation (4) for $C\,\kappa\,e^{\kappa a}$,

$$F\,\kappa\,e^{ika} \;-\; D\,\kappa\,e^{-\kappa a} \;-\; D\,\kappa\,e^{-\kappa a} \;=\; F\,ik\,e^{ika}$$

$$-2D\,\kappa\,e^{-\kappa a} \;=\; -F\kappa\,e^{ika} \;+\; F\,ik\,e^{ika} \;=\; F\,(-\kappa + ik)\,e^{ika}$$

$$\Rightarrow \quad D\,e^{-\kappa a} \;=\; \frac{1}{2}\left(1 - \frac{ik}{\kappa}\right) F\,e^{ika}. \tag{7}$$

(c) The signs on the exponentials in equations (6) and (7) are opposite those in equation (5), so

$$C\,e^{\kappa a} \;=\; \frac{1}{2}\left(1 + \frac{ik}{\kappa}\right) Fe^{ika} \quad \Rightarrow \quad C\,e^{-\kappa a} \;=\; \frac{1}{2}\left(1 + \frac{ik}{\kappa}\right) F\,e^{ika}e^{-2\kappa a},$$

$$D\,e^{-\kappa a} \;=\; \frac{1}{2}\left(1 - \frac{ik}{\kappa}\right) F\,e^{ika} \quad \Rightarrow \quad D\,e^{\kappa a} \;=\; \frac{1}{2}\left(1 - \frac{ik}{\kappa}\right) F\,e^{ika}e^{2\kappa a},$$

and now the signs of the exponentials are consistent. Substituting these into equation (5),

$$\Rightarrow \quad 2A\,e^{-ika} \;=\; \left(1 - \frac{i\kappa}{k}\right)\frac{1}{2}\left(1 + \frac{ik}{\kappa}\right) F\,e^{ika}e^{-2\kappa a} \;+\; \left(1 + \frac{i\kappa}{k}\right)\frac{1}{2}\left(1 - \frac{ik}{\kappa}\right) F\,e^{ika}e^{2\kappa a}$$

$$= \frac{F\,e^{ika}}{2}\left(1 - \frac{i\kappa}{k} \;+\; \frac{ik}{\kappa} \;+\; \frac{\kappa k}{\kappa k}\right)e^{-2\kappa a} \;+\; \frac{F\,e^{ika}}{2}\left(1 + \frac{i\kappa}{k} \;-\; \frac{ik}{\kappa} \;+\; \frac{\kappa k}{\kappa k}\right)e^{2\kappa a}$$

$$= \frac{F\,e^{ika}}{2}\left(2e^{-2\kappa a} \;-\; \frac{i\kappa}{k}e^{-2\kappa a} \;+\; \frac{ik}{\kappa}e^{-2\kappa a} \;+\; 2e^{2\kappa a} \;+\; \frac{i\kappa}{k}e^{2\kappa a} \;-\; \frac{ik}{\kappa}e^{2\kappa a}\right)$$

$$= \frac{F\,e^{ika}}{2}\left[2\left(e^{-2\kappa a} \;+\; e^{2\kappa a}\right) \;-\; \frac{i\kappa^2}{k\kappa}e^{-2\kappa a} \;+\; \frac{ik^2}{k\kappa}e^{-2\kappa a} \;+\; \frac{i\kappa^2}{k\kappa}e^{2\kappa a} \;-\; \frac{ik^2}{k\kappa}e^{2\kappa a}\right]$$

$$= \frac{F\,e^{ika}}{2}\left[2\left(e^{-2\kappa a} \;+\; e^{2\kappa a}\right) \;+\; \frac{i\kappa^2}{k\kappa}\left(e^{2\kappa a} \;-\; e^{-2\kappa a}\right) \;-\; \frac{ik^2}{k\kappa}\left(e^{2\kappa a} \;-\; e^{-2\kappa a}\right)\right]$$

$$= F\,e^{ika}\left[2\left(\frac{e^{2\kappa a} \;+\; e^{-2\kappa a}}{2}\right) \;+\; \frac{i\,(\kappa^2 - k^2)}{k\kappa}\left(\frac{e^{2\kappa a} \;-\; e^{-2\kappa a}}{2}\right)\right]$$

$$\Rightarrow \quad A\,e^{-ika} \;=\; F\,e^{ika}\left[\cosh(2\kappa a) \;+\; \frac{i\,(\kappa^2-k^2)}{2k\kappa}\,\sinh(2\kappa a)\right].$$

(d) The transmission coefficient is the ratio of intensity transmitted, represented by $|\,F\,|^2$, to the intensity incident, represented by $|\,A\,|^2$. It is conventional to calculate the reciprocal of this ratio to arrive at a compact expression. Both sides are in the polar form of complex numbers, *i.e.*, magnitude and phase. The last result can be arranged as the ratio

$$\left|\frac{A\,e^{-ika}}{F\,e^{ika}}\right| \;=\; \left|\left[\cosh(2\kappa a) \;+\; \frac{i\,(\kappa^2-k^2)}{2k\kappa}\,\sinh(2\kappa a)\right]\right|.$$

Now $\left|\dfrac{A\,e^{-ika}}{F\,e^{ika}}\right| \;=\; \left[\dfrac{A\,e^{-ika}}{F\,e^{ika}}\,\dfrac{A^*e^{ika}}{F^*e^{-ika}}\right]^{1/2} \;=\; \left[\dfrac{A\,A^*}{F\,F^*}\right]^{1/2} \;=\; \dfrac{\left[\,A\,A^*\,\right]^{1/2}}{\left[\,F\,F^*\,\right]^{1/2}} \;=\; \dfrac{|\,A\,|}{|\,F\,|}$ and

$$\frac{|\,A\,|^2}{|\,F\,|^2} \;=\; \left|\left[\cosh(2\kappa a) \;+\; \frac{i\,(\kappa^2-k^2)}{2k\kappa}\,\sinh(2\kappa a)\right]\right|^2 \;=\; \cosh^2(2\kappa a) + \left(\frac{(\kappa^2-k^2)}{2k\kappa}\right)^2 \sinh^2(2\kappa a),$$

where we have used the fact that the product of complex conjugates is the sum of the squares of the real part and the imaginary part. Recalling that $\cosh^2(x) \;=\; 1+\sinh^2(x)$,

$$\begin{aligned}
\frac{|\,A\,|^2}{|\,F\,|^2} \;&=\; 1 \;+\; \sinh^2(2\kappa a) + \left(\frac{\kappa^4-2k^2\kappa^2+k^4}{4k^2\kappa^2}\right)\sinh^2(2\kappa a) \\
&=\; 1 \;+\; \left(1+\frac{\kappa^4-2k^2\kappa^2+k^4}{4k^2\kappa^2}\right)\sinh^2(2\kappa a) \\
&=\; 1 \;+\; \left(\frac{4k^2\kappa^2+\kappa^4-2k^2\kappa^2+k^4}{4k^2\kappa^2}\right)\sinh^2(2\kappa a) \\
&=\; 1 \;+\; \left(\frac{\kappa^4+2k^2\kappa^2+k^4}{4k^2\kappa^2}\right)\sinh^2(2\kappa a) \\
&=\; 1 \;+\; \frac{\left(\kappa^2+k^2\right)^2}{4k^2\kappa^2}\,\sinh^2(2\kappa a).
\end{aligned}$$

Substituting $k \;=\; \sqrt{2mE}\,/\,\hbar$ and $\kappa \;=\; \sqrt{2m\,(V_0-E)}\,/\,\hbar$,

$$\begin{aligned}
\frac{|\,A\,|^2}{|\,F\,|^2} \;&=\; 1 \;+\; \frac{\left(\dfrac{2m}{\hbar^2}(V_0-E) \;+\; \dfrac{2m}{\hbar^2}E\right)^2}{4\left(\dfrac{2m}{\hbar^2}E\right)\left(\dfrac{2m}{\hbar^2}(V_0-E)\right)}\sinh^2\left(\frac{2a}{\hbar}\sqrt{2m\,(V_0-E\,)}\right) \\
&=\; 1 \;+\; \frac{\dfrac{4m^2}{\hbar^4}\,(V_0-E+E)^2}{\dfrac{4m^2}{\hbar^4}\,4E\,(V_0-E)}\sinh^2\left(\frac{2a}{\hbar}\sqrt{2m\,(V_0-E)}\right) \\
\Rightarrow \quad \frac{|\,A\,|^2}{|\,F\,|^2} \;&=\; T^{-1} \;=\; 1 \;+\; \frac{V_0^2}{4E\,(V_0-E)}\,\sinh^2\left(\frac{2a}{\hbar}\sqrt{2m\,(V_0-E\,)}\right).
\end{aligned}$$

Postscript: A tunneling wave function is depicted in figure 9–5. The transmission coefficient is greater than zero at $x > a$. Now picture the probability density; the square of the wave function. There is non-zero probability that the particle can be found at any x including $-a < x < a$. These are classical impossibilities. That a quantum mechanical particle not having enough energy to go "over" a barrier can be in it or go through it is a significant element in many aspects of physics, chemistry, and engineering.

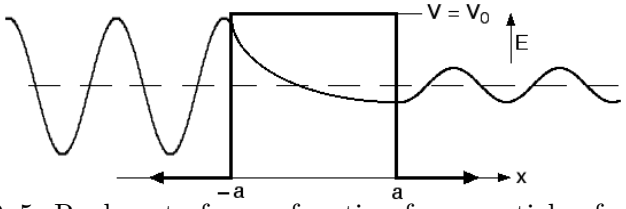


Figure 9–5. Real part of wave function for a particle of $E < V_0$.

Some texts use $x = 0$ to $x = a$ for the size of their barrier. The physics is the same, the mathematics is changed cosmetically, as is the precise mathematical description of the transmission coefficient. The quantum mechanical facts remain that an electron can "appear" within a barrier or on the far side of an electrical potential greater than its own energy.

9–4. Determine the transmission coefficient for a particle with $E = V_0$ incident from the left on the rectangular barrier defined in the last problem.

The intent of this problem is to further develop your skills applying boundary conditions. Require continuity of the wave function and its first derivative at all boundaries.

The first step, which is non-trivial, is to write a proper wave function, which can be puzzling in region 2 where $E = V_0$. The wave function must satisfy the Schrodinger postulate, thus

$$-\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E(x)\psi(x) \quad \Rightarrow \quad -\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\,\psi(x) = E\psi(x)$$

but for $E = V_0$ this means

$$-\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\,\psi(x) = V_0\psi(x) \quad \Rightarrow \quad -\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2} = 0 \quad \Rightarrow \quad \frac{d^2\psi(x)}{dx^2} = 0$$

in region 2. Integrating twice

$$\frac{d\psi(x)}{dx} = D \quad \Rightarrow \quad \psi(x) = C + Dx$$

where C and D are constants of integration. The wave function can then be written

$$\begin{aligned}
\psi_1(x) &= A\,e^{ikx} + B\,e^{-ikx} \qquad \text{for} \qquad x < -a\,,\\
\psi_2(x) &= C + D\,x \qquad \text{for} \qquad -a < x < a\,,\\
\psi_3(x) &= F\,e^{ikx} \qquad \text{for} \qquad x > a\,.
\end{aligned}$$

The wavenumber is the same in regions 1 and 3 because particle energy is the same height above the "floor," and is zero in region 2 for either possible definition because $E = V_0$. Follow parts (b) through (d) of problem 9–3 to get the reciprocal of the transmission coefficient,

$$T^{-1} = 1 + \frac{2mE}{\hbar^2}a^2\,.$$

When $E = V_0$, the wavenumber in the region $-a < x < a$ is $k = \sqrt{2m(V_0 - E)}/\hbar = 0$,

so the wave function can be written $\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for } x < -a, \\ C + Dx & \text{for } -a < x < a, \\ Fe^{ikx} & \text{for } x > a. \end{cases}$

Continuity of the wave function at $x = -a$ means

$$A\,e^{-ika} + B\,e^{ika} = C - D\,a, \tag{1}$$

$$\text{and at } x = a, \quad C + D\,a = F\,e^{ika}. \tag{2}$$

Continuity of the derivative of the wave function at $x = -a$ means

$$A\,ik\,e^{-ika} - B\,ik\,e^{ika} = D, \tag{3}$$

$$\text{and at } x = a, \quad D = F\,ik\,e^{ika}. \tag{4}$$

Multiplying equation (1) by ik and solving for the term with the coefficient B yields

$$B\,ik\,e^{ika} = ik\,C - ik\,D\,a - A\,ik\,e^{-ika}.$$

Substituting this into equation (3) eliminates the unknown coefficient B,

$$A\,ik\,e^{-ika} - ik\,C + ik\,D\,a + A\,ik\,e^{-ika} = D$$

$$\Rightarrow \quad 2A\,ik\,e^{-ika} = ik\,C + D\,(1 - ika). \tag{5}$$

Equation (2) can be written $C = F\,e^{ika} - D\,a$, and substituting this into equation (5),

$$\begin{aligned} 2A\,ik\,e^{-ika} &= ik\,(Fe^{ika} - D\,a) + D\,(1 - ika) \\ &= ik\,Fe^{ika} - ik\,D\,a + D\,(1 - ika) \\ &= ik\,F\,e^{ika} + D\,(1 - 2ika)\,. \end{aligned}$$

Substituting equation (4) into the last equation eliminates the unknown coefficient D,

$$\begin{aligned} & 2A\,ik\,e^{-ika} = ik\,F\,e^{ika} + F\,ik\,e^{ika}\,(1 - 2ika) \\ \Rightarrow \quad & 2A\,e^{-ika} = F\,e^{ika} + F\,e^{ika}\,(1 - 2ika) \\ \Rightarrow \quad & 2A\,e^{-ika} = F\,e^{ika}\,(2 - 2ika) \\ \Rightarrow \quad & A\,e^{-ika} = F\,e^{ika}\,(1 - ika) \\ \Rightarrow \quad & \frac{A\,e^{-ika}}{F\,e^{ika}} = 1 - ika \\ \text{and} \quad & \left|\frac{A\,e^{-ika}}{F\,e^{ika}}\right| = \left|\frac{A}{F}\right| = \frac{|A|}{|F|} \qquad \text{as previously shown,} \\ \Rightarrow \quad & \frac{|A|^2}{|F|^2} = |1 - ika|^2 = 1 + k^2a^2. \end{aligned}$$

Substituting $k = \sqrt{2mE}/\hbar$, $\quad \dfrac{|A|^2}{|F|^2} = T^{-1} = 1 + \dfrac{2mE}{\hbar^2}a^2$ for $E = V_0$.

9–5. Show as $E \rightarrow V_0$ from below, that the results of problems 9–3 and 9–4 are equivalent.

The intent of this problem is to demonstrate self-consistency by examining a limiting case. It is a technique that is difficult to teach and important to learn. Start with the result of problem 9–3. Expand $\sinh(x)$ and ignore the higher order terms so that $\sinh(x) \approx x$ since $E \approx V_0$. Of course, in the limit $E \rightarrow V_0$ the results of problem 9–3 and 9–4 must be the same.

Start with the reciprocal of the transmission coefficient from problem 9–3. Ignoring higher order terms as negligible in the series expansion of $\sinh(x) \Rightarrow \sinh(x) \approx x$,

$$\begin{aligned} T^{-1} &= 1 + \frac{V_0^2}{4E(V_0 - E)} \left(\frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right)^2 \\ &= 1 + \frac{V_0^2}{4E(V_0 - E)} \left(\frac{4a^2}{\hbar^2} 2m(V_0 - E) \right) \\ &= 1 + \frac{V_0^2}{E} \left(\frac{a^2}{\hbar^2} 2m \right) \\ &= 1 + \frac{2mV_0^2}{\hbar^2 E} a^2 . \end{aligned}$$

Remembering that $E \approx V_0$, $\quad T^{-1} \approx 1 + \dfrac{2mE}{\hbar^2} a^2 .$

9–6. (a) A particle of energy $E > V_0$ is incident on a rectangular barrier of width $2a$. Solve for the value of the transmission coefficient and locate the positions of the maxima and minima in terms of wave number. Plot transmission coefficient versus barrier width for a particle of constant energy and variable barrier width.

(b) Locate the positions of the maxima in terms of particle energy. Plot transmission coefficient versus particle energy where $E > V_0$ and barrier width is fixed.

Problem 9–3 discusses the $E < V_0$ case in order to address barrier penetration and tunneling. The general solution to $E > V_0$ case is left to the student as exercise 9–11. This problem uses results from exercise 9–11 in order to introduce a phenomenon known as **resonance scattering**. At certain values of particle wavenumber (energy), there is 100% transmission and no reflection. Part (a) should illustrate resonance scattering for an incident particle of fixed energy and a barrier width that is variable. Part (b) illustrates the same phenomenon where particle energy is variable and barrier width is fixed. Start with an intermediate result from exercise 9–11,

$$\frac{1}{T} = 1 + \frac{1}{4} \left(\frac{k_1^2 - k_2^2}{k_1 k_2} \right)^2 \sin^2(2k_2 a) .$$

Solve for T instead of its reciprocal. The maxima occur where the sine term is zero at barrier widths of $2a = n\pi/k_2$. The minima occur where the sine term is one, where the transmission coefficient has the value $T = \left(\dfrac{2k_1 k_2}{k_1^2 + k_2^2} \right)^2$. Part (b) is started with

$$\frac{1}{T} = 1 + \frac{V_0^2}{4E(E - V_0)} \sin^2 \left(\frac{2a}{\hbar} \sqrt{2m(E - V_0)} \right) ,$$

the result of exercise 9–11 in terms of energy. Again, solve for T instead of its reciprocal. This plot is more difficult because the independent variable E appears in five places including within the square root of the argument of the sine squared term. The important part of this graph is the shape. If you do not have access to a commercial graphing package, try to imagine what the graph should look like, and skip to the solution. You should find the maxima at

$$E \;=\; \frac{\pi^2\hbar^2}{8ma^2}\,n^2 \;+\; V_0\,.$$

You may recognize this result is closely related to the energy eigenvalues of the infinite square well.

$$\text{(a)}\quad \frac{1}{T} \;=\; 1 \;+\; \frac{1}{4}\left(\frac{k_1^2-k_2^2}{k_1k_2}\right)^2 \sin^2(2k_2a) \;=\; \frac{4k_1^2k_2^2}{4k_1^2k_2^2} \;+\; \frac{k_1^4 \;-\; 2k_1^2k_2^2 \;+\; k_2^4}{4k_1^2k_2^2}\sin^2(2k_2a)$$

$$= \frac{4k_1^2k_2^2 \;+\; \left(k_1^4 \;-\; 2k_1^2k_2^2 \;+\; k_2^4\right)\sin^2(2k_2a)}{4k_1^2k_2^2}$$

$$\Rightarrow \quad T \;=\; \frac{4k_1^2k_2^2}{4k_1^2k_2^2 \;+\; \left(k_1^4 \;-\; 2k_1^2k_2^2 \;+\; k_2^4\right)\sin^2(2k_2a)}\,.$$

Maxima of $T = 1$ occur where $\sin^2(2k_2a) = 0$, *i.e.*, where $2k_2a = n\pi \quad\Rightarrow\quad 2a = \dfrac{n\pi}{k_2}$ are the barrier widths at which maxima occur, noting that the width of the barrier is given to be $2a$. The minima occur where the sine squared term is one, so minima occur at

$$T \;=\; \frac{4k_1^2k_2^2}{4k_1^2k_2^2 \;+\; \left(k_1^4 \;-\; 2k_1^2k_2^2 \;+\; k_2^4\right)\cdot 1} \;=\; \frac{4k_1^2k_2^2}{k_1^4 \;+\; 2k_1^2k_2^2 \;+\; k_2^4} \quad\Rightarrow\quad T \;=\; \left(\frac{2k_1k_2}{k_1^2 \;+\; k_2^2}\right)^2.$$

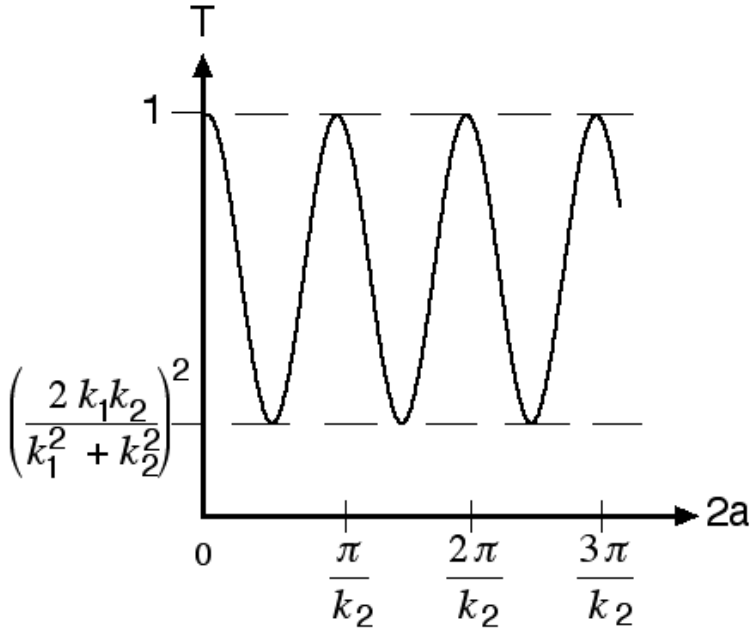


Figure 9–6. Transmission coefficient as width of barrier is varied.

(b) In terms of particle energy,

$$\begin{aligned}
\frac{1}{T} &= 1 + \frac{V_0^2}{4E\,(E-V_0)}\,\sin^2\left(\frac{2a}{\hbar}\sqrt{2m\,(E-V_0)}\right) \\
&= \frac{4E\,(E-V_0) + V_0^2\,\sin^2\left(\frac{2a}{\hbar}\sqrt{2m\,(E-V_0)}\right)}{4E\,(E-V_0)} \\
\Rightarrow \quad T &= \frac{4E\,(E-V_0)}{4E\,(E-V_0) + V_0^2\,\sin^2\left(\frac{2a}{\hbar}\sqrt{2m\,(E-V_0)}\right)}\,.
\end{aligned}$$

The maxima occur where the sine squared term is zero, so

$$\begin{aligned}
&\frac{2a}{\hbar}\sqrt{2m\,(E-V_0)} = n\pi \quad \Rightarrow \quad \sqrt{2m\,(E-V_0)} = \frac{n\pi\hbar}{2a} \\
\Rightarrow \quad &2m\,(E-V_0) = \frac{\pi^2\hbar^2}{4a^2}\,n^2 \quad \Rightarrow \quad E - V_0 = \frac{\pi^2\hbar^2}{8ma^2}\,n^2 \\
\Rightarrow \quad &E_n = \frac{\pi^2\hbar^2}{8ma^2}\,n^2 + V_0
\end{aligned}$$

which are energies closely related to the eigenenergies of a particle in an infinite square well.

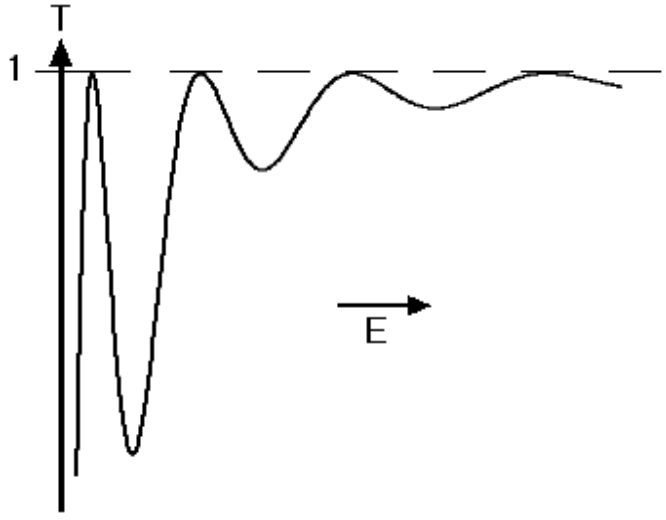


Figure 9–7. Transmission coefficient, fixed barrier width, increasing energy.

Postscript: Resonance scattering is the circumstance where 100% transmission occurs. There are two significant things to observe in the last figure. First, as long as the barrier is finite, there will be maxima. This means that 100% transmission occurs at selected energies for any barrier not of infinite width. Secondly, the maxima are not periodic. Rather, the spacing between maxima varies as n^2 for a fixed barrier width.

9–7. (a) Show in position space that

$$\Delta\left(\psi'(x)\right) \;=\; \frac{2m}{\hbar^2}\,\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx$$

is the general value of the discontinuity in the first derivative for an infinite potential.

(b) Calculate the value of the discontinuity in the first derivative for a particle interacting with the potential well $V(x) = -\alpha\,\delta(x)$.

ψ and ψ' must be continuous at any boundary of a finite potential. There must, however, be a discontinuity in the first derivative at all infinite boundaries. If the value of the discontinuity can be calculated, the boundary condition for the first derivative is again useful. The method of calculating the value of the discontinuity is to put the potential into the Schrodinger equation, integrate around the infinite boundary, and let the limits approach zero from both sides.

For a general potential $V(x)$, the Schrodinger equation in position space is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} \;+\; V(x)\,\psi(x) \;=\; E\,\psi(x).$$

If we integrate around the point which is the discontinuity, this is

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi(x)}{dx^2}\,dx \;+\; \int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx \;=\; E\int_{-\epsilon}^{\epsilon}\psi(x)\,dx,$$

which assumes that the infinite boundary is at $x = 0$. The quantity ϵ is infinitesimal. If we let $\epsilon \to 0$, the right side of the equation is zero. The integral of a finite quantity, $\psi(x)$, over an arbitrarily small interval is zero. The term with the potential does not vanish because the integral of an infinite quantity, the potential, can be non-zero even for an arbitrarily small interval. So,

$$\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi(x)}{dx^2}\,dx \;=\; \frac{2m}{\hbar^2}\,\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx$$

$$\Rightarrow \quad \frac{d\psi(x)}{dx}\Big|_{\epsilon\to 0} - \frac{d\psi(x)}{dx}\Big|_{-\epsilon\to 0} \;=\; \frac{2m}{\hbar^2}\,\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx$$

$$\Rightarrow \quad \Delta\left(\psi'(x)\right) \;=\; \frac{2m}{\hbar^2}\,\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} V(x)\,\psi(x)\,dx \tag{1}$$

is the general value of the discontinuity in the first derivative.

(b) A delta function potential is infinite, so employing equation (1),

$$\Delta\big(\psi'(x)\big)\Big|_{x=0} \;=\; \frac{2m}{\hbar^2}\,\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon}\big(-\alpha\,\delta(x)\big)\,\psi(x)\,dx \;=\; -\frac{2m}{\hbar^2}\,\alpha\,\psi(0),$$

because regardless of how closely ϵ approaches zero, $-\epsilon < 0 < \epsilon$, meaning that zero is within the limits of integration. Since the value of the delta function that makes its argument zero is

within the limits of integration, the integral is the wave function evaluated at the point that makes the argument of the delta function zero.

Postscript: An infinite potential models a perfectly rigid and perfectly impenetrable wall. The wave function must be zero at an infinite potential barrier, such as the wall of an infinite square well, because the product $V(x)\,\psi(x)$ in the Schrodinger equation would be infinite for $\psi \neq 0$. There is a non-smooth "corner" in the wave function as it goes to zero at any position other than $\pm\infty$, thus there is a discontinuity in the first derivative of the wave function. The delta function potential with only "one wall" is useful to understanding concepts, is mathematically tractable, and is a first approximation to an abrupt and large potential that is thin.

9–8. Calculate the reflection and transmission coefficients for a particle incident on the potential

$$V(x) \;=\; -\alpha\,\delta(x) \qquad \text{given} \qquad E \;>\; 0\,.$$

This problem is intended to demonstrate how a potential that includes a delta function is treated specifically, and one treatment of a discontinuity. First, write the wave function for two regions because the delta function is of "zero" width. The wavenumber is the same in regions 1 and 2 because the particle energy is the same height above the potential "floor" in both regions. A $\psi(0)$ is required. Use either $\psi_1(0)$ or $\psi_2(0)$, because the condition of continuity of the wave function at the boundary ensures that they are the same. We use $\psi_2(0)$ because it has one fewer term than $\psi_1(0)$. Classically, the reflection coefficient must be zero. The quantum mechanical result is non-zero.

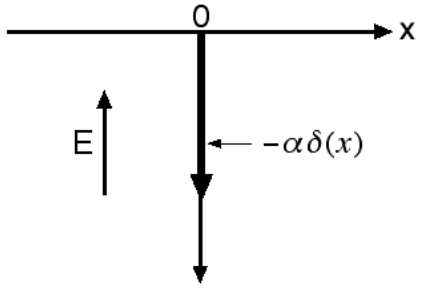


Figure 9–8. Negative delta function potential.

The solution to the Schrodinger equation in position space is

$$\psi_1(x) \;=\; A\,e^{ikx} \;+\; B\,e^{-ikx}, \;\; x \;<\; 0\,, \qquad\qquad \psi_2(x) \;=\; C\,e^{ikx}, \;\; x \;>\; 0\,,$$

where the infinite potential well is at $x = 0$. Continuity of the wave function means

$$A\,e^{ik(0)} \;+\; B\,e^{-ik(0)} \;=\; C\,e^{ik(0)} \qquad \Rightarrow \qquad A \;+\; B \;=\; C\,.$$

The first derivatives in regions 1 and 2 are

$$\psi_1'(x) \;=\; ik\,A\,e^{ikx} \;-\; ik\,B\,e^{-ikx}, \qquad\qquad \psi_2'(x) \;=\; ik\,C\,e^{ikx}.$$

We calculated the general value of the discontinuity of the first derivative in problem 9–7. This is the difference of the first derivatives in regions 1 and 2, meaning

$$\psi_1'(0) \;-\; \psi_2'(0) \;=\; -\frac{2m}{\hbar^2}\,\alpha\,\psi(0)$$

$$\Rightarrow \quad ik\,A\,e^{ik(0)} \;-\; ik\,B\,e^{-ik(0)} \;-\; ik\,C\,e^{ik(0)} \;=\; -\frac{2m}{\hbar^2}\,\alpha\,\psi\,(0)\,.$$

Using $\quad \psi\,(x) \;=\; \psi_2\,(x)\,, \quad$ where $\quad \psi_2(0) \;=\; C\,e^{ik(0)} \;=\; C$

$$\Rightarrow \quad ik\,A \;-\; ik\,B \;-\; ik\,C \;=\; -\frac{2m}{\hbar^2}\,\alpha\,C$$

$$\Rightarrow \quad ik\,A \;-\; ik\,B \;=\; C\left(ik - \frac{2m}{\hbar^2}\alpha\right),$$

and we use the continuity condition, $A \;+\; B \;=\; C\,,$ to eliminate C, so

$$ik\,A \;-\; ik\,B \;=\; \Big(A + B\Big)\left(ik - \frac{2m}{\hbar^2}\,\alpha\right)$$

$$\Rightarrow \quad ik\,A \;-\; ik\,B \;=\; A\left(ik - \frac{2m}{\hbar^2}\,\alpha\right) \;+\; B\left(ik - \frac{2m}{\hbar^2}\,\alpha\right)$$

$$\Rightarrow \quad A\left(\cancel{ik} \;-\; \cancel{ik} \;+\; \frac{2m}{\hbar^2}\,\alpha\right) \;=\; B\left(ik + ik - \frac{2m}{\hbar^2}\,\alpha\right)$$

$$\Rightarrow \quad A\left(\frac{2m}{\hbar^2}\,\alpha\right) \;=\; B\left(2ik - \frac{2m}{\hbar^2}\,\alpha\right)$$

$$\Rightarrow \quad B \;=\; A\left[\left(\frac{2m}{\hbar^2}\,\alpha\right) \Big/ \left(2ik - \frac{2m}{\hbar^2}\,\alpha\right)\right] \;=\; \frac{m\alpha A}{ik\hbar^2 - m\alpha}\,.$$

The reflection coefficient is

$$R \;=\; \frac{\big|\,B\,\big|^2}{\big|\,A\,\big|^2} \;=\; \left(\frac{m\alpha A^*}{-ik\hbar^2 - m\alpha}\right)\left(\frac{m\alpha A}{ik\hbar^2 - m\alpha}\right)\frac{1}{|\,A\,|^{\,2}} \;=\; \frac{m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2} \;=\; \frac{1}{1 + k^2\hbar^4/m^2\alpha^2}\,.$$

The transmission coefficient is

$$T \;=\; 1 - R \;=\; 1 - \frac{m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2} \;=\; \frac{k^2\hbar^4 + m^2\alpha^2 - m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2} \;=\; \frac{k^2\hbar^4}{k^2\hbar^4 + m^2\alpha^2} \;=\; \frac{1}{1 + m^2\alpha^2/k^2\hbar^4}\,.$$

Postscript: Any curve that has a sharp corner has a discontinuity in it's next order derivative. Delta functions and theta functions can be useful in describing discontinuities. Techniques seen in problems 9–7 and 9–8 are useful in a number of areas, the use of delta functions in particular is becoming increasingly popular, and you will see these techniques in future chapters.

The negative delta function potential is an infinitely deep, infinitely thin potential energy well. It is a limiting case of a finite square well (chapter 11), so will be encountered again.

9–9. Qualitatively discuss how boundary value techniques may be applied to more realistic potential energy functions.

The vertical step potential and the rectangular barrier potential are idealizations having the advantage that they have exact solutions. A realistic potential energy function will vary smoothly rather than have precisely square corners and vertical walls.

First, idealized potentials may be viewed as a limiting case of a smooth function.

Figure 9–9. Idealized potentials as approximations to smoothly varying functions.

Any realistic potential energy function can be better approximated using multiple rectangular barriers (and/or wells). While not completely prohibitive, there would be nine regions and five

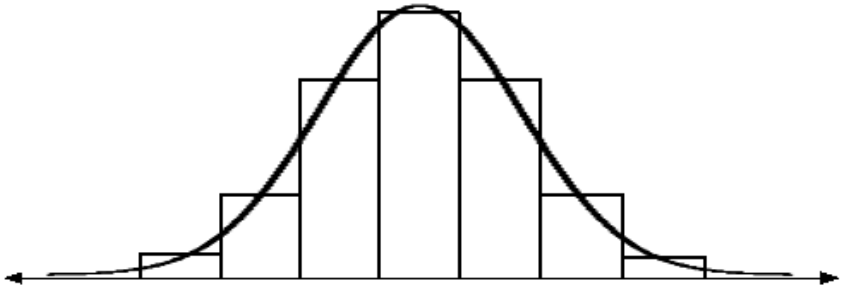


Figure 9–10. A Gaussian barrier being approximated by seven adjacent rectangular barriers.

different wavenumbers to consider for the symmetric case sketched in figure 9–10. Should the realistic potential be asymmetric, the number of wavenumbers increases.

A realistic potential barrier is better addressed using the **Wentzel–Kramers–Brillouin (WKB) approximation** which will yield

$$\left| T \right|^2 \;=\; \exp\left(-2 \int \sqrt{\frac{2m}{\hbar^2} \left(V\left(x\right) - E \right)} \, dx \right)$$

for a slowly varying potential energy function. The same approximation can be obtained from multiple thin rectangular barriers in the limit of an infinite number of barriers that approach zero width for large κa, and assuming that transmission through multiple barriers is multiplicative[1]. The second book in this series addresses the WKB approximation.

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[1] Gasiorwicz *Quantum Physics* (John Wiley & Sons, New York, 1974), pp.84-86.

Exercises

9–10. For a particle that encounters a vertical step potential of height V_0 (figure 9–1), calculate the reflection and transmission coefficients for the particle energies

(a) $E = 2V_0$,

(b) $E = 3V_0/2$,

(c) $E = 1.1V_0$, and

(d) $E = V_0$.

(e) Explain the result of part (d).

This problem is intended primarily to reinforce the quantum mechanical effect that reflection occurs at a step even when $E > V_0$. It should further familiarize you with reflection and transmission coefficients. The boundary value problem for a vertical step potential is solved in problem 9–1, resulting in the general forms of the reflection and transmission coefficients

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad \text{and} \qquad T = 1 - R = \frac{4\,k_1\,k_2}{(k_1 + k_2)^2}\,.$$

Express the wavenumbers in terms of energies for parts (a) through (d) to obtain the reflection and transmission coefficients using these equations. There is an increasing amount of reflection as the energy of the particle gets closer to the energy of the potential barrier, until at $E = V_0$, the transmission coefficient is zero. The reason for this is there are artificialities built into the model to make it more mathematically tractable. The barrier of figure 9–4 with $+a \to \infty$ is the vertical step potential of figure 9–1. Use this and the result of problem 9–4 to answer part (e).

9–11. Determine the transmission coefficient for a particle with $E > V_0$ incident from the left on the rectangular barrier defined in problem 9–3.

Reflection from a potential barrier, depicted in figure 9–4, of energy less than that of the incident particle is another solely quantum mechanical phenomenon. Start with the wave function

$$\psi(x) = \begin{cases} A\,e^{ik_1 x} + B\,e^{-ik_1 x}, & \text{for} \quad x < -a\,, \\ C\,e^{ik_2 x} + D\,e^{-ik_2 x}, & \text{for} \quad -a < x < a\,, \\ F\,e^{ik_1 x}, & \text{for} \quad x > a\,. \end{cases}$$

Require continuity of the wave function and its first derivative at all boundaries. Follow the procedures of problem 9–3. Define $k_1 = \sqrt{2mE}\,/\,\hbar$ and $k_2 = \sqrt{2m\,(E - V_0)}\,/\,\hbar$, to find

$$T^{-1} = 1 + \frac{V_0^2}{4E\,(E - V_0)}\,\sin^2\left(\frac{2a}{\hbar}\sqrt{2m\,(E - V_0)}\right).$$

9–12. Show in the limit $E \to V_0$ from above, that the result of problems 9–4 and exercise 9–11 are equivalent.

This exercise has the same intent as problem 9–5. Start with the result of exercise 9–11. Expand $\sin(x)$ and ignore the higher order terms so that $\sin(x) \approx x$ since $E \approx V_0$. You must find that in the limit $E \to V_0$, the results of problems 9–4 and exercise 9–11 are the same.

9–13. Sketch probability density versus distance for the particle/potential system of problem 9–3.

Figure 9–5 illustrates the real part of a particle wave function for a particle approaching a rectangular barrier from the left. To obtain probability density, start with

$$\psi(x) = \begin{cases} A\,e^{ikx} + B\,e^{-ikx}, & \text{for} \quad x < -a\,, \\ C\,e^{\kappa x} + D\,e^{-\kappa x}, & \text{for} \quad -a < x < a\,, \\ F\,e^{ikx}, & \text{for} \quad x > a\,, \end{cases}$$

form the corresponding $\left|\psi(x)\right|^2 = \psi^*(x)\,\psi(x)$ in each region, and sketch these in each region versus x. The coefficients A, B, C, etc., are constants. Assume $D >> C$.

9–14. A particle of $E > 0$ approaches the negative vertical step potential

$$V(x) = \begin{cases} 0, & \text{for} \quad x < 0\,, \\ -V_0 & \text{for} \quad x > 0\,. \end{cases}$$

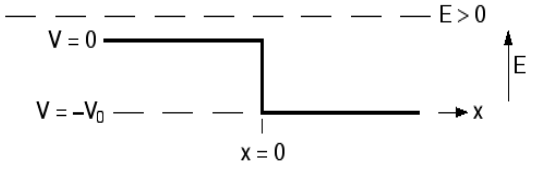

Figure 9–11. Negative vertical step potential.

What are the reflection and transmission coefficients if $E = V_0/3$, and $E = V_0/8$?

This problem parallels the discussion of the vertical step potential. It is intended to reinforce the methods of addressing a boundary value problem. It also illustrates another completely non-classical phenomenon. Classically, we expect the reflection coefficients to be zero for any $E > 0$.

(a) Write the wave function. You have only two regions to consider. You should recognize that the general form of the wave function is

$$\psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x} \quad \text{for} \quad x < 0\,,$$

$$\psi_2(x) = Ce^{ik_2 x} + De^{-ik_2 x} \quad \text{for} \quad x > 0\,,$$

where $k_1 = \sqrt{2mE}\,/\,\hbar$ and $k_2 = \sqrt{2m\,(E-(-V_0))}\,/\,\hbar = \sqrt{2m\,(E+V_0)}\,/\,\hbar$. Can you conclude that $D = 0$ because it is the coefficient of an oppositely directed incident wave?

(b) Apply the continuity conditions to the wave function and its first derivative at $x = 0$. You should have two equations in three unknowns. The square of the coefficient A is the intensity of incidence, and the square of the coefficient B is the intensity of reflection. Since A and B are

the two coefficients you want to compare, you should combine your two equations to eliminate C. You should find that $A\,(k_1 - k_2) \;=\; B\,(k_1 + k_2)$.

(c) The reflection coefficient is the ratio $|\,B\,|^2/|\,A\,|^2$, which you can form from your result of part (b). Use the definitions of the wavenumbers to establish R in terms of E and V_0, then substitute $E = V_0/3$ and $E = V_0/8$ to get numerical answers. You should find $R = 1/9$ and $1/4$, respectively, and the transmission coefficients follow directly using $R + T = 1$.

9–15. (a) Find the transmission coefficient for a particle with $E > 0$ that encounters the rectangular well

$$V\,(x) \;=\; \begin{cases} -V_0\,, & \text{for } -a < x < a\,, \\ 0\,, & \text{for } |\,x\,| > a\,. \end{cases}$$

(b) Show that $T = 1$ in the limit that $V_0 \to 0$.

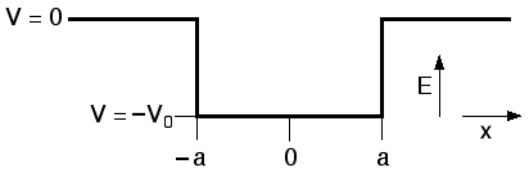

Figure 9–12. Rectangular well potential.

This is a finite square well (square corners) addressed in greater depth in chapter 11. The procedures for this problem strongly parallel the boundary value problem 9–3. You should find

$$T^{-1} \;=\; 1 \;+\; \frac{V_0^2}{4E\,(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m\,(E+V_0)}\right)$$

using $k_1 = \sqrt{2mE}\,/\,\hbar$ and $k_2 = \sqrt{2m\,(E-(-V_0))}\,/\,\hbar \;=\; \sqrt{2m\,(E+V_0)}\,/\,\hbar$. Consider the width and depth of the well when $V_0 \to 0$ for part (b).

9–16. The transmission coefficient a particle of $E < V_0$ approaching a barrier of width $2a$ is

$$T \;=\; \frac{1}{1 \;+\; \dfrac{V_0^2}{4E\,(V_0-E)}\,\sinh^2\left(\dfrac{2a}{\hbar}\sqrt{2m\,(V_0-E)}\right)} \qquad \text{from problem 9–3.}$$

(a) Calculate the transmission coefficient for the case $E = V_0/2$ and $2a = 2\lambda$.

(b) Draw a sketch of T versus a for $E = V_0/2$ for a single particle.

(c) Find T for $2a = \lambda/4$ and $\lambda/2$ at $E = V_0/2$ for a single particle.

This exercise provides numerical context for barrier transmission/tunneling. The transmission coefficient quickly becomes vanishingly small for barriers of even modest width for a single particle.

Substitute $E = V_0/2$ and $2a = 2\lambda$. Use the de Broglie relation to express V_0 in terms of λ. Remember that

$$\sinh\,(x) \;=\; \frac{e^x - e^{-x}}{2}\,.$$

The sketch should start at $a = 0$, which is no barrier, and will quickly approach the horizontal axis as a gets larger. But it approaches only asymptotically, thus, $T > 0$ for all a. Offered only as food for thought, how many would tunnel if an Avogadro's number of single particles were incident on a barrier of width $2a = 2\lambda$ at $E = V_0/2$?

9–17. Plot barrier width versus transmission coefficient for a particle incident on a rectangular barrier of width $2a$ at $E = V_0$. What widths of the barrier result in 10%, 1%, 0.1%, and 0.01% transmission when particle energy is equal to barrier height?

This exercise continues the context of the last, and illustrates that even a thin barrier prevents most transmission of a single particle at particle energy the same as barrier height. Answers should be in terms of wavelengths. A barrier a few wavelengths in width results in miniscule transmission. Start with the reciprocal of the transmission coefficient from problem 9–4 expressed in terms of energy and half barrier width a. Use the de Broglie relationship to express the energy in terms of wavelength, then solve for the barrier width $2a$. The barrier width that results in 10% transmission is slightly less than one particle wavelength.

9–18. Calculate the reflection and transmission coefficients for a particle incident on the potential

$$V(x) \;=\; \alpha\,\delta(x-a)\,.$$

This exercise is quite similar to problem 9–8, though this potential is positive and is located at $x = a$. Use the result of problem 9–7 (a) to obtain the value of the discontinuity of the first derivatives. The fact that this potential is positive forces some sign considerations, and that the delta function is located at other than zero requires carrying exponentials. For instance,

$$B \;=\; \frac{-m\,\alpha\,e^{2ika}}{ik\hbar^2 \;+\; m\,\alpha}A\;.$$

Remember that the square of a norm is just the product of the complex conjugates. You need $|A|^2$ and $|B|^2$ rather than just A and B.

What should differ from problem 9–8 in your overall answers just because the delta function is inverted and displaced from zero? Do you expect to obtain the same reflection and transmission coefficients as problem 9–8?

9–19. (a) Qualitatively discuss what would be expected for a particle incident on a "saw tooth" potential from the left with $E > V_0$.

(b) Qualitatively discuss what would be expected for a particle incident on a "saw tooth" potential from the left with $E < V_0$.

(c) Draw a sketch approximating the "saw tooth" potential with two rectangular barriers.

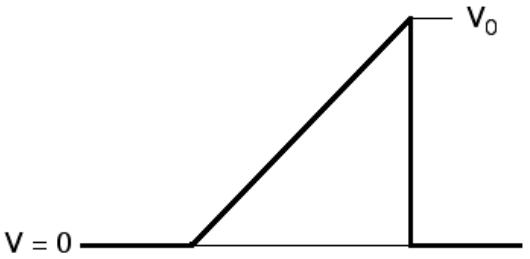

Figure 9–13. Saw tooth potential.

Make no attempt to address this exercise quantitatively. The intent of problem 9–9 and this exercise is to convey the concept that if quantum mechanical phenomena occur for rectangular barriers, and all barriers can be viewed as a sequence of rectangular barriers, then quantum mechanical phenomena should be expected for all barriers. Answers to parts (a) and (b) should be a few sentences describing reflection, transmission, barrier penetration, etc. A quantitative discussion of realistic potential energy functions will ensue when the WKB approximation is addressed.

9–20. Briefly discuss the form of a wave function for a particle incident from the left on a rectangular barrier for $E < V_0$ in the interval $-a < x < a$.

Tunneling means that a particle appears on the other side of a barrier that it does not have the energy to surmount. Barrier penetration is often considered synonymous with tunneling, though barrier penetration is really a more encompassing phenomenon. A particle has a non-zero probability of being located within the barrier! A particle may penetrate the barrier's leading edge, be transmitted (tunnel) by leaving the trailing edge, or become reflected. The barrier can be penetrated without the particle tunneling.

Problem 9–3 and figures 9–4 and 9–5 may be helpful. Notice that in region 2 of the rectangular barrier of figure 9–4 the wave function is

$$\psi(x) = C e^{\kappa x} + D e^{-\kappa x} \qquad \text{for} \qquad -a < x < a$$

where $\kappa = \sqrt{2m(V_0 - E)}/\hbar$. Consider that κ must be real and positive for $E < V_0$. Then this exercise amounts to explaining the meanings of the terms $C e^{\kappa x}$ and $D e^{-\kappa x}$. It may be helpful to shift the edges of the barrier to $0 < x < 2a$ to absorb the point of this exercise.

Given $E < V_0$ for a particle incident from the left on a rectangular barrier of height V_0, there is a non-zero probability the particle will be reflected, a non-zero probability that the particle will be transmitted, and a non-zero probability that the particle could be located within the barrier.

The particle could penetrate the barrier and then be reflected. This is the phenomenon this exercise intends to highlight. It is a quantum mechanical phenomenon associated with a particle incident on any potential energy barrier that is not purely vertical and of infinite height and also of infinite width. The infinite square well is the only potential energy well or barrier encountered in this text for which barrier penetration, often resulting in reflection, does not occur.

Chapter 10

The Simple Harmonic Oscillator

The infinite square well is useful to illustrate many concepts including energy quantization, but the infinite square well is a limiting case of a realistic potential. The simple harmonic oscillator (SHO), in contrast, is a realistic and commonly encountered potential energy function. It is one of the most important problems in quantum mechanics and physics in general. It is often used as a first approximation to more complex phenomena. It is dominantly popular in modeling a multitude of cooperative phenomena. The electrical bonds between the atoms or molecules in a crystal lattice are often modeled as "little springs," so group phenomena is modeled by a system of coupled SHO's. The phonons of solid state physics and the quantum mechanical description of electromagnetic fields in free space use multiple coupled phonons and photons modeled by simple harmonic oscillators. The rudiments are the same as classical mechanics; small oscillations in a smooth potential are modeled well by the SHO.

If a particle is confined in any potential, it demonstrates the same basic qualitative behavior as a particle confined to an infinite square well. Energy is quantized in all bound systems. The energy levels of the SHO are different than an infinite square well because the "geometry" of the potential energy function is different. Look for other similarities in these two systems. For instance, compare the shapes of the eigenfunctions between the infinite square well and the SHO.

Part 1 outlines the basic concepts and focuses on the arguments of linear algebra using **raising and lowering operators** and matrix operators. This approach is more elegant than brute force solutions of differential equations in position space, and uses and reinforces Dirac notation, which depends upon the arguments of linear algebra. The raising and lowering operators, or **ladder operators**, are the predecessors of the creation and annihilation operators used in the quantum mechanical description of interacting photons. The arguments of linear algebra provide a variety of raising and lowering equations that yield the eigenvalues of the SHO,

$$E_n \;=\; \left(n \;+\; \frac{1}{2}\right)\hbar\omega,$$

and their eigenfunctions. The eigenfunctions of the SHO can be described using **Hermite polynomials** (pronounced "her meet") in position space.

Part 2 will explain why the Hermite polynomials are applicable and reinforce the results of part 1. Part 2 emphasizes the method of **power series solutions** of a differential equation. Chapter 8 introduced the separation of variables, which is usually the first method applied in an attempt to solve a partial differential equation. Power series solutions apply to ordinary differential equations. In the case the partial differential equation is separable, it may be appropriate to solve one or more of the resulting ordinary differential equations using a power series method. The power series method is often used to address the hydrogen atom. You should leave this chapter understanding how an ordinary differential equation is solved using a power series solution.

We do not reach the coupled harmonic oscillator in this text. Of course, the SHO is an important building block in reaching the coupled harmonic oscillator. There are numerous physical systems described by a single harmonic oscillator. The SHO approximates any individual bond, such as the bond encountered in a diatomic molecule like O_2 or N_2. The SHO applies to any system that demonstrates smooth, small amplitude vibration.

Part 1, Ladder Operators and Hermite Polynomials

10–1. Justify the use of a simple harmonic oscillator potential, $V(x) = kx^2/2$, for a particle confined to any smooth potential well. Write the time–independent Schrodinger equation in abstract Hilbert space for a system described as a simple harmonic oscillator.

The sketches may be illustrative. Problem 2–19 addresses the Hamiltonian operator for an SHO.

The functional form of an SHO from classical mechanics is $V(x) = \frac{1}{2}kx^2$. Its graph is a parabola as seen in the figure on the left. Any relative minimum in a smooth potential energy curve can be approximated by a simple harmonic oscillator if the energy is small compared to the height of the well meaning that oscillations have small amplitudes.

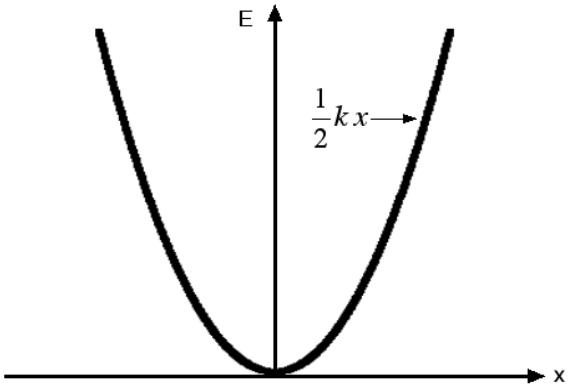

Figure 10–1. SHO potential well.

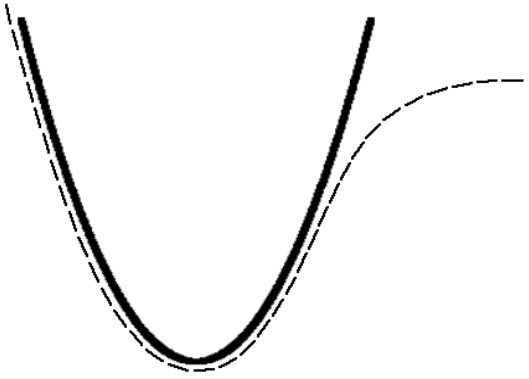

Figure 10–2. Relative potential energy minimum.

Expanding an arbitrary potential energy function in a Taylor series, where x_0 is the minimum,

$$V(x) = V(x_0) + \frac{dV}{dx}\Big|_{x_0}(x-x_0) + \frac{1}{2!}\frac{d^2V}{dx^2}\Big|_{x_0}(x-x_0)^2 + \frac{1}{3!}\frac{d^3V}{dx^3}\Big|_{x_0}(x-x_0)^3 + \cdots$$

defining $V(x_0) = 0$, $\frac{dV}{dx}\Big|_{x_0} = 0$ because the slope is zero at the bottom of a minimum, and if $E \ll$ the height of the potential well, then $x \approx x_0$ so terms where the difference $(x - x_0)$ has a power of 3 or greater are negligible. The Taylor series expansion reduces to

$$V(x) = \frac{1}{2}\frac{d^2V}{dx^2}\Big|_{x_0}(x-x_0)^2 \qquad \text{where} \qquad \frac{d^2V}{dx^2}\Big|_{x_0} = k\,.$$

The definition $x_0 = 0 \;\Rightarrow\; V(x) = \frac{1}{2}kx^2$. Since $k = m\omega^2$, $V(x) = \frac{1}{2}m\omega^2x^2$. Using this potential to form a Hamiltonian operator, the time–independent Schrodinger equation is

$$\mathcal{H}\,|\,\psi> \;=\; E_n\,|\,\psi> \quad \Rightarrow \quad \left[\frac{\mathcal{P}^2}{2m} + \frac{1}{2}m\omega^2\mathcal{X}^2\right]|\,\psi> \;=\; E_n\,|\,\psi>\,.$$

Postscript: Notice that this Schrodinger equation is basis independent. The momentum and position operators are represented only in abstract Hilbert space.

10–2. Show that the time-independent Schrodinger Equation for the SHO can be written

$$\hbar\omega\left(a^\dagger\, a + \frac{1}{2}\right)\,|\,\psi> \;=\; E_n\,|\,\psi>\;.$$

$$a \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \;+\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P} \qquad \text{and} \qquad a^\dagger \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X}^\dagger \;-\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}^\dagger.$$

For reasons that will become apparent, a is called the **lowering operator**, and $a^\dagger$ is known as the **raising operator**. Since $\mathcal{X}$ and $\mathcal{P}$ are Hermitian, $\mathcal{X}^\dagger = \mathcal{X}$ and $\mathcal{P}^\dagger = \mathcal{P}$, so the raising operator can be written

$$a^\dagger \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \;-\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}.$$

Remember that $\mathcal{X}$ and $\mathcal{P}$ do not commute. They are fundamentally canonical, $\big[\,\mathcal{X},\,\mathcal{P}\,\big] \;=\; i\hbar\,.$

$$\begin{aligned}
\hbar\omega\left(a^\dagger\, a + \frac{1}{2}\right) \;&=\; \hbar\omega\left\{\left[\Big(\frac{m\omega}{2\hbar}\Big)^{1/2}\mathcal{X} \;-\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}\right]\left[\Big(\frac{m\omega}{2\hbar}\Big)^{1/2}\mathcal{X} \;+\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P}\right] + \frac{1}{2}\right\} \\
&=\; \hbar\omega\left[\Big(\frac{m\omega}{2\hbar}\Big)\,\mathcal{X}^2 \;+\; i\left(\frac{1}{4\hbar^2}\right)^{1/2}\mathcal{X}\mathcal{P} \;-\; i\left(\frac{1}{4\hbar^2}\right)^{1/2}\mathcal{P}\mathcal{X} \;+\; \left(\frac{1}{2m\omega\hbar}\right)\mathcal{P}^2 + \frac{1}{2}\right] \\
&=\; \hbar\omega\left[\frac{m\omega}{2\hbar}\mathcal{X}^2 \;+\; \frac{1}{2m\omega\hbar}\mathcal{P}^2 \;+\; \frac{i}{2\hbar}\Big(\mathcal{X}\mathcal{P} \;-\; \mathcal{P}\mathcal{X}\Big) \;+\; \frac{1}{2}\right] \\
&=\; \hbar\omega\left[\frac{1}{2m\omega\hbar}\mathcal{P}^2 \;+\; \frac{m\omega}{2\hbar}\mathcal{X}^2 \;+\; \frac{i}{2\hbar}\Big[\,\mathcal{X},\,\mathcal{P}\,\Big] \;+\; \frac{1}{2}\right] \\
&=\; \hbar\omega\left[\frac{1}{2m\omega\hbar}\mathcal{P}^2 \;+\; \frac{m\omega}{2\hbar}\mathcal{X}^2 \;+\; \frac{i}{2\hbar}\,i\hbar \;+\; \frac{1}{2}\right] \\
&=\; \hbar\omega\left[\frac{1}{2m\omega\hbar}\mathcal{P}^2 \;+\; \frac{m\omega}{2\hbar}\mathcal{X}^2 \;-\; \frac{1}{2} \;+\; \frac{1}{2}\right] \;=\; \left[\frac{1}{2m}\mathcal{P}^2 \;+\; \frac{m\omega^2}{2}\mathcal{X}^2\right] \;=\; \mathcal{H}
\end{aligned}$$

$$\Rightarrow \qquad \left[\frac{1}{2m}\mathcal{P}^2 \;+\; \frac{m\omega^2}{2}\mathcal{X}^2\right]\,|\,\psi> \;=\; E_n\,|\,\psi> \;\iff\; \hbar\omega\left(a^\dagger\, a + \frac{1}{2}\right)\,|\,\psi> \;=\; E_n\,|\,\psi>\;.$$

Postscript: The Schrodinger equation is $\big[\,\mathcal{P}^2 \,+\, \mathcal{X}^2\,\big]\,|\,\psi> \;=\; E_n\,|\,\psi>,$ when constant factors are excluded. The sum $\mathcal{P}^2 + \mathcal{X}^2 = \mathcal{X}^2 + \mathcal{P}^2$ would appear to factor as $\big(\mathcal{X} + i\mathcal{P}\big)\big(\mathcal{X} - i\mathcal{P}\big)\,,$ so

$$\big[\,\mathcal{P}^2+\mathcal{X}^2\,\big]\,|\,\psi> = E_n\,|\,\psi> \;\Rightarrow\; \big[\,\mathcal{X}^2+\mathcal{P}^2\,\big]\,|\,\psi> = E_n\,|\,\psi> \;\Rightarrow\; \big(\,\mathcal{X}+i\mathcal{P}\,\big)\big(\,\mathcal{X}-i\mathcal{P}\,\big)\,|\,\psi> = E_n\,|\,\psi>$$

This is only a qualified type of factoring because the order of the "factors" cannot be changed; $\mathcal{X}$ and $\mathcal{P}$ are fundamentally canonical and simply do not commute. Nevertheless, the parallel with

common factoring into complex conjugate quantities is part of the motivation for the raising and lowering operators. In fact, some authors refer to this approach as the **method of factorization**.

Notice that $a^\dagger a \;=\; \dfrac{1}{\hbar\omega}\,\mathcal{H} \;-\; \dfrac{1}{2}\,.$

Notice also that though $\mathcal{X}$ and $\mathcal{P}$ are Hermitian, a and $a^\dagger$ are not.

10–3. Show that the commutator $\big[\,a,\,a^\dagger\,\big] \;=\; 1\,.$

Problems 10–3 and 10–4 develop tools for the eigenvector/eigenvalue problem of the SHO.

We want $\big[\,a,\,a^\dagger\,\big] \;=\; a\,a^\dagger - a^\dagger a$ in terms the definitions of problem 10–2. Letting

$$C \;=\; \Big(\frac{m\omega}{2\hbar}\Big)^{1/2}, \qquad \text{and} \qquad D \;=\; \Big(\frac{1}{2m\omega\hbar}\Big)^{1/2} \qquad \text{to simplify notation,}$$

$$\begin{aligned}
\big[\,a,\,a^\dagger\,\big] \;&=\; \big(C\mathcal{X} \;+\; iD\mathcal{P}\big)\big(C\mathcal{X} \;-\; iD\mathcal{P}\big) \;-\; \big(C\mathcal{X} \;-\; iD\mathcal{P}\big)\big(C\mathcal{X} \;+\; iD\mathcal{P}\big) \\
&=\; \cancel{C^2\mathcal{X}^2} - \;iCD\mathcal{X}\,\mathcal{P} \;+\; iDC\mathcal{P}\,\mathcal{X} \;+\; \cancel{D^2\mathcal{P}^2} - \;\cancel{C^2\mathcal{X}^2} - \;iCD\mathcal{X}\,\mathcal{P} \;+\; iDC\mathcal{P}\,\mathcal{X} \;-\; \cancel{D^2\mathcal{P}^2} \\
&=\; 2iCD\big(\,\mathcal{P}\,\mathcal{X} \;-\; \mathcal{X}\,\mathcal{P}\,\big) \\
&=\; 2i\Big(\frac{m\omega}{2\hbar}\Big)^{1/2}\Big(\frac{1}{2m\omega\hbar}\Big)^{1/2}\Big[\,\mathcal{P},\,\mathcal{X}\,\Big] \\
&=\; \frac{2i}{2\hbar}\big(-i\hbar\big) \;=\; 1, \quad \text{since} \quad \Big[\,\mathcal{P},\,\mathcal{X}\,\Big] \;=\; -\Big[\,\mathcal{X},\,\mathcal{P}\,\Big] \;=\; -i\hbar\,.
\end{aligned}$$

10–4. Show that $\mathcal{H}\,a^\dagger \;=\; a^\dagger\mathcal{H} \;+\; a^\dagger\hbar\omega\,.$

This is a tool used to solve the eigenvector/eigenvalue problem for the SHO, though it should also build some familiarity with the raising and lowering operators and commutator algebra.

$$\mathcal{H} \;=\; \hbar\omega\Big(a^\dagger a \;+\; \frac{1}{2}\Big) \quad \Rightarrow \quad \frac{\mathcal{H}}{\hbar\omega} \;=\; a^\dagger a \;+\; \frac{1}{2}$$

$$\begin{aligned}
\Big[\,a^\dagger,\,\frac{\mathcal{H}}{\hbar\omega}\,\Big] \;&=\; \Big[\,a^\dagger,\,a^\dagger a \;+\; \frac{1}{2}\,\Big] \;=\; a^\dagger a^\dagger a \;+\; a^\dagger\cancel{\frac{1}{2}} \;-\; a^\dagger a a^\dagger \;-\; \frac{1}{2}\cancel{a^\dagger} \\
&=\; a^\dagger\big(a^\dagger a - a a^\dagger\big) \;=\; -a^\dagger\Big[\,a,\,a^\dagger\,\Big] \;=\; -a^\dagger
\end{aligned}$$

$$\Rightarrow \quad \big[\,a^\dagger,\,\mathcal{H}\,\big] \;=\; -a^\dagger\hbar\omega \quad \Rightarrow \quad a^\dagger\mathcal{H} \;-\; \mathcal{H}\,a^\dagger \;=\; -a^\dagger\hbar\omega \quad \Rightarrow \quad \mathcal{H}\,a^\dagger \;=\; a^\dagger\mathcal{H} \;+\; a^\dagger\hbar\omega\,.$$

Postscript: We will also use $\mathcal{H}\,a \;=\; a\,\mathcal{H} \;-\; a\hbar\omega\,,$ though proof is left as an exercise.

10–5. Find the effect of the raising and lowering operators using the results of problem 10–4.

We have usually written the time–independent Schrodinger equation as $\mathcal{H}\,|\,\psi> \;=\; E_n\,|\,\psi>$. Since the Hamiltonian is the energy operator, the eigenvalues are necessarily energy eigenvalues. The state vector is a linear combination of all energy eigenvectors. If we specifically measure the eigenvalue E_n, then the state vector is necessarily the associated eigenvector which can be denoted $|\,E_n>$. The time–independent Schrodinger equation written as $\mathcal{H}\,|\,E_n> \;=\; E_n\,|\,E_n>$ is likely a better expression for the development that follows.

If $\mathcal{H}\,|\,E_n> \;=\; E_n\,|\,E_n>$ where E_n is an energy eigenvalue and $|\,\psi> \;=\; |\,E_n>$,

$$\begin{aligned}\mathcal{H}\,a^\dagger\,|\,E_n> \;&=\; \big(a^\dagger\mathcal{H} \;+\; a^\dagger\hbar\omega\big)\,|\,E_n> \;=\; a^\dagger\mathcal{H}\,|\,E_n> \;+\; a^\dagger\hbar\omega\,|\,E_n> \\ &=\; a^\dagger E_n\,|\,E_n> \;+\; a^\dagger\hbar\omega\,|\,E_n> \;=\; \big(E_n+\hbar\omega\big)\,a^\dagger\,|\,E_n> \quad \text{or} \\ \mathcal{H}\Big(a^\dagger\,|\,E_n>\Big) \;&=\; \big(E_n \;+\; \hbar\omega\big)\Big(a^\dagger\,|\,E_n>\Big).\end{aligned}$$

This means that $a^\dagger\,|\,E_n>$ is an eigenvector of $\mathcal{H}$ with an eigenvalue of $E_n+\hbar\omega$. This is exactly $\hbar\omega$ more than the eigenvalue of the eigenvector $|\,E_n>$. The effect of $a^\dagger$ acting on $|\,E_n>$ is to "raise" the eigenvalue by $\hbar\omega$, thus $a^\dagger$ is known as the raising operator.

Again, given that $\mathcal{H}\,|\,E_n> \;=\; E_n\,|\,E_n>$,

$$\begin{aligned}\mathcal{H}\,a\,|\,E_n> \;&=\; \big(a\mathcal{H} \;-\; a\hbar\omega\big)\,|\,E_n> \;=\; a\mathcal{H}\,|\,E_n> \;-\; a\hbar\omega\,|\,E_n> \\ &=\; aE_n\,|\,E_n> \;-\; a\hbar\omega\,|\,E_n> \;=\; \big(E_n \;-\; \hbar\omega\big)\,a\,|\,E_n> \quad \text{or} \\ \mathcal{H}\Big(a\,|\,E_n>\Big) \;&=\; \big(E_n \;-\; \hbar\omega\big)\Big(a\,|\,E_n>\Big).\end{aligned}$$

Here $a\,|\,E_n>$ is an eigenvector of $\mathcal{H}$ with an eigenvalue of $E_n-\hbar\omega$. This is $\hbar\omega$ less than the eigenvalue of the eigenvector $|\,E_n>$. The effect of a acting on $|\,E_n>$ is to "lower" the eigenvalue by $\hbar\omega$, thus a is known as the lowering operator.

10–6. What is the effect of the lowering operator on the ground state, E_g?

This is another step toward finding the eigenvalues of the SHO.

Given $\mathcal{H}\,|\,E_g> \;=\; E_g\,|\,E_g>$, the effect of the lowering operator is to lower the eigenvalue by $\hbar\omega$, $\mathcal{H}\,a\,|\,E_g> \;=\; \big(E_g-\hbar\omega\big)\,a\,|\,E_g>$. This is physically impossible; there cannot be an energy less than ground state energy. The only physical possibility of the lowering operator acting on the ground state is zero; this means that there is no physical system. Thus, $a\,|\,E_g> \;=\; 0$.

Postscript: The quantum number $n=0$ is the ground state of the SHO. The quantum number of the SHO is sufficient to uniquely identify the eigenstate so $|\,E_3> \;=\; |\,3>$, $|\,E_7> \;=\; |\,7>$, and $|\,E_g> \;=\; |\,E_0> \;=\; |\,0>$. A zero result is an absence of a physical system, which should not be confused with the eigenstate $|\,0>$ representing the ground state.

10–7. Calculate a value for the ground state energy of the SHO.

Remember that $a\,|\,0> = 0$ from the previous problem. Orthonormality of eigenstates is required. The strategy is to calculate the expectation value of the ground state two different ways.

$\mathcal{H}\,|\,0> = E_0\,|\,0> \quad \Rightarrow \quad <0\,|\,\mathcal{H}\,|\,0> = <0\,|\,E_0\,|\,0> \quad \Rightarrow \quad <0\,|\,\mathcal{H}\,|\,0> = E_0\,<0\,|\,0> = E_0$ because $<0\,|\,0> = 1$ due to the orthonormality of eigenstates. This expectation value can also be expressed in terms of the raising and lowering operators

$$\begin{aligned} E_0 &= <0\,|\,\mathcal{H}\,|\,0> = <0\,|\,\hbar\omega\left(a^\dagger a + \frac{1}{2}\right)|\,0> = <0\,|\,\hbar\omega a^\dagger a + \frac{\hbar\omega}{2}\,|\,0> \\ &= <0\,|\,\hbar\omega a^\dagger a\,|\,0> + <0\,|\,\frac{\hbar\omega}{2}\,|\,0> \\ &= <0\,|\,\hbar\omega a^\dagger\Big(a\,|\,0>\Big) + \frac{\hbar\omega}{2}\,<0\,|\,0> = 0 + \frac{\hbar\omega}{2} = \frac{\hbar\omega}{2} \end{aligned}$$

is the ground state energy of the SHO.

10–8. Derive the eigenenergies of the SHO

Per problem 10–5, $\mathcal{H}\left(a^\dagger\,|\,E_n>\right) = \left(E_n + \hbar\omega\right)\left(a^\dagger\,|\,E_n>\right)$ so $a^\dagger\,|\,E_n>$ is an eigenvector of $\mathcal{H}$ with the eigenvalue $E_n + \hbar\omega$. Similarly, that $a^\dagger\,|\,E_n>$ is an eigenvector of $\mathcal{H}$,

$$\Rightarrow \quad \mathcal{H}\left[a^\dagger\Big(a^\dagger\,|\,E_n>\Big)\right] = \left(E_n + \hbar\omega + \hbar\omega\right)\left[a^\dagger\Big(a^\dagger\,|\,E_n>\Big)\right]$$

so $a^\dagger\left(a^\dagger\,|\,E_n>\right) = a^\dagger a^\dagger\,|\,E_n>$ is an eigenvector of $\mathcal{H}$ with the eigenvalue $E_n + 2\hbar\omega$. Successively applying the raising operator yields successive eigenvalues. The eigenvalue of the ground state is fixed at $\hbar\omega/2$ so all the eigenvalues can be obtained in terms of the ground state eigenvalue.

$$\begin{aligned} \mathcal{H}\,|\,0> = E_0\,|\,0> = \frac{\hbar\omega}{2}\,|\,0> \quad &\Rightarrow \quad \mathcal{H}\,a^\dagger\,|\,0> = \left(\frac{\hbar\omega}{2} + \hbar\omega\right)|\,0> \\ &\Rightarrow \quad \mathcal{H}\,a^\dagger a^\dagger\,|\,0> = \left(\frac{\hbar\omega}{2} + 2\hbar\omega\right)|\,0> \\ &\Rightarrow \quad \mathcal{H}\,a^\dagger a^\dagger a^\dagger\,|\,0> = \left(\frac{\hbar\omega}{2} + 3\hbar\omega\right)|\,0> \quad \text{and in general} \\ &\Rightarrow \quad \mathcal{H}\left(a^\dagger\right)^n\,|\,0> = \left(\frac{\hbar\omega}{2} + n\hbar\omega\right)|\,0> \end{aligned}$$

$$\Rightarrow \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad \text{are the eigenenergies of the SHO.}$$

Postscript: Notice that the eigenvectors $a^\dagger\,|\,0>,\ a^\dagger a^\dagger\,|\,0>, \ldots, \left(a^\dagger\right)^n\,|\,0>$ are not identified.

10–9. Find energy space representations for the eigenvectors of the SHO.

Explicit eignvalues given $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$ are $E_0 = \frac{1}{2}\hbar\omega$, $E_1 = \frac{3}{2}\hbar\omega$, $E_2 = \frac{5}{2}\hbar\omega$, $E_3 = \frac{7}{2}\hbar\omega$, ... The eigenvector/eigenvalue equations must remain

$$\mathcal{H}\,|\,0> \;=\; E_0\,|\,0>, \qquad \mathcal{H}\,|\,1> \;=\; E_1\,|\,1>, \qquad \mathcal{H}\,|\,2> \;=\; E_2\,|\,2>, \;\ldots,\; \mathcal{H}\,|\,n> \;=\; E_n\,|\,n> .$$

Combining these eigenvalue/eigenvector relations with those obtained earlier using the raising operator provides the ability to explicitly represent the eigenvectors.

$$\begin{aligned}
\mathcal{H}\,|\,1> \;=\; \frac{3}{2}\hbar\omega\,|\,1> \;=\; \mathcal{H}\,a^\dagger\,|\,0> \quad &\Rightarrow \quad |\,1> \;\propto\; a^\dagger\,|\,0> \\
\mathcal{H}\,|\,2> \;=\; \frac{5}{2}\hbar\omega\,|\,2> \;=\; \mathcal{H}\,a^\dagger a^\dagger\,|\,0> \quad &\Rightarrow \quad |\,2> \;\propto\; a^\dagger a^\dagger\,|\,0> \;\propto\; a^\dagger\,|\,1> \\
\mathcal{H}\,|\,3> \;=\; \frac{7}{2}\hbar\omega\,|\,3> \;=\; \mathcal{H}\,a^\dagger a^\dagger a^\dagger\,|\,0> \quad &\Rightarrow \quad |\,3> \;\propto\; a^\dagger a^\dagger a^\dagger\,|\,0> \;\propto\; a^\dagger\,|\,2> \quad \text{and} \\
\mathcal{H}\,|\,n> \;=\; \left(n + \frac{1}{2}\right)\hbar\omega\,|\,n> \;=\; \mathcal{H}\left(a^\dagger\right)^n\,|\,0> \quad &\Rightarrow \quad |\,n> \;\propto\; \left(a^\dagger\right)^n\,|\,0> \;\propto\; a^\dagger\,|\,n-1>
\end{aligned}$$

$$\Rightarrow \quad C\,(n)\,|\,n> \;=\; a^\dagger\,|\,n-1> \quad \text{in general, where } C\,(n) \text{ is a proportionality constant.}$$

Postscript: The relation of proportionality is appropriate for this argument because of the nature of the eigenvalue/eigenvector equation. Any vector that is proportional to the eigenvector will work in the eigenvalue/eigenvector equation. Consider

$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}$ whose eigenvalues are 2 and 1, corresponding to the eigenvectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

$$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \;=\; 2\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} 2 \\ 0 \end{pmatrix} \;=\; \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \quad \text{but any vector}$$

proportional to $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ also yields a true statement in the eigenvalue/eigenvector equation, *e.g.*,

$$\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 2 \\ 0 \end{pmatrix} \;=\; 2\begin{pmatrix} 2 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} 4 \\ 0 \end{pmatrix} \;=\; \begin{pmatrix} 4 \\ 0 \end{pmatrix}.$$

In fact, the proportionality condition is equivalent to the normalization condition in this case.

The n in the equation $C\,(n)\,|\,n> \;=\; a^\dagger\,|\,n-1>$ is one eigenstate higher than $n-1$. The raising operator acting on an eigenstate increases the state to the next higher eigenstate.

10–10. Normalize $C(n)\,|\,n> \;=\; a^\dagger\,|\,n-1>$.

This problem is a good example of (a) forming adjoints and applying the normalization condition, (b) using commutator algebra, and (c) using eigenvalue/eigenvector equations. Remember orthonormality requires that $<n\,|\,n> \;=\; <n-1\,|\,n-1> \;=\; 1$, and also that $\left[\,a\,,\,a^\dagger\,\right] \;=\; 1$.

(a) $C(n)\,|\,n> \;=\; a^\dagger\,|\,n-1> \;\Rightarrow\; <n\,|\,C^*(n) \;=\; <n-1\,|\left(a^\dagger\right)^\dagger \;=\; <n-1\,|\,a$ is the adjoint equation $\Rightarrow$ $<n\,|\,C^*(n)\,C(n)\,|\,n> \;=\; <n-1\,|\,a\,a^\dagger\,|\,n-1>$ are the innner products. We have an expression for $a^\dagger a$, but need to develop an expression for $a\,a^\dagger$.

(b) $$\mathcal{H} \;=\; \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \;\Rightarrow\; a^\dagger a \;=\; \frac{\mathcal{H}}{\hbar\omega} - \frac{1}{2} \;\Rightarrow\; a^\dagger a - a\,a^\dagger \;=\; \frac{\mathcal{H}}{\hbar\omega} - \frac{1}{2} - a\,a^\dagger$$

subtracting $a\,a^\dagger$ from both sides. $\left[\,a\,,\,a^\dagger\,\right] \;=\; 1 \;\Rightarrow\; \left[\,a^\dagger\,,\,a\,\right] \;=\; -1\,,$

$$\Rightarrow \quad \left[\,a^\dagger\,,\,a\,\right] \;=\; \frac{\mathcal{H}}{\hbar\omega} \;-\; \frac{1}{2} \;-\; a\,a^\dagger \quad \Rightarrow \quad -1 \;=\; \frac{\mathcal{H}}{\hbar\omega} \;-\; \frac{1}{2} \;-\; a\,a^\dagger \quad \Rightarrow \quad a\,a^\dagger \;=\; \frac{\mathcal{H}}{\hbar\omega} \;+\; \frac{1}{2}\,.$$

Returning to part (a)

(c) $$\left|\,C(n)\,\right|^2 <n\,|\,n> \;=\; <n-1\,|\,\frac{\mathcal{H}}{\hbar\omega} \;+\; \frac{1}{2}\,|\,n-1>$$

$$\Rightarrow \quad \left|\,C(n)\,\right|^2 \;=\; <n-1\,|\,\frac{\mathcal{H}}{\hbar\omega}\,|\,n-1> \;+\; <n-1\,|\,\frac{1}{2}\,|\,n-1>$$

$$\Rightarrow \quad \left|\,C(n)\,\right|^2 \;=\; <n-1\,|\,\frac{1}{\hbar\omega}\left(n-1+\frac{1}{2}\right)\hbar\omega\,|\,n-1> \;+\; \frac{1}{2}\,<n-1\,|\,n-1>$$

where $\mathcal{H}$ acts on $|\,n-1>$ resulting in the eigenvalue in the first term on the right. Then

$$\left|\,C(n)\,\right|^2 \;=\; <n-1\,|\,n-\frac{1}{2}\,|\,n-1> \;+\; \frac{1}{2} \;=\; <n-1\,|\,n\,|\,n-1> \;-\; <n-1\,|\,\frac{1}{2}\,|\,n-1> \;+\; \frac{1}{2}$$

$$=\; n\,<n-1\,|\,n-1> \;-\; \frac{1}{2}\,<n-1\,|\,n-1> \;+\; \frac{1}{2} \;=\; n \;-\; \frac{1}{2} \;+\; \frac{1}{2} \;=\; n\,,$$

$$\Rightarrow \quad C(n) \;=\; \sqrt{n} \quad \Rightarrow \quad \sqrt{n}\,|\,n> \;=\; a^\dagger\,|\,n-1>\,.$$

Postscript: An alternate way of writing this result is $a^\dagger\,|\,n> \;=\; \sqrt{n+1}\,|\,n+1>$. The effect of the lowering operator is $a\,|\,n> \;=\; \sqrt{n}\,|\,n-1>$, and is left as an exercise.

10–11. Find a general relation for an arbitrary eigenstate of the SHO in terms of the ground state and the raising operator.

The general relation for one state in terms of the higher adjacent state and the raising operator is $a^\dagger \,|\, n> \;=\; \sqrt{n+1}\,|\, n+1>$. Apply this relation to the ground state and adjacent states.

$$\left(a^\dagger\right)^1 |\, 0> \;=\; \sqrt{0+1}\,|\, 0+1> \;=\; \sqrt{1}\,|\, 1>$$

$$\left(a^\dagger\right)^2 |\, 0> \;=\; a^\dagger\sqrt{1}\,|\, 1> \;=\; \sqrt{1}\,a^\dagger\,|\, 1> \;=\; \sqrt{1}\sqrt{1+1}\,|\, 1+1> \;=\; \sqrt{1}\sqrt{2}\,|\, 2>$$

$$\left(a^\dagger\right)^3 |\, 0> \;=\; a^\dagger\sqrt{1}\sqrt{2}\,|\, 2> = \sqrt{1}\sqrt{2}\,a^\dagger\,|\, 2> = \sqrt{1}\sqrt{2}\sqrt{2+1}\,|\, 2+1> = \sqrt{1}\sqrt{2}\sqrt{3}\,|\, 3> \;.$$

For arbitrary n this pattern yields

$$\begin{aligned}
\left(a^\dagger\right)^n |\, 0> \;&=\; a^\dagger\sqrt{1}\sqrt{2}\sqrt{3}\sqrt{4}\cdots\sqrt{n-1}\,|\, n-1> \\
&=\; \sqrt{1}\sqrt{2}\sqrt{3}\sqrt{4}\cdots\sqrt{n\,-1}\,a^\dagger\,|\, n-1> \\
&=\; \sqrt{1}\sqrt{2}\sqrt{3}\sqrt{4}\cdots\sqrt{n-1}\sqrt{n}\,|\, n> \\
&=\; \sqrt{n!}\,|\, n> \\
\Rightarrow \qquad |\, n> \;&=\; \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n |\, 0> \;.
\end{aligned}$$

10–12. Develop a matrix operator representation of the Hamiltonian of the SHO.

It is convenient to use unit vectors to express eigenstates for the SHO. The first few are written

$$|\, 0> \;=\; \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \qquad |\, 1> \;=\; \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \qquad |\, 2> \;=\; \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \qquad |\, 3> \;=\; \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}.$$

Notice that all the eigenkets are of infinite dimension and that they are orthonormal. This problem is an application of earlier addressed mathematics applied to a realistic system.

The Hamiltonian is Hermitian so can be diagonalized to have unit vectors as basis vectors. The Hamiltonian that is diagonal must, therefore, have eigenvalues on the main diagonal, *i.e.*,

$$\mathcal{H} \;=\; \hbar\omega \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 3/2 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 5/2 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 7/2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 9/2 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

10–13. (a) Develop the matrix representation of the lowering operator for the SHO.

(b) Lower the third excited state of the SHO using explicit matrix multiplication, and

(c) demonstrate equivalence to $a\,|\,n> \;=\; \sqrt{n}\,|\,n-1> \quad \text{for} \quad n\,=\,3\,.$

An individual element of any matrix can be calculated using Dirac notation by sandwiching the operator between the bra representing the row of interest and the ket representing the column of interest (forming a braket). In general for the lowering operator,

$$\begin{aligned} <n\,|\,a\,|\,m> \;&=\; <n\,|\,\sqrt{m}\,|\,m-1> \\ &=\; \sqrt{m}\,<n\,|\,m-1> \\ &=\; \sqrt{m}\;\delta_{n,\,m-1}, \end{aligned}$$

where the lowering operator acted to the right in the first line. The Kronecker delta reflects orthonormality. It says that the element in row n and column $m-1$ is zero unless $n\,=\,m-1\,.$

(a) Trying a few values on the main diagonal,

$$\begin{aligned} <0\,|\,a\,|\,0> \;&=\; \sqrt{0}\;\delta_{0,-1} \;=\; \sqrt{0}\,(0) \;=\; 0\,, \\ <1\,|\,a\,|\,1> \;&=\; \sqrt{1}\;\delta_{1,\,0} \;=\; \sqrt{1}\,(0) \;=\; 0\,, \quad \text{and} \\ <2\,|\,a\,|\,2> \;&=\; \sqrt{2}\;\delta_{2,\,1} \;=\; \sqrt{2}\,(0) \;=\; 0\,. \end{aligned}$$

In fact, all elements on the main diagonal are zero. The Kronecker delta indicates that the column must be one greater than the row to be non–zero, so

$$\begin{aligned} <0\,|\,a\,|\,1> \;&=\; \sqrt{1}\;\delta_{0,\,0} \;=\; \sqrt{1}\,(1) \;=\; \sqrt{1}\,, \\ <1\,|\,a\,|\,2> \;&=\; \sqrt{2}\;\delta_{1,\,1} \;=\; \sqrt{2}\,(1) \;=\; \sqrt{2}\,, \\ <2\,|\,a\,|\,3> \;&=\; \sqrt{3}\;\delta_{2,\,2} \;=\; \sqrt{3}\,(1) \;=\; \sqrt{3}\,, \end{aligned}$$

and the pattern continues to yield

$$a \;=\; \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

(b) $$a\,|\,3> \;=\; \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \;=\; \begin{pmatrix} 0 \\ 0 \\ \sqrt{3} \\ 0 \\ 0 \\ \vdots \end{pmatrix} \;=\; \sqrt{3} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \;=\; \sqrt{3}\,|\,2>\,,$$

(c) which is the same as $a\,|\,3> \;=\; \sqrt{3}\,|\,3-1> \;=\; \sqrt{3}\,|\,2>\,.$ (Of course, these must be the same. The relation used for part (c) is also the relation used to build the matrix representation).

Postscript: The upper left element of matrix operators used to describe the SHO is row zero, column zero. This is because the zero is an allowed quantum number for the SHO and $|0>$ is the ground state. The upper left element in most other matrices is row one, column one.

The matrix representation of the raising operator is similarly developed and is

$$a^\dagger \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

10–14. Find the matrix representation of $\mathcal{X}$ for the SHO.

The operators $\mathcal{X}$, $\mathcal{P}$, and $\mathcal{H}$, correspond to position, momentum, and energy, which are dynamical variables in classical mechanics, but operators in quantum mechanics. Remember

$$a \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \;+\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P},$$

$$a^\dagger \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \;-\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P},$$

are the definitions of the "ladder" operators in terms of the position and momentum operators. Since we have matrix representations of a and $a^\dagger$, the matrix representation of $\mathcal{X}$, $\mathcal{P}$, and $\mathcal{H}$, are a matter of chapter 1 matrix addition and multiplicative constants.

Adding the equations for a and $a^\dagger$,

$$a + a^\dagger \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \;+\; i\left(\frac{1}{2m\cancel{\omega}\hbar}\right)^{1/2}\mathcal{P} \;+\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \;-\; i\left(\frac{1}{2m\cancel{\omega}\hbar}\right)^{1/2}\mathcal{P}$$

$$= \; 2\left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \qquad \Rightarrow \qquad \mathcal{X} \;=\; \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a + a^\dagger\right)$$

$$= \; \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left[\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \;+\; \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}\right]$$

$$= \; \left(\frac{\hbar}{2m\omega}\right)^{1/2}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Postscript: Subtract a from $a^\dagger$ to find the matrix representation of $\mathcal{P}$, which is

$$\mathcal{P} \;=\; i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

10–15. Use the position space representations of the position and momentum operators in the lowering operator to obtain the ground state eigenfunction of the SHO in position space.

The position space representation of the lowering operator is

$$\begin{aligned} a \;&=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\mathcal{X} \;+\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\mathcal{P} \\ &=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}x \;+\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}\left(-i\hbar\frac{d}{dx}\right) \\ &=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}x \;+\; \left(\frac{\hbar}{2m\omega}\right)^{1/2}\frac{d}{dx}\,. \end{aligned}$$

The idea is to use this to obtain a position space representation. The ground state will follow.

Just to simplify the notation, we are going to change variables. Let

$$y \;=\; \left(\frac{m\omega}{\hbar}\right)^{1/2}x \quad\Rightarrow\quad dy \;=\; \left(\frac{m\omega}{\hbar}\right)^{1/2}dx$$

$$\Rightarrow\quad x \;=\; \left(\frac{\hbar}{m\omega}\right)^{1/2}y \qquad\text{and}\qquad dx \;=\; \left(\frac{\hbar}{m\omega}\right)^{1/2}dy$$

$$\Rightarrow\quad a \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(\frac{\hbar}{m\omega}\right)^{1/2}y \;+\; \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\frac{m\omega}{\hbar}\right)^{1/2}\frac{d}{dy} \quad\Rightarrow\quad a \;=\; \frac{1}{\sqrt{2}}\left(y+\frac{d}{dy}\right).$$

The eigenkets $|\,n>$ in abstract Hilbert space and $\psi_n(y)$ in position space are equivalent expressions, and we used the fact that $a\,|\,0> \;=\; 0$ to obtain eigenenergies earlier, so

$$|\,n> \;=\; \psi_n(y) \quad\Rightarrow\quad a\,|\,n> \;=\; a\,\psi_n(y) \quad\Rightarrow\quad a\,|\,0> \;=\; a\,\psi_0(y) \quad\Rightarrow\quad a\,\psi_0(y) \;=\; 0\,,$$

therefore
$$\begin{aligned} \frac{1}{\sqrt{2}}\left(y+\frac{d}{dy}\right)\psi_0(y) \;&=\; 0 \\ \Rightarrow\quad \frac{d\,\psi_0(y)}{\psi_0(y)} \;&=\; -y\,dy \\ \Rightarrow\quad \ln\psi_0(y) \;&=\; -\frac{1}{2}\,y^2 \;+\; C \\ \Rightarrow\quad \psi_0(y) \;&=\; A_0\,e^{-y^2/2} \quad\text{where the constant of integration } C \text{ is} \end{aligned}$$

absorbed into the constant A_0. Returning to the variable x,

$$\psi_0(x) \;=\; A_0\, e^{-m\omega x^2/\,2\hbar}$$

is the unnormalized ground state eigenfunction of the SHO in position space.

Postscript: Notice that the ground state eigenfunction of the SHO in position space is a Gaussian function. The normalized ground state eigenfunction is $\psi_0(x) \;=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/\,2\hbar}$.

10–16. (a) Find a generating function for the eigenstates of the SHO in position space in general.

(b) Find the eigenfunction for the first excited state of the SHO in position space.

Employ the result of problem 10–11,

$$|\,n> \;=\; \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n |\,0>,$$

using the position space representation of the raising operator,

$$a^\dagger \;=\; \left(\frac{m\omega}{2\hbar}\right)^{1/2} x \;-\; \left(\frac{\hbar}{2m\omega}\right)^{1/2} \frac{d}{dx}\,.$$

This is cleaner using y as defined in problem 10–15. Use the result of part (a) for $n = 1$ to complete part (b). Eliminate y to express ψ_1 in terms of x to finish.

(a) Using y as defined in problem 10–15, $a^\dagger \;=\; \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)$, the result of problem 10–11 is

$$\psi_n(y) \;=\; \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^n \psi_0(y)$$

$$\Rightarrow \quad \psi_n(y) \;=\; \frac{1}{\sqrt{n!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^n \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-y^2/2}.$$

(b) The first excited state of the SHO means $n = 1$, so

$$\begin{aligned}
\psi_1(y) \;&=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{1!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^1 e^{-y^2/2} \\
&=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}}\left(y\, e^{-y^2/2} - \frac{d}{dy}\, e^{-y^2/2}\right) \\
&=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}}\left(y\, e^{-y^2/2} \;-\; (-y)\, e^{-y^2/2}\right) \\
&=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}}\, 2y\, e^{-y^2/2} \\
\Rightarrow \quad \psi_1(x) \;&=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{2}\, \left(\frac{m\omega}{\hbar}\right)^{1/2} x\, e^{-m\omega x^2/\,2\hbar} \\
&=\; \left(\frac{4}{\pi}\left(\frac{m\omega}{\hbar}\right)^3\right)^{1/4} x\, e^{-m\omega x^2/\,2\hbar}.
\end{aligned}$$

10–17. Find the eigenfunction for the ground state and first excited state of the SHO in position space using Hermite polynomials.

Eigenstates of the SHO can be expressed using Hermite polynomials. The n^{th} eigenstate is

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2} \qquad \text{where} \qquad \xi = \sqrt{\frac{m\omega}{\hbar}}\, x \tag{1}$$

and the H_n are Hermite polynomials. The first few Hermite polynomials are

$$\begin{aligned}
H_0(\xi) &= 1 \\
H_1(\xi) &= 2\xi \\
H_2(\xi) &= 4\xi^2 - 2 \\
H_3(\xi) &= 8\xi^3 - 12\xi \\
H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\
H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi \\
H_6(\xi) &= 64\xi^6 - 480\xi^4 + 720\xi^2 - 120 \\
H_7(\xi) &= 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi
\end{aligned}$$

Table 10 – 1. The First Eight Hermite Polynomials.

Hermite polynomials can be generated using the recurrence relation

$$H_{n+1}(\xi) = 2x\, H_n(\xi) - 2n\, H_{n-1}(\xi).$$

The Schrodinger equation in position space for the SHO is a naturally occurring form of Hermite's equation. The solutions to Hermite's equation are the Hermite polynomials. We will solve this differential equation thereby deriving the Hermite polynomials using a power series solution in part 2 of this chapter. Using equation (1) with the appropriate Hermite polynomial is likely the easiest way to obtain a position space eigenfunction for the quantum mechanical SHO.

$$\begin{aligned}
\psi_0(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^0\, 0!}} H_0\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} (1)\, e^{-m\omega x^2/2\hbar} \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}, \qquad \text{in agreement with our earlier calculation.}
\end{aligned}$$

$$\begin{aligned}
\psi_1(x) &= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^1\, 1!}} H_1\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2}}\, 2\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-m\omega x^2/2\hbar} \\
&= \left(\frac{4}{\pi}\left(\frac{m\omega}{\hbar}\right)^3\right)^{1/4} x\, e^{-m\omega x^2/2\hbar}, \qquad \text{also in agreement with our earlier calculation.}
\end{aligned}$$

Postscript: Hermite polynomials are not square integrable. The products of a Hermite polynomial and the Gaussian envelope $e^{-\xi^2/2}$ are, however, square integrable over all space so are acceptable wave functions. The constants $\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}$ are simply normalization constants.

The adjective form of Charles Hermite's name is Hermitian, as in Hermitian operator.

10–18. Show that $H_1(\xi)$ is orthogonal to $H_2(\xi)$.

The Hermite polynomials are orthogonal when both are weighted by $e^{-\xi^2/2}$.

Including the weighting functions, the orthogonality condition is

$$\int_{-\infty}^{\infty} H_1(\xi)\, e^{-\xi^2/2}\, H_2(\xi)\, e^{-\xi^2/2}\, d\xi \;=\; \int_{-\infty}^{\infty} 2\xi\left(4\xi^2-2\right) e^{-\xi^2}\, d\xi$$

$$=\; \int_{-\infty}^{\infty}\left(8\xi^3-4\xi\right) e^{-\xi^2}\, d\xi \;=\; 8\int_{-\infty}^{\infty}\xi^3\, e^{-\xi^2}\, d\xi - 4\int_{-\infty}^{\infty}\xi\, e^{-\xi^2}\, d\xi\,.$$

The integrands are both odd functions integrated between symmetric limits. The integrands are therefore, both zero, so their difference is zero. Since

$$\int_{-\infty}^{\infty} H_1(\xi)\, e^{-\xi^2/2}\, H_2(\xi)\, e^{-\xi^2/2}\, d\xi \;=\; 0, \qquad H_1(\xi) \text{ is orthogonal to } H_2(\xi)\,.$$

Postscript: This is a calculation for two specific Hermite polynomials. To show the Hermite polynomials are orthogonal in general, we need to show

$$|A|^2 \int_{-\infty}^{\infty} H_n(\xi)\; e^{-\xi^2/2}\, H_m(\xi)\, e^{-\xi^2/2}\, d\xi \;=\; \delta_{n,m}.$$

This calculation is done in Byron and Fuller[1], and other texts. The weighting function is necessary to demonstrate orthogonality which is a fact that is not always stated explicitly.

The infinite set of Hermite polynomials is complete. Table 10–1 shows that each successive $H_n(\xi)$ contains the successive power of ξ. This guarantees the uniqueness of the final expression of a polynomial function in terms of H_n because there is exactly one way to represent the highest power term of any given polynomial function. Any function (or eigenfunction) in polynomial space can be constructed from a linear combination of Hermite polynomials (see problem 5–5).

The infinite set of unit vectors is orthonormal and is complete. The infinite set of sines and cosines used for the infinite square well is orthogonal so can be made orthonormal and is complete. The infinite set of Hermite polynomials used for the SHO is orthogonal so can be made orthonormal and is complete. We will encounter infinite sets of associated Laguerre polynomials,

[1] Byron and Fuller *Mathematics of Classical and Quantum Physics* (Dover Publications, New York, 1970), pp 261-273.

Legendre functions, spherical harmonic functions, and other sets of polynomials and functions which are orthogonal so can be made orthonormal and are complete. Each of these infinite sets form a basis in the same sense as the unit vectors form a basis.

10–19. Sketch the first five eigenenergies on an energy versus position plot for an SHO potential. Then superimpose the first five eigenfunctions on corresponding eigenenergies on a similar plot. Finally, plot the probability densities of the first five eigenfunctions in the same manner.

Examine the three sketches that follow. The graphs for the wave functions and probability densities are larger in scale than that for the eigenenergies so that the barrier penetration outside of the SHO

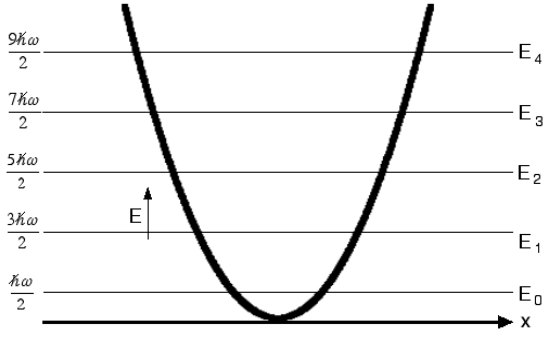

Figure 10–3. First five SHO eigenenergies.

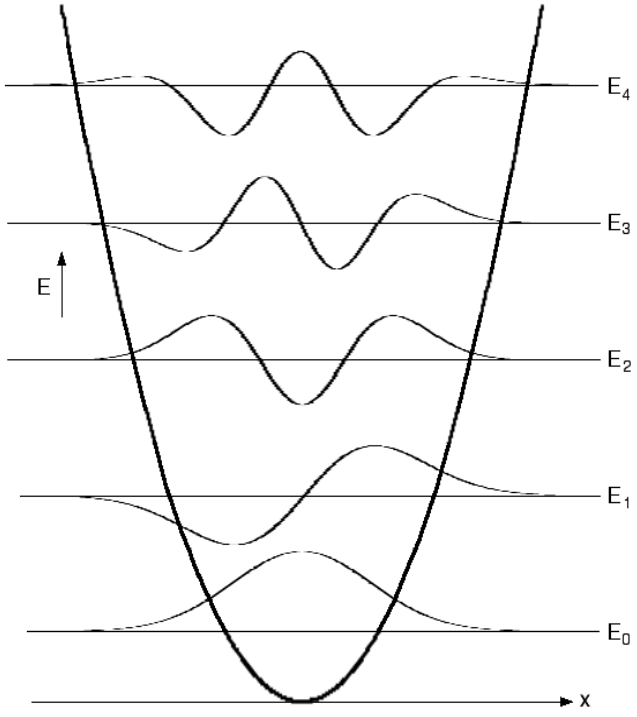

Figure 10–4. First five SHO eigenfunctions.

potential well can be seen. The eigenfunctions and probability densities are sketched at the level of the corresponding eigenenergy, however, each horizontal line represents zero amplitude in figures 10–4 and 10–5. Notice in all three figures that the ground state energy is $\hbar\omega/2$ above zero, but that the energy levels are evenly spaced by $\hbar\omega$ above E_0. Notice that the eigenfunctions do not have an amplitude of zero at the boundaries. The eigenfunctions approach zero asymptotically outside the potential well indicating regions of non-zero probability density outside the well, thus there is a finite probability of finding the particle outside of the well. There are locations inside the well where the probability density is zero for all wave functions except the ground state. Also, there are regions of maximal and minimal probability which differ in position for each eigenfunction.

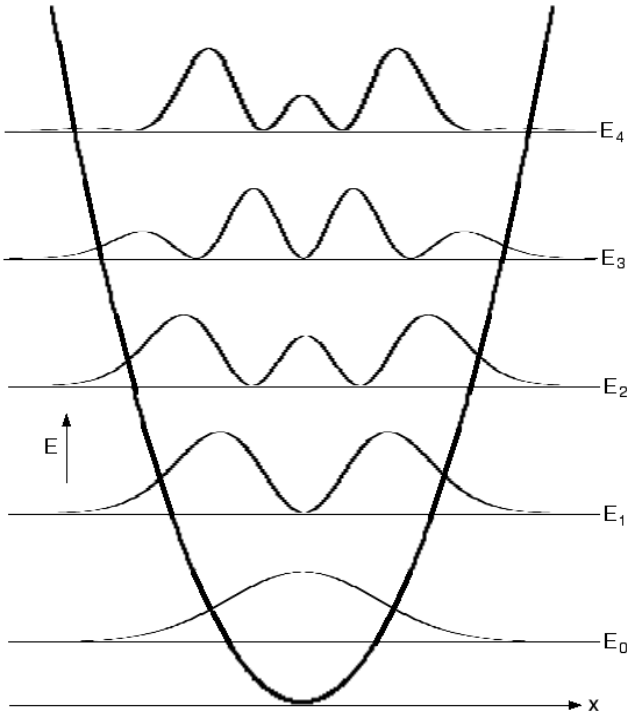

Figure 10–5. First five SHO probability densities.

Postscript: That there is a non-zero probability density outside the well is a feature of all but infinite, vertical potential energy walls. Barrier penetration, though not necessarily complete tunneling, is a quantum mechanical phenomenon expected for all realistic potential energy functions.

10–20. Sketch the linear combination $\Psi(x) = 2\psi_0(x) + \psi_1(x)$ for the SHO.

A general wave function of the SHO is a superposition or linear combination of its eigenfunctions,

$$\Psi(x) = c_0\psi_0(x) + c_1\psi_1(x) + c_2\psi_2(x) + c_3\psi_3(x) + \cdots = \sum_{n=0}^{\infty} c_n\psi_n(x), \quad \text{in general, or}$$

$$|\Psi> = c_0|0> + c_1|1> + c_2|2> + c_3|3> + \cdots = \sum_{n=0}^{\infty} c_n|n> \quad \text{for the SHO.}$$

Imagine two parts of the big lump that is the ground state minus the negative portion of the first excited state to the left of zero while adding the positive portion to the right of zero.

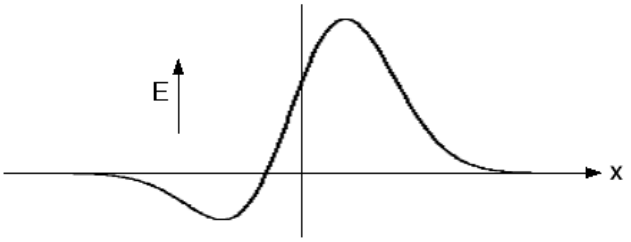

Figure 10–6. Sketch of $|\Psi> = 2|0> + |1>$ for SHO.

Postscript: The c_n are constants that provide the relative contributions of each eigenfunction. The c_n can be any scalars so $\Psi(x)$ can have any shape. As before, if the general wave function is normalized, $\left|\Psi(x)\right|^2 = 1$, the relative magnitudes of the c_n are fixed. Also as before, the orthogonality of the eigenfunctions of the SHO ensures that the c_n are unique.

Problems 10–21 through 10–27 use the linear combination of two eigenstates,

$$|\Psi> = A\Big[\,2|0> + 5|2>\Big],$$

which is the general linear combination of eigenstates for $c_0 = 2$, $c_2 = 5$, and all other $c_n = 0$.

10–21. (a) Normalize the wave function $|\Psi>$ using row and column vectors, and

(b) using Dirac notation.

(a) $$<\Psi|\Psi> = 1 \quad \Rightarrow \quad (2,\ 0,\ 5,\ 0,\ 0,\cdots)^*\, A^* A \begin{pmatrix} 2 \\ 0 \\ 5 \\ 0 \\ 0 \\ \vdots \end{pmatrix} = 1$$

$$\Rightarrow \quad (4+25)\left|A\right|^2 = 1 \quad \Rightarrow \quad A = \frac{1}{\sqrt{29}} \quad \Rightarrow \quad |\Psi> = \frac{1}{\sqrt{29}}\Big[\,2|0> + 5|2>\Big].$$

(b) $$<\Psi|\Psi> = 1 \quad \Rightarrow \quad \Big[<0|2^* + <2|5^*\Big]\, A^* A\Big[2|0> + 5|2>\Big] = 1$$

$$\Rightarrow \quad |A|^2\Big[4<0|0> + 10<0|2> + 10<2|0> + 25<2|2>\Big] = 1.$$

Orthonormality, $<i|j> = \delta_{ij} \Rightarrow <0|0> = <2|2> = 1$, and $<0|2> = <2|0> = 0$,

$$\Rightarrow \quad |A|^2\Big[4 + 25\Big] = 1 \quad \Rightarrow \quad A = \frac{1}{\sqrt{29}} \quad \Rightarrow \quad |\Psi> = \frac{1}{\sqrt{29}}\Big[\,2|0> + 5|2>\Big].$$

Postscript: The row and column vector representation is likely easier to visualize, but normalizing $A\left[\,5\,|\,0>\,+\,6\,|\,100>\,\right]$ or any large system using the row and column method would be awkward. Both of these approaches are significantly easier than the same calculation in position space that requires evaluation of at least two integrals.

A portion of the utility of abstract Hilbert space is that calculations are usually dramatically simpler than in any specific representation, such as position space. Abstract Hilbert space also allows maximum generality in that you can represent your work in any appropriate basis at any time. Working in Hilbert space until a representation is necessary is the norm. Without a reason to represent the results of the last calculation in any specific basis, it remains in Hilbert space.

10–22. Find the normalized wave function $|\,\Psi>$ in position space.

Use procedures similar to those seen in problem 10–17.

$$\psi_2\,(x) \;=\; \left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(2\,\frac{m\omega}{\hbar}\,x^2-1\right)e^{-m\omega x^2/\,2\hbar}$$

using table 10–1. Combining with the ground state from problem 10–17,

$$\begin{aligned}\Psi\,(x) \;&=\; \frac{1}{\sqrt{29}}\left[2\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-m\omega x^2/\,2\hbar}\;+\;5\left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\left(2\,\frac{m\omega}{\hbar}\,x^2-1\right)e^{-m\omega x^2/\,2\hbar}\right]\\ &=\; \frac{1}{\sqrt{29}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left[2\;+\;\frac{5\sqrt{2}}{2}\,\left(2\,\frac{m\omega}{\hbar}\,x^2-1\right)\right]e^{-m\omega x^2/\,2\hbar}.\end{aligned}$$

10–23. Calculate the probability of measuring $E\,=\,\dfrac{5}{2}\,\hbar\omega$ for the $|\,\Psi>$ given.

This is application of the eigenvalue and probability postulates. The only possible results of a measurement of energy are the eigenvalues $E_n\,=\,\left(n+\dfrac{1}{2}\right)\hbar\omega\,.$ The state vector contains only the two eigenstates $|\,n=0>$ and $|\,n=2>,$ so $E_0\,=\,\dfrac{1}{2}\,\hbar\omega$ and $E_2\,=\,\dfrac{5}{2}\,\hbar\omega$ are the only possible results. Then $P\,(E=E_n)\;=\;|\,<n\,|\,\Psi>\,|^{\,2}\,.$

$$\begin{aligned}P\,(E=E_2)\;&=\;\left|\;(0,\;0,\;1,\;0,\cdots)\;\frac{1}{\sqrt{29}}\begin{pmatrix}2\\0\\5\\0\\\vdots\end{pmatrix}\right|^2\\ &=\;\left|\;\frac{1}{\sqrt{29}}\,(0+0+5+0+\cdots)\right|^2\;=\;\left|\;\frac{5}{\sqrt{29}}\;\right|^2\;=\;\frac{25}{29}\,,\end{aligned}$$

using unit vector notation. The same calculation in Dirac notation looks like

$$P\,(E=E_2) \;=\; \big|\,<2\,|\,\Psi>\,\big|^2 \;=\; \left|\,<2\,|\,\frac{1}{\sqrt{29}}\Big(\,2\,|\,0>\;+\;5\,|\,2>\Big)\,\right|^2$$
$$=\;\frac{1}{29}\big|\,2\,<2\,|\,0>\;+\;5\,<2\,|\,2>\,\big|^2 \;=\; \frac{1}{29}\big|\,5\,\big|^2 \;=\; \frac{25}{29}\,,$$

where the inner products are $<i\,|\,j> \;=\; \delta_{ij}\,,$ meaning $<2\,|\,0> \;=\; 0$ and $<2\,|\,2> \;=\; 1\,.$

10–24. Calculate the expectation value of energy for the $|\,\Psi>$ given.

This problem demonstrates the calculation using matrix and Dirac notation. The calculation using the position space representations is written, though not completed, in the postscript to demonstrate the relative degree of difficulty.

$$<E> \;=\; <\mathcal{H}>_\psi \;=\; <\psi\,|\,\mathcal{H}\,|\,\psi> \;=\frac{1}{\sqrt{29}}\,\big(\,2,\;0,\;5,\;\cdots\big)^*\begin{pmatrix}\frac{1}{2} & 0 & 0 & \cdots\\ 0 & \frac{3}{2} & 0 & \cdots\\ 0 & 0 & \frac{5}{2} & \cdots\\ \vdots & \vdots & \vdots & \ddots\end{pmatrix}\hbar\omega\,\frac{1}{\sqrt{29}}\begin{pmatrix}2\\0\\5\\\vdots\end{pmatrix}$$

$$=\;\frac{\hbar\omega}{29}\,\big(\,2,\;0,\;5,\;\cdots\big)\begin{pmatrix}\frac{1}{2}\,(2)\\ \\ \frac{3}{2}\,(0)\\ \\ \frac{5}{2}\,(5)\\ \\ \vdots\end{pmatrix} \;=\; \frac{\hbar\omega}{29}\left(2+\frac{125}{2}\right) \;=\; \frac{129}{58}\,\hbar\omega\,.$$

The same calculation in Dirac notation using the direct action of the Hamiltonian is

$$\begin{aligned}
<E> \;&=\; <\psi\,|\,\mathcal{H}\,|\,\psi>\\
&=\; \left[\frac{1}{\sqrt{29}}\,\big(\,<0\,|\,2^*\;+\;<2\,|\,5^*\big)\right]\,\mathcal{H}\,\left[\frac{1}{\sqrt{29}}\,\big(\,2\,|\,0>\;+\;5\,|\,2>\big)\right] && (1)\\
&=\; \frac{1}{29}\Big[\;<0\,|\,2\;+\;<2\,|\,5\Big]\left[\,2\left(\frac{1}{2}\,\hbar\omega\right)\,|\,0>\;+\;5\left(\frac{5}{2}\,\hbar\omega\right)\,|\,2>\right] && (2)\\
&=\; \frac{1}{29}\left[\,2\cdot 2\cdot\left(\frac{1}{2}\,\hbar\omega\right)<0\,|\,0>\;+\;5\cdot 5\cdot\left(\frac{5}{2}\,\hbar\omega\right)<2\,|\,2>\right] && (3)\\
&=\; \frac{\hbar\omega}{29}\left[\,2\;+\;\frac{125}{2}\,\right] \;=\; \frac{129}{58}\,\hbar\omega,
\end{aligned}$$

where the Hamiltonian operating to the right on the two eigenstates in equation (1) results in the energy eigenvalues times the corresponding eigenstate in equation (2). The orthonormality of eigenstates results in equation (3) where the inner product of terms that are known to be zero are

excluded. Excluding known zeros is the norm, and in fact, inner products such as $<0\,|\,0>$ and $<2\,|\,2>$ that are known to be one are normally not explicitly written.

Postscript: The calculation of expectation value for the given $|\,\Psi>$ in position space would be

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{29}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left[2 + \frac{5\sqrt{2}}{2}\left(2\,\frac{m\omega}{\hbar}\,x^2 - 1\right)\right] e^{-m\omega x^2/\,2\hbar} \left[\frac{1}{2m}\left(-i\hbar\,\frac{d}{dx}\right)^2 + \frac{1}{2}\,kx^2\right]$$

$$\times\ \frac{1}{\sqrt{29}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left[2 + \frac{5\sqrt{2}}{2}\left(2\,\frac{m\omega}{\hbar}\,x^2 - 1\right)\right] e^{-m\omega x^2/\,2\hbar}\,dx\,,$$

which is intended only as a statement that matrix methods and Dirac notation may be worthwhile.

10–25. Calculate the expectation value of energy for the $|\,\Psi>$ given using the ladder operator representation of the Hamiltonian.

This problem is an explicit example of ladder operators calculations. It is not the easiest way to calculate an expectation value. The ladder operators though, are prototypes for the creation and annihilation operators used in field theoretic descriptions of photons, electrons, phonons, etc. In other words, the raising and lowering operators become increasingly important as you progress.

$\mathcal{H} \;=\; \left(a^\dagger a \;+\; \frac{1}{2}\right)\hbar\omega\,, \qquad a^\dagger\,|\,n> \;=\; \sqrt{n+1}\,|\,n+1>\,, \qquad a\,|\,n> \;=\; \sqrt{n}\,|\,n-1>\,,$ and

$<E> \;=\; <\psi\,|\,\mathcal{H}\,|\,\psi>$ are relations used in this problem.

$$\begin{aligned}
<E> \;&=\; \left[\frac{1}{\sqrt{29}}\left(<0\,|\,2^* \;+\; <2\,|\,5^*\right)\right]\left[\left(a^\dagger a + \frac{1}{2}\right)\hbar\omega\right]\left[\frac{1}{\sqrt{29}}\left(2\,|\,0> \;+\; 5\,|\,2>\right)\right] \\
&=\; \frac{\hbar\omega}{29}\Big[\,2<0|\;+\;5<2|\,\Big]\left[2\,a^\dagger a\,|\,0> \;+\; 5\,a^\dagger a\,|\,2> \;+\; \frac{2}{2}\,|\,0> \;+\; \frac{5}{2}\,|\,2>\right] \\
&=\; \frac{\hbar\omega}{29}\Big[\,2<0|\;+\;5<2|\,\Big]\left[2\,\cancel{a^\dagger}\,\vec{0} \;+\; 5\,a^\dagger\sqrt{2}\,|\,1> \;+\; |\,0> \;+\; \frac{5}{2}\,|\,2>\right] \qquad (1) \\
&=\; \frac{\hbar\omega}{29}\Big[\,2<0|\;+\;5<2|\,\Big]\left[5\sqrt{2}\cdot\sqrt{2}\,|\,2> \;+\; |\,0> \;+\; \frac{5}{2}\,|\,2>\right]
\end{aligned}$$

As before, the raising operator acting on the zero vector is zero so that term is struck in equation (1). The only non-zero contributions are from the $<0\,|\,0>$ and $<2\,|\,2>$ terms since these inner products are 1, the $<0\,|\,2>$ and $<2\,|\,0>$ products are 0, therefore,

$$<E> = \frac{\hbar\omega}{29}\left[2<0\,|\,0> + 5\cdot5\cdot2<2\,|\,2> + 5\cdot\frac{5}{2}<2\,|\,2>\right] = \frac{\hbar\omega}{29}\left[2 + 5\cdot5\cdot2 + 5\cdot\frac{5}{2}\right] = \frac{129}{58}\,\hbar\omega.$$

10–26. Express the state of the system described by $|\Psi>$ at time t,

(a) in Hilbert space in terms of the abstract $|n>$'s,

(b) in position space in terms of the $\psi_n(x)$'s,

(c) in momentum space in terms of the $\widehat{\psi}_n(p)$'s, and

(d) in energy space in terms of the $\widetilde{\psi}_n(E)$'s.

Do not evaluate the specific $|n>$'s, $\psi_n(x)$'s, $\widehat{\psi}_n(p)$'s, or $\widetilde{\psi}_n(E)$'s.

Stationary state time dependence is

$$|\psi(t)> = \sum_n^\infty |n><n|\psi(0)>\, e^{-iE_nt/\hbar} \quad \text{where} \quad |\psi(0)> = \frac{1}{\sqrt{29}}\Big[2|0> + 5|2>\Big] \quad \text{here.}$$

$$\text{(a)} \quad |\psi(t)> = \frac{1}{\sqrt{29}}\Big[|0><0|\Big(2|0>+5|2>\Big)e^{-iE_0t/\hbar} + |2><2|\Big(2|0>+5|2>\Big)e^{-iE_2t/\hbar}\Big]$$

$$= \frac{1}{\sqrt{29}}\Big[|0>\Big(2<0|0>+5<0\not{|}2>,\Big)e^{-iE_0t/\hbar} + |2>\Big(2<2\not{|}0> + 5<2|2>\Big)e^{-iE_2t/\hbar}\Big]$$

$$= \frac{1}{\sqrt{29}}\Big[2\,e^{-iE_0t/\hbar}|0> + 5\,e^{-iE_2t/\hbar}|2>\Big]$$

retaining only the non-zero terms. Using the eigenenergies $E_n = \big(n+\frac{1}{2}\big)\hbar\omega$,

$$|\psi(t)> = \frac{1}{\sqrt{29}}\Big[2|0>e^{-i\omega t/2} + 5|2>e^{-i5\omega t/2}\Big].$$

Parts (b) through (d) require only operation on both sides of this equation with the appropriate bra so are essentially exercises in notation.

(b) Remembering that $<x|\psi(t)> = \psi(x,t)$,

$$<x|\psi(t)> = \frac{1}{\sqrt{29}}\Big[2<x|0>e^{-i\omega t/2} + 5<x|2>e^{-i5\omega t/2}\Big]$$

$$\Rightarrow \quad \psi(x,t) = \frac{1}{\sqrt{29}}\Big[2\,\psi_0(x)\,e^{-i\omega t/2} + 5\,\psi_2(x)\,e^{-i5\omega t/2}\Big].$$

(c) To transition to momentum space, $<p|\psi(t)> = \widehat{\psi}(p,t)$,

$$<p|\psi(t)> = \frac{1}{\sqrt{29}}\Big[2<p|0>e^{-i\omega t/2} + 5<p|2>e^{-i5\omega t/2}\Big]$$

$$\Rightarrow \quad \widehat{\psi}(p,t) = \frac{1}{\sqrt{29}}\Big[2\,\widehat{\psi}_0(p)\,e^{-i\omega t/2} + 5\,\widehat{\psi}_2(p)\,e^{-i5\omega t/2}\Big].$$

(d) To find the wave function in energy space, remember that $<E\,|\,\psi\,(t)> \;=\; \widetilde{\psi}\,(E,t)\,,$

$$<E\,|\,\psi\,(t)> \;=\; \frac{1}{\sqrt{29}}\left[\,2\,<E\,|\,0>\;e^{-i\omega t/2} \;+\; 5\,<E\,|\,2>\;e^{-i5\omega t/2}\,\right]$$

$$\Rightarrow \quad \widetilde{\psi}\,(E,t) \;=\; \frac{1}{\sqrt{29}}\left[\,2\,\widetilde{\psi}_0\,(E)\,e^{-i\omega t/2} \;+\; 5\,\widetilde{\psi}_2\,(E)\,e^{-i5\omega t/2}\,\right].$$

10–27. Calculate the probability of measuring $E \,=\, \dfrac{5}{2}\,\hbar\omega$ at time t for the $|\,\Psi>$ given.

Likely the best choice of representation is the abstract state vector. You will find that the same calculation is much more arduous in position space in one of the exercises at the end of this part. Remember that the square of a magnitude is the product of the complex conjugates.

Since the state vector is normalized, probability is $P\,(E=E_n) \;=\; |<n\,|\,\psi\,(t)>|^2\,,$ then

$$\begin{aligned} P\,(E=E_2) \;&=\; \left|\,<2\,|\,\frac{1}{\sqrt{29}}\left[\,2\,|\,0>\,e^{-i\omega t/2} \;+\; 5\,|\,2>\,e^{-i5\omega t/2}\right]\,\right|^2 \\ &=\; \frac{1}{29}\Big|\,2\;<2\!\not|\,0>\,e^{-i\omega t/2} \;+\; 5\;<2\,|\,2>\,e^{-i5\omega t/2}\,\Big|^2, \end{aligned}$$

where the first term is struck because the eigenstates of the SHO are orthonormal so the inner product of unlike vectors is zero. Orthonormality also means that $<2\,|\,2> \;=\; 1\,.$ Then

$$P\,(E=E_2) \;=\; \frac{1}{29}\left|\,5\,e^{-i5\omega t/2}\,\right|^2 \;=\; \frac{1}{29}\Big(5\,e^{i5\omega t/2}\Big)\Big(5\,e^{-i5\omega t/2}\Big) \;=\; \frac{1}{29}\Big(25\,e^{0}\Big) \;=\; \frac{25}{29}\,,$$

necessarily identical to the time independent case for all stationary state probability calculations.

Postscript: This problem ends this sequence.

10–28. Calculate $<\mathcal{P}>$ using the SHO state vector

$$|\,\Phi\,(t)> \;=\; \frac{1}{\sqrt{30}}\left[\,2\,|\,0>\,e^{-i\omega t/2} \;+\; |\,1>\,e^{-i3\omega t/2} \;+\; 5\,|\,2>\,e^{-i5\omega t/2}\,\right].$$

Time never appears in any probability of a stationary state. The exponential stationary state time dependence does affect other calculations, however, such as an expectation value of a dynamic variable. We use $<\mathcal{P}> \;=\; <\Phi\,(t)\,|\,\mathcal{P}\,|\,\Phi\,(t)>$ to demonstrate both (a) vector/matrix operator and (b) Dirac notation/ladder operator calculation of a time-dependent expectation value. The principles are the same for $<\mathcal{H}>\,,$ $<\mathcal{X}>\,,$ and $<m\omega^2\mathcal{X}^2/2>\,,$ or other classically dynamical variables. This calculation using the two-dimensional $|\,\Psi>$ of the last six problems presents too many zeros to be a good example, thus the three-dimensional $|\,\Phi>\,.$

(a) Using the matrix operator representation of $\mathcal{P}$ for the SHO given earlier,

$$<\mathcal{P}> = <\Phi(t)\,|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{4} & 0 & -\sqrt{5} & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}\frac{1}{\sqrt{30}}\begin{pmatrix} 2e^{-i\omega t/2} \\ e^{-i3\omega t/2} \\ 5e^{-i5\omega t/2} \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$$

$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(2\,e^{+i\omega t/2},\ e^{+i3\omega t/2},\ 5\,e^{+i5\omega t/2},\ 0,\cdots\right)\begin{pmatrix} -e^{-i3\omega t/2} \\ 2\,e^{-i\omega t/2} - 5\sqrt{2}\,e^{-i5\omega t/2} \\ \sqrt{2}\,e^{-i3\omega t/2} \\ 5\sqrt{3}\,e^{-i5\omega t/2} \\ \vdots \end{pmatrix}$$

$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(-2\,e^{-i\omega t} \ + \ 2\,e^{+i\omega t} \ - \ 5\sqrt{2}\,e^{-i\omega t} \ + \ 5\sqrt{2}\,e^{+i\omega t} \ + \ 0\right)$$

$$= \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2} 2i\left(2\frac{(e^{+i\omega t} - e^{-i\omega t})}{2i} \ + \ 5\sqrt{2}\,\frac{(e^{+i\omega t} - e^{-i\omega t})}{2i}\right)$$

$$= -\frac{1}{15}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(2\sin(\omega t) \ + \ 5\sqrt{2}\sin(\omega t)\right) \ = \ -\left(\frac{2+5\sqrt{2}}{15}\right)\left(\frac{m\omega\hbar}{2}\right)^{1/2}\sin(\omega t)\,.$$

(b) The momentum operator is $\mathcal{P} \ = \ i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^\dagger - a)$ in terms of the ladder operators, so

$$\begin{aligned} <\mathcal{P}> \ &= \ <\Phi(t)\,\big|\,\mathcal{P}\,\big|\Phi(t)> \\ &= \ <\Phi(t)\,\big|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(a^\dagger - a)\big|\frac{1}{\sqrt{30}}\left(2\,|\,0>e^{-i\omega t/2} \ + \ |\,1>e^{-i3\omega t/2} \ + \ 5\,|\,2>e^{-i5\omega t/2}\right) \\ &= \ <\Phi(t)\,\big|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{1}{\sqrt{30}}\Big(2\,a^\dagger\,|\,0>e^{-i\omega t/2} \ - \ 2\,a\,|\,0>e^{-i\omega t/2} \ + \ a^\dagger\,|\,1>e^{-i3\omega t/2} \\ &\qquad\qquad - \ a\,|\,1>e^{-i3\omega t/2} \ + \ 5\,a^\dagger\,|\,2>e^{-i5\omega t/2} \ - \ 5\,a\,|\,2>e^{-i5\omega t/2}\Big) \end{aligned}$$

$$= \; <\Phi\,(t)\,|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{1}{\sqrt{30}}\Big(2\sqrt{1}\,|\,1>e^{-i\omega t/2} \;-\; 0 \;+\; \sqrt{2}\,|\,2>e^{-i3\omega t/2} \;-\; \sqrt{1}\,|\,0>e^{-i3\omega t/2}$$
$$+\; 5\sqrt{3}\,|\,3>e^{-i5\omega t/2} \;-\; 5\sqrt{2}\,|\,1>e^{-i5\omega t/2}\Big)$$

$$= \; <\Phi\,(t)\,|\,i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{1}{\sqrt{30}}\Big(-\;\;|\,0>e^{-i3\omega t/2} \;+\; |\,1>\Big[\,2\,e^{-i\omega t/2}-5\sqrt{2}\,e^{-i5\omega t/2}\,\Big]$$
$$+\;\;|\,2>\sqrt{2}\,e^{-i3\omega t/2} \;+\; |\,3>5\sqrt{3}\,e^{-i5\omega t/2}\Big)$$

$$= \; \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big(2<0\,|\,e^{+i\omega t/2}+\;<1\,|\,e^{+i3\omega t/2} \;+\; 5<2\,|\,e^{+i5\omega t/2}\Big) \;\times$$

$$\Big(\,|\,0>\Big[-e^{-i3\omega t/2}\Big]+|\,1>\Big[2e^{-i\omega t/2}-5\sqrt{2}\,e^{-i5\omega t/2}\Big]+|\,2>\Big[\sqrt{2}\,e^{-i3\omega t/2}\Big]+|\,3>\Big[5\sqrt{3}\,e^{-i5\omega t/2}\Big]\,\Big)$$

$$= \; \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2}\Big(-2e^{-i\omega t} \;+\; 2\,e^{+i\omega t} \;-\; 5\sqrt{2}\,e^{-i\omega t} \;+\; 5\sqrt{2}\,e^{+i\omega t}\Big) \qquad (1)$$

$$= \; \frac{i}{30}\left(\frac{m\omega\hbar}{2}\right)^{1/2} 2i\left(2\,\frac{(e^{+i\omega t}-e^{-i\omega t})}{2i} \;+\; 5\sqrt{2}\,\frac{(e^{+i\omega t}-e^{-i\omega t})}{2i}\right)$$

$$= \; -\left(\frac{2+5\sqrt{2}}{15}\right)\;\left(\frac{m\omega\hbar}{2}\right)^{1/2}\sin\,(\omega t\,)\,.$$

Postscript: This calculation is made shorter by dropping all but the $|\,0>,\;\;|\,1>$, and $|\,2>$ terms right after letting the ladder operators act. Only these terms will survive when the inner products are calculated. Orthonormality of eigenstates is used to obtain equation (1) though other economies are ignored in order to show the new "machinery" explicitly in this example.

Exercises

10–29. Show that the time-independent Schrodinger equation for the SHO can be written

$$\hbar\omega\left(a\,a^{\dagger}-\frac{1}{2}\right)\,|\,\psi>\;=\;E_n\,|\,\psi>\;.$$

Practice in operator algebra using the raising and lowering operators. See problem 10–2.

10–30. Show that a and $a^{\dagger}$ are not Hermitian.

More practice using the raising and lowering operators. Does $a^{\dagger}\;=\;a\,?$ Assuming that these operators are Hermitian leads to a straightforward proof by contradiction.

10–31. Show that $\mathcal{H}\,a\;=\;a\,\mathcal{H}\;-\;a\hbar\omega\,.$

Parallel problem 10–4. Start with the $\mathcal{H}$ of exercise 10–29.

10–32. Normalize $a\,|\,n>\;=\;C\,(n)\,|\,n-1>\,.$

See problem 10–10. The answer is in the postscript.

10–33. Show that $\mathcal{H}\,|\,2>\;=\;\frac{5}{2}\,\hbar\omega\,|\,2>$ by explicit matrix multiplication.

Use the unit vector $|\,2>$ and matrix representation of $\mathcal{H}$ given in problem 10–12.

10–34. Express the matrix elements

(a) $<n\,|\,a\,|\,m>\,,$
(b) $<n\,|\,a^{\dagger}|\,m>\,,$
(c) $<n\,|\,\mathcal{X}\,|\,m>\,,$
(d) $<n\,|\,\mathcal{P}\,|\,m>\,,$ and
(e) $<n\,|\,\mathcal{H}\,|\,m>\,,$ in terms of quantum numbers and Kronecker deltas.

The condition of orthonormality, $<i\,|\,j> = \delta_{i,\,j}$, can also be expressed $<n\,|\,m-1> = \delta_{n,\,m-1}$. The action of $a^\dagger$ on a general ket $|\,m>$ is given by $a^\dagger|\,m> = \sqrt{m+1}\,|\,m+1>$. Then consider the inner product with the bra $<n\,|$ to obtain

$$<n\,|\,a^\dagger|\,m> \;=\; <n\,|\sqrt{m+1}\,|\,m+1> \;=\; \sqrt{m+1}\,<n\,|\,m+1> \;=\; \sqrt{m+1}\,\delta_{n,\,m+1}\,.$$

In other words, $<n\,|\,a^\dagger|\,m> = \sqrt{m+1}$ for $n = m+1$, and $<n\,|\,a^\dagger|\,m> = 0$ otherwise. Part (b) is now done for you. Part (a) is done in problem 10–13. Problems 10–2, 10–12, and 10–14 may be helpful. The $\mathcal{X}$, $\mathcal{P}$, and $\mathcal{H}$ operators can be expressed in terms of the ladder operators. You should find

$$<n\,|\,\mathcal{X}\,|\,m> \;=\; \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(\sqrt{m}\;\delta_{n,\,m-1} \;+\; \sqrt{m+1}\;\delta_{n,\,m+1}\right) \quad \text{for instance.}$$

10–35. Use the results of the previous exercise to calculate the matrix elements

(a) $<7\,|\,a\,|\,8>$,
(b) $<7\,|\,a^\dagger|\,8>$,
(c) $<7\,|\,\mathcal{X}\,|\,8>$,
(d) $<7\,|\,\mathcal{P}\,|\,8>$, and
(e) $<14\,|\,\mathcal{H}\,|\,14>$.

This exercise illustrates that it may be useful to have skills with Kronecker deltas per exercise 10–34. One line suffices for each part. This process may negate the need to build a large matrix.

10–36. (a) Use the result of part (b) of exercise 10–34 to develop the matrix representation of the raising operator for the SHO.

(b) Use the result of part (d) of exercise 10–34 to develop the matrix representation of the momentum operator for the SHO.

If you have successfully navigated the last two exercises, using $<n\,|\,a^\dagger\,|\,m> = \sqrt{m+1}\,\delta_{n,\,m+1}$ to create the matrix operator $a^\dagger$ and $<n\,|\,\mathcal{P}\,|\,m> = i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(\sqrt{m+1}\,\delta_{n,\,m+1} - \sqrt{m}\,\delta_{n,\,m-1}\right)$ to obtain the matrix form of $\mathcal{P}$ should be straightforward. Remember that since 0 is an acceptable quantum number for an SHO potential energy function, the upper left element of pertinent matrices is row 0, column 0; rather than row 1, column 1 as it is in most other matrix operators. Problem 10–13 provides the answer for part (a), and problem 10–14 provides the answer to part (b).

Exercises 10–37 through 10–45 concern a particle in an SHO potential that is initially in the state

$$|\,\psi\,(t=0)> \;=\; N\,[\,3\,|\,0> \;+\; 2\,|\,1> \;+\; 1\,|\,5>]\,.$$

10–37. Calculate the normalization constant using

(a) row and column vectors, and

(b) Dirac notation.

See problem 10–21.

10–38. Energy is measured at $t = 0$.

(a) What results are possible and what is the probability of each possibility?

(b) Calculate probabilities using row and column vectors.

(c) Calculate probabilities using Dirac notation.

Apply the eigenvalue postulate for part (a), and the probability postulate for parts (b) and (c). See problem 10–23.

10–39. Find the expectation value $<E>$.

Use the matrix representation of the Hamiltonian derived in problem 10–12. It is convenient to work in the six by six subspace that includes all of the non-zero elements of the given wave function. No other dimensions will contribute. Problem 10–24 should also be helpful.

10–40. Find the uncertainty of energy.

Remember that $\triangle E = \sqrt{<\psi|\,(\mathcal{H}-<\mathcal{H}>)^2\,|\psi>}$. Multiply $<\mathcal{H}>$ from the previous exercise by the identity matrix to obtain the matrix form of $<\mathcal{H}>$. Subtract this from $\mathcal{H}$ and square the result. You should find

$$(\mathcal{H} - <\mathcal{H}>)^2 = \begin{pmatrix} \frac{81}{196} & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & \frac{25}{196} & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & \frac{361}{196} & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & \frac{1089}{196} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \frac{2209}{196} & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \frac{3721}{196} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \hbar^2\omega^2 .$$

Next calculate $\triangle E^2 = <\psi|\,(\mathcal{H} - <\mathcal{H}>)^2\,|\psi>$, and take the square root to find

$$\triangle E = \sqrt{<\psi|\,(\mathcal{H} - <\mathcal{H}>)^2\,|\psi>} = \sqrt{\frac{325}{196}\hbar^2\omega^2} \approx 1.288\,\hbar\omega .$$

10–41. Verify the results of the last two exercises by calculating

$$\text{(a)} \quad <E> \;=\; \sum_i P(E_i)\, E_i \qquad \text{and} \qquad \text{(b)} \quad \triangle E \;=\; \sqrt{\sum_i P(E_i)\left[\, E_i - <E> \,\right]^2}\,.$$

Another way to get $<E>$, also denoted $<\mathcal{H}>$, is to multiply each of the possible eigenvalues by the probability of measuring that eigenvalue and add the products. Calculating uncertainty using probabilities is common. Of course, you must obtain the same answers.

10–42. Sketch your calculated probabilities $P(E_i)$ versus E. Show your expectation value and uncertainty on the plot. Explain how the expectation value and the uncertainty are related to the outcome of a series of energy measurements.

The range of probability is 0 to 1 on the vertical axis. Use units of $\hbar\omega$ on the horizontal axis. The requested graph has only three discrete spikes at the energies of the eigenvalues, a discrete value at $<E>$, and a lower and upper limit for $\triangle E$. Expectation value is simply a weighted average, and uncertainty is simply a measure of spread. Where should these be located on a graph with three discrete values of different heights?

10–43. Calculate the state of the system at time t. Express your answer

(a) in the Hilbert space in terms of the abstract $|\,n>$'s,

(b) in position space in terms of the $\psi_n(x)$'s,

(c) in momentum space in terms of the $\widehat{\psi}_n(p)$'s, and

(d) in energy space in terms of the $\widetilde{\psi}_n(E)$'s.

Do not evaluate the specific $|\,n>$'s, $\psi_n(x)$'s, $\widehat{\psi}_n(p)$'s, or $\widetilde{\psi}_n(E)$'s.

This exercise is designed to help you assimilate the notation of quantum mechanics using an SHO state vector as a vehicle. It is largely an exercise in notation. This exercise is asking only for the form of the state vector in different spaces. See problem 10–26.

10–44. Calculate the time-dependent expectation values

(a) $<\mathcal{H}>$,
(b) $<\mathcal{P}>$,
(c) $<\mathcal{X}>$,
(d) $<\mathcal{P}^2/2m>$,
(e) $<m\omega^2\mathcal{X}^2/2>$.

This exercise demonstrates that the factor $e^{-iE_nt/\hbar}$ can be consequential for stationary states when describing dynamic variables. There are multiple options to calculate the five expectation

values. Matrix arguments are likely the most straightforward. Part (a) is $< \psi(t) \,|\, \mathcal{H} \,|\, \psi(t) >$ where $\mathcal{H}$ is seen in problem 10–12. In ket form, the state vector is

$$\psi(t) \;=\; \frac{1}{\sqrt{14}} \begin{pmatrix} 3\, e^{-i\omega t/2} \\ 2\, e^{-i3\omega t/2} \\ 0 \\ 0 \\ 0 \\ e^{-i11\omega t/2} \\ \vdots \end{pmatrix} .$$

$< \mathcal{H} >$ is independent of time and the same as previously calculated. You should find that $< \mathcal{P}^2/2m > \;=\; < m\omega^2 \mathcal{X}^2/2 > \;=\; 4\hbar\omega/\,7\,.$ You will also find

$$< \mathcal{P} > \;=\; -\,\frac{6}{7} \left(\frac{m\hbar\omega}{2} \right)^{1/2} \sin(\omega t) \qquad \text{and} \qquad < \mathcal{X} > \;=\; \frac{6}{7} \left(\frac{\hbar}{2m\omega} \right)^{1/2} \cos(\omega t)$$

See problems 10–14 and 10–28.

10–45. (a) Show that this state vector obeys the quantum mechanical virial theorem for the SHO, which states that the expectation value of the kinetic energy is equal to the expectation value of the potential energy, $< T > \;=\; < V >$.

(b) Show that your values of $< T >$ and $< V >$ are consistent with previous calculations of $< E >$.

The general virial theorem is deeper than the statement given here, but this is a simple example that the expectation value of the kinetic energy will equal the expectation value of the potential energy. Examine the parts (d) and (e) of the last exercise. If you can recognize kinetic and potential energy in those expectation values, you have essentially completed both parts (a) and (b). Part (b) means that the expectation values of kinetic and potential energies must sum to the expectation value of the total energy which you have from exercise 10–39.

This is the final exercise in this sequence.

10–46. (a) Write the time-independent Schrodinger equation for the SHO in position space, and

(b) in momentum space.

This is primarily an exercise in notation and representation. The time-independent Schrodinger equation is $\mathcal{H} \,|\, \psi > \;=\; E \,|\, \psi >$ in abstract Hilbert space, where the Hamiltonian is the total energy operator $\mathcal{H} \;=\; \mathcal{T} \;+\; \mathcal{V}$. Remember that in position space,

$$\mathcal{P} \;\rightarrow\; -i\hbar \frac{\partial}{\partial x}\,, \qquad \mathcal{X} \;\rightarrow\; x\,, \qquad \text{and} \qquad < x \,|\, \psi > \;\rightarrow\; \psi(x)\,,$$

$$\text{and in momentum space,} \quad \mathcal{P} \;\rightarrow\; p\,, \qquad \mathcal{X} \;\rightarrow\; i\hbar \frac{\partial}{\partial p}\,, \qquad \text{and} \qquad < p \,|\, \psi > \;\rightarrow\; \widehat{\psi}(p)\,.$$

10–47. Find the ground state energy for a 1 gram mass on a $k = 0.1\,N/m$ spring. Calculate the approximate quantum number of this oscillator if its energy is $k_BT/2$ where $T = 300\,K$ and k_B is Boltzmann's constant. At what temperature would this oscillator be in its ground state?

This numerical problem should give you some appreciation of the magnitudes involved. Ground state energy, also known as zero point energy, means $n = 0$ for an SHO. You should find that the ground state energy is on the order of $10^{-34}\,J$ for this system, and that ground state temperature is on the order of $10^{-11}\,K$. $T = 300\,K$ is approximately room temperature where the quantum number is just less than 2×10^{12}. Notice that n is inversely proportional to $\hbar\omega$ to calculate the quantum number at large n, *i.e.*, at 300 K. MKS units are likely easiest given that the spring constant is in N/m. $k_B = 1.38 \times 10^{-23}\,J/K$ and $\hbar = 1.06 \times 10^{-34}\,J \cdot s$ in MKS units. The assumption that the energy is $k_BT/2$ is a statement of the equipartition theorem[2]. Finally, remember that $\omega = \sqrt{k/m}$, $E = k_BT/2$, and $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$.

10–48. (a) Find $\psi_2(x)$ for the SHO using the Hermite polynomials given in Table 10–1.

(b) Verify this eigenfunction using the generating function of problem 10–16.

Hermite polynomials are well known so part (a) is likely an easier method to obtain an excited state of the SHO in position space than using the generating function. The eigenfunction $\psi_2(x)$ is given in problem 10–22. Use the procedures of problem 10–17 to obtain this.

Problems 10–15 and 10–16 address the generating function for part (b). The generating function for the second excited state in position space is

$$\psi_2(y) = \frac{1}{\sqrt{2!}}\left(\frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)\right)^2\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-y^2/2} = \frac{1}{2\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(y - \frac{d}{dy}\right)^2 e^{-y^2/2}.$$

The two terms in the operator $\left(y - \frac{d}{dy}\right)^2$ do not commute. The operator can be applied as

$$\left(y - \frac{d}{dy}\right)\left(y - \frac{d}{dy}\right) \quad \text{or} \quad y^2 - y\frac{d}{dy} - \frac{d}{dy}y + \frac{d}{dy}\frac{d}{dy}, \quad \text{but not as} \quad y^2 - 2y\frac{d}{dy} - \frac{d^2}{dy^2}.$$

Remember that $y = \sqrt{\frac{m\omega}{\hbar}}\,x$ to obtain the final form. Parts (a) and (b) must agree, of course.

10–49. Show that $H_1(\xi)$ is orthogonal to $H_3(\xi)$ when both are weighted with the factor $e^{-\xi^2/2}$.

To be useful for quantum mechanics, a basis must be orthonormal. If the basis is orthogonal, it can be made orthonormal. The intent of this problem is to demonstrate orthogonality for a selected pair of Hermite polynomials. When weighted by $e^{-\xi^2/2}$, the recurrence relation immediately

[2] Atkins *Quanta* (Oxford University Press, Oxford, 1991), pp 111-112.

below table 10–1 leads to a differential equation that is self-adjoint and the solutions to a self-adjoint differential equation are orthogonal[3]. Byron and Fuller show by methods of integration that Hermite polynomials are orthogonal in general when weighted by $e^{-\xi^2/2}$ per footnote 1.

Like problem 10–18, weighting each Hermite polynomial by $e^{-\xi^2/2}$ means to multiply both $H_1(\xi)$ and $H_3(\xi)$ by $e^{-\xi^2/2}$ in the orthogonality condition which may be written

$$\int_{-\infty}^{\infty} H_1(\xi)\, e^{-\xi^2/2}\, H_3(\xi)\, e^{-\xi^2/2}\, d\xi\,.$$

This results in a difference of two integrals that are both even. These are equal to twice the same integrand from the limits zero to infinity. Both integrals can be evaluated using

$$\int_0^{\infty} x^{2n}\, e^{-px^2} dx \;=\; \frac{(2n-1)!!}{2\,(2p)^n}\,\sqrt{\frac{\pi}{p}}\,, \qquad p\,>\,0\,, \qquad n\,=\,0\,,1\,,2\,,\ldots$$

10–50. Express the position space state function

$$\Psi(x,\,t) \;=\; \frac{1}{\sqrt{14}}\left[\,3\,\psi_0(x)\,e^{-i\omega t/2} \;+\; 2\,\psi_1(x)\,e^{-i3\omega t/2} \;+\; \psi_5(x)\,e^{-i11\omega t/2}\right]$$

in functional form in terms of the independent variable x.

This question was deliberately not addressed in the sequence exercises 10–37 through 10–45 to first provide greater exposure to Hermite polynomials. This exercise caps that sequence.

Express the three $\psi_n(x)$'s in terms of x. You have $\psi_0(x)$ and $\psi_1(x)$ from previous exercises. You need only to find $\psi_5(x)$, which is likely easiest using table 10–1, and then substitute the three eigenfunctions into the given wave function. Remember $0!\,=\,1$, and let our answer

$$\Psi(x,t) \;=\; \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}\left\{\frac{3}{\sqrt{14}}\,e^{-i\omega t/2} \;+\; \frac{4}{\sqrt{14}}\left(\frac{m\omega}{2\hbar}\right)^{1/2} x\,e^{-i3\omega t/2}\right.$$

$$\left. +\,\frac{1}{\sqrt{210}}\left[\,2\left(\frac{m\omega}{\hbar}\right)^{5/2} x^5 \;-\; 10\left(\frac{m\omega}{\hbar}\right)^{3/2} x^3 \;+\; \frac{15}{2}\left(\frac{m\omega}{\hbar}\right)^{1/2} x\,\right] e^{-i11\omega t/2}\right\}$$

guide you in organizing constants and concluding numerics. Obtaining representations in various spaces is a necessary skill, however, the relative inelegance of this answer may serve as additional encouragement to prefer bras and kets in Hilbert space over representations where possible.

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[3] Arfken *Mathematical Methods for Physicists* (Academic Press, New York, 1970, 2nd ed.), pp 424-432 and 611.

10–51. What are the ground state, and the first two excited states of a one-dimensional SHO in momentum space?

The intent of this exercise is to address the momentum space description of the SHO, but also to demonstrate the use of the raising operator in a momentum representation. First employ a quantum mechanical Fourier transform to $\psi_0(x)$ to find $\widehat{\psi}_0(p)$. The Fourier transform is

$$\widehat{\psi}(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x)\,e^{-ipx/\hbar}\,dx \quad \text{which is of the form} \quad \int_{-\infty}^{\infty}e^{-a^2x^2-bx}\,dx \;=\; \frac{\sqrt{\pi}}{a}\,e^{b^2/4a^2}$$

for the ground state. You can also obtain $\widehat{\psi}_n(p)$ from the Fourier transform of $\psi_n(x)$. Rather, use the raising operator in momentum space which is

$$a^\dagger \;=\; i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\frac{\partial}{\partial p} \;-\; i\left(\frac{1}{2m\omega\hbar}\right)^{1/2}p \;=\; i\left[\left(\frac{\alpha}{2}\right)^{1/2}\frac{d}{dp} \;-\; \left(\frac{1}{2\alpha}\right)^{1/2}p\right]$$

where $\alpha = m\omega\hbar$ is used to reduce clutter. Calculate $\widehat{\psi}_1(p)$ using this raising operator on $\widehat{\psi}_0(p)$,

$$\widehat{\psi}_1(p) \;=\; a^\dagger\,\widehat{\psi}_0(p) \;=\; i\left[\left(\frac{\alpha}{2}\right)^{1/2}\frac{\partial}{\partial p} \;-\; \left(\frac{1}{2\alpha}\right)^{1/2}p\right]\widehat{\psi}_0(p)$$

and then obtain $\widehat{\psi}_2(p)$ by raising $\widehat{\psi}_1(p)$. You should find

$$\widehat{\psi}_2(p) \;=\; \frac{\sqrt{2}}{(\pi)^{1/4}(m\omega\hbar)^{3/4}}\left[\left(\frac{m\omega\hbar}{2}\right)^{1/2} \;-\; \left(\frac{2}{m\omega\hbar}\right)^{1/2}p^2\right]e^{-p^2/\,2m\omega\hbar}\,.$$

You should see that you can form $\widehat{\psi}_{n+1}(p)$ from $\widehat{\psi}_n(p)$ for any n. This is often more economic than evaluating integrals created from a Fourier transform for even moderate n.

10–52. Use the raising operator in position space to find $\psi_1(x)$ from $\psi_0(x)$.

We hope that this exercise cements the utility of the ladder operators, the predecessors of the creation and annihilation operators. You were asked in the previous exercise to use the raising operator in the momentum basis, here you are asked to employ the raising operator in the position representation. You should use

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}x \;-\; \left(\frac{\hbar}{2m\omega}\right)^{1/2}\frac{d}{dx}$$

in position space. You have $\psi_0(x)$ and $\psi_1(x)$ from the numerous problems and exercises. Of course, this must work, and is intended as a demonstration that it does work.

Part 2, Power Series Solution to the SHO

10–53. Show that Schrodinger's equation in position space can be written

$$\frac{d^2\,\psi\,(x)}{dx^2} \;+\; \left(\lambda - \alpha^2 x^2\right)\psi\,(x) \;=\; 0 \qquad \text{for an SHO in one dimension.}$$

Part 2 emphasizes the procedures for solving an ordinary differential equation (ODE) using a **power series solution**. Power series solutions to ODE's are useful in numerous areas of physics.

The Schrodinger equation for the SHO potential in one dimension in position space is

$$\left(-\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2} \;+\; \frac{1}{2}\,kx^2\right)\psi\,(x) \;=\; E\,\psi\,(x) \quad \Rightarrow \quad \frac{d^2\,\psi\,(x)}{dx^2} \;+\; \frac{2m}{\hbar^2}\left(E - \frac{1}{2}\,kx^2\right)\psi\,(x) \;=\; 0\,.$$

$$\text{Let} \quad \lambda \;=\; \frac{2mE}{\hbar^2} \quad \text{and} \quad \alpha^2 \;=\; \frac{mk}{\hbar^2} \quad \Rightarrow \quad \frac{d^2\,\psi\,(x)}{dx^2} \;+\; \left(\lambda - \alpha^2 x^2\right)\psi\,(x) \;=\; 0\,.$$

10–54. Discuss the procedures for solving an ODE using a power series solution.

Power series solutions to ODE's are longer problems. Breaking longer problems into smaller segments will often make the overall solution more accessible, so here is a six step procedure.

Power Series Solution Road Map

1. Find the solution as x approaches infinity, *i.e.*, the asymptotic solution.

2. Assume that the product of the asymptotic solution and an arbitrary function, $f\,(x)$, is a solution. Use this solution in the homogeneous ODE and simplify.

3. Assume the arbitrary function can be expressed as an infinite power series, *i.e.*,

$$f\,(x) \;=\; a_0 \;+\; a_1 x \;+\; a_2 x^2 \;+\; a_3 x^3 \;+\; \cdots \;=\; \sum_{i\,=\,0}^{\infty} a_i x^i\,.$$

4. Evaluate the derivatives where $f\,(x)$ is expressed as the power series of step 3, and substitute these into the ODE.

5. Group like powers of x such that each power of x has its own coefficient.

6. The expressions that are the coefficients must vanish individually. Express this fact as a recursion relation in closed form if possible.

Postscript: The fact given in step 6 "The expressions that are the coefficients must vanish individually," is not obvious. Each power of x may be viewed as a basis vector. The different basis vectors cannot mix, so in the homogeneous series $a_0 + a_1x + a_2x^2 + a_3x^3 + \cdots = 0$, each term must be zero individually. The coefficients are usually expressions like $(\lambda - n)$ rather than individual scalars so that each coefficient can vanish individually. Arfken[4] provides a more formal discussion. Problem 10–59 in this sequence will likely be illustrative.

10–55. Find the asymptotic solution to $\dfrac{d^2\psi(x)}{dx^2} + (\lambda - \alpha^2x^2)\psi(x) = 0$.

An asymptotic solution means the solution as $|x| \gg 0$. The solution is a wave function. A wave function over all space must approach zero as $|x| \gg 0$ to be normalizable.

$$|x| \gg 0 \;\Rightarrow\; \alpha^2x^2 \gg \lambda, \text{ so at large } x \text{ the ODE approaches } \frac{d^2\psi(x)}{dx^2} - \alpha^2x^2\psi(x) = 0. \quad (1)$$

The solution to this asymptotic form of the rearranged time independent Schrodinger equation is

$$\psi(x) = Ae^{-\alpha x^2/2} + Be^{\alpha x^2/2} = Ae^{-\alpha x^2/2}, \quad (2)$$

where $B = 0$ because the exponential term with the positive argument approaches infinity so is not normalizable and is discarded. To show that equation (2) is a solution to equation (1),

$$\frac{d}{dx}\psi(x) = -\alpha xAe^{-\alpha x^2/2} \Rightarrow \frac{d^2}{dx^2}\psi(x) = \frac{d}{dx}\left(-\alpha xAe^{-\alpha x^2/2}\right) = \alpha^2x^2Ae^{-\alpha x^2/2} - \alpha A\cancel{e^{-\alpha x^2/2}}$$

where the last term is struck because it is negligible under the assumption $x \gg 0$. Substituting into equation (1) yields

$$\alpha^2x^2Ae^{-\alpha x^2/2} - \alpha^2x^2Ae^{-\alpha x^2/2} = 0,$$

so equation (2) is the asymptotic form sought. Now we know the "long distance" behavior. Step 1 of the road map is complete.

10–56. Caste $\dfrac{d^2\psi(x)}{dx^2} + (\lambda - \alpha^2x^2)\psi(x) = 0$ into an ODE valid over the entire domain.

The domain is $-\infty < x < \infty$. Step 2 is substitute

$$\psi(x) = Ae^{-\alpha x^2/2}f(x)$$

and reduce. The asymptotic behavior is modeled by the exponential term, and the unknown function $f(x)$ is assumed to model the behavior of $\psi(x)$ within and near the potential well. It is not known if such an $f(x)$ exists. Further it is also not known that $\psi(x)$ can be expressed as

[4] Arfken *Mathematical Methods for Physicists* (Academic Press, New York, 1970, 2nd ed.), pp 267–270.

a product. Should a solution be found subject to these assumptions, the assumptions are valid. If a solution cannot be found, at least one of the assumptions is incorrect and another approach is necessary. In this case, however, this approach does work.

Substituting the product of an unknown $f(x)$ and the asymptotically decaying exponential into the problem 10–53 form of the Schrodinger equation,

$$\frac{d^2}{dx^2}\, e^{-\alpha x^2/2} f(x) \;+\; \left(\lambda - \alpha^2 x^2\right) e^{-\alpha x^2/2} f(x) \;=\; 0\,, \tag{1}$$

where we have divided both sides by the constant A so it does not appear. The second derivative of the composite function is required, so

$$\frac{d^2}{dx^2}\, e^{-\alpha x^2/2} f(x) \;=\; \frac{d}{dx}\left(-\alpha x\, e^{-\alpha x^2/2} f(x) \;+\; e^{-\alpha x^2/2} \frac{d}{dx} f(x)\right)$$

$$= -\alpha\, e^{-\alpha x^2/2} f(x) + \alpha^2 x^2 e^{-\alpha x^2/2} f(x) - \alpha x\, e^{-\alpha x^2/2} f'(x) - \alpha x\, e^{-\alpha x^2/2} f'(x) + e^{-\alpha x^2/2} f''(x).$$

Using this in equation (1),

$$-\alpha\, e^{-\alpha x^2/2} f(x) \;+\; \alpha^2 x^2 e^{-\alpha x^2/2} f(x) \;-\; 2\,\alpha x\, e^{-\alpha x^2/2} \frac{d}{dx} f(x)$$
$$+\; e^{-\alpha x^2/2} \frac{d^2}{dx^2} f(x) \;+\; \left(\lambda - \alpha^2 x^2\right) e^{-\alpha x^2/2} f(x) \;=\; 0$$

Each of the six terms on the left contains the same exponential. Dividing both sides by the exponential and striking terms that sum to zero,

$$-\alpha f(x) \;+\; \alpha^2 \cancel{x^2} f(x) \;-\; 2\alpha\, x \frac{d}{dx} f(x) \;+\; \frac{d^2}{dx^2} f(x) \;+\; \lambda f(x) \;-\; \alpha^2 \cancel{x^2} f(x) = \; 0$$

$$\Rightarrow \quad \frac{d^2}{dx^2} f(x) \;-\; 2\alpha x \frac{d}{dx} f(x) \;+\; \left(\lambda - \alpha\right) f(x) \;=\; 0\,,$$

and that concludes step 2.

Postscript: Notice that though the exponential factor is no longer part of the equation, it was necessary to the reduction. The second derivative, which requires the use of the chain rule, would be invalid without it. We are left to find $f(x)$ assumed to model the behavior of $\psi(x)$ within and near the well. The exponential factor remains a portion of $\psi(x)$.

10–57. Change the independent variable to $\xi \;=\; \sqrt{\alpha}\, x$.

A change of variables is used to caste an expression or equation into a more favorable form. This is an optional technique prior to step 3.

$$\xi \;=\; \sqrt{\alpha}\,x \qquad \Rightarrow \qquad d\xi \;=\; \sqrt{\alpha}\,dx \qquad \Rightarrow \qquad \frac{d\xi}{dx} \;=\; \sqrt{\alpha}\,.$$

To change variables, also needed is $\dfrac{d}{dx}\,f\,(x) \;=\; \dfrac{d}{d\xi}\,\dfrac{d\,\xi}{dx}\,f\,(\xi) \;=\; \dfrac{d}{d\xi}\,\sqrt{\alpha}\,f\,(\xi) \;=\; \sqrt{\alpha}\,\dfrac{d}{d\xi}\,f\,(\xi)$

$$\Rightarrow \qquad \frac{d^2}{dx^2}\,f\,(x) \;=\; \frac{d}{dx}\,\sqrt{\alpha}\,\frac{d}{d\xi}\,f\,(\xi) \;=\; \frac{d}{d\xi}\,\frac{d\xi}{dx}\,\sqrt{\alpha}\,\frac{d}{d\xi}\,f\,(\xi) \;=\; \frac{d}{d\xi}\,\alpha\,\frac{d}{d\xi}\,f\,(\xi) \;=\; \alpha\,\frac{d^2}{d\xi^2}\,f\,(\xi)\,,$$

therefore, $\dfrac{d^2}{dx^2}\,f\,(x) \;-\; 2\alpha x\,\dfrac{d}{dx}\,f\,(x) \;+\; \big(\lambda - \alpha\big)f\,(x) \;=\; 0$ becomes

$$\alpha\,\frac{d^2}{d\xi^2}\,f\,(\xi) \;-\; 2\alpha\,\frac{\xi}{\sqrt{\alpha}}\,\sqrt{\alpha}\,\frac{d}{d\xi}\,f\,(\xi) \;+\; \big(\lambda - \alpha\big)f\,(\xi) \;=\; 0$$

$$\Rightarrow \qquad \frac{d^2}{d\xi^2}\,f\,(\xi) \;-\; 2\,\xi\,\frac{d}{d\xi}\,f\,(\xi) \;+\; \left(\frac{\lambda}{\alpha} \;-\; 1\right) f\,(\xi) \;=\; 0\,,$$

and this is **Hermite's equation**. The arbitrary function $f\,(\xi)$ is often represented $H_n\,(\xi)\,,$ or

$$\frac{d^2}{d\xi^2}\,H_n\,(\xi) \;-\; 2\xi\,\frac{d}{d\xi}\,H_n\,(\xi) \;+\; \left(\frac{\lambda}{\alpha} - 1\right) H_n\,(\xi) \;=\; 0\,.$$

The solutions to Hermite's equation are the Hermite polynomials denoted $H_n\,(\xi)\,.$

10–58. Express Hermite's equation in terms of an infinite power series.

Solutions to Schrodinger's equation with the SHO potential are $\psi\,(x) \;=\; A\,H_n\,(\xi)\,e^{-\alpha x^2/\,2}$ where a normalization constant A and an exponential factor $e^{-\alpha x^2/\,2}$ have been divided from the ODE. Should Hermite's equation be recognized, the $H_n\,(\xi)$ are the solutions and the rest of the road map is unnecessary. We continue the process to illustrate the remaining procedures of completing a power series solution. Generally,

$$f\,(x) \;=\; a_0 \;+\; a_1\,x \;+\; a_2\,x^2 \;+\; a_3\,x^3 \;+\; \cdots \;=\; \sum_{i\,=\,0}^{\infty} a_i\,x^i\,,$$

but in terms of $\xi\,,$

$$f\,(\xi) \;=\; a_0 \;+\; a_1\,\xi \;+\; a_2\,\xi^2 \;+\; a_3\,\xi^3 \;+\; \cdots \;=\; \sum_{i\,=\,0}^{\infty} a_i\,\xi^i\,.$$

$$\frac{d}{d\xi}\,f(\xi) \;=\; a_1 \;+\; 2a_2\,\xi \;+\; 3a_3\,\xi^2 \;+\; 4a_4\,\xi^3 \;+\; \cdots \;=\; \sum_{i\,=\,1}^{\infty} i\,a_i\,\xi^{i-1},$$

$$\frac{d^2}{d\xi^2}\,f\,(\xi) \;=\; 1\cdot 2a_2 \;+\; 2\cdot 3a_3\,\xi \;+\; 3\cdot 4a_4\,\xi^2 \;+\; 4\cdot 5a_5\,\xi^3 \;+\; \cdots \;=\; \sum_{i\,=\,2}^{\infty}(i-1)i\,a_i\,\xi^{i-2}.$$

Inserting these derivatives into Hermite's equation,

$$\begin{aligned} &1\cdot 2a_2 \;+\; 2\cdot 3a_3\,\xi \;+\; 3\cdot 4a_4\,\xi^2 \;+\; 4\cdot 5a_5\,\xi^3 \;+\; \cdots \\ &\qquad -\; 2\xi\left(a_1 \;+\; 2a_2\,\xi \;+\; 3a_3\,\xi^2 \;+\; 4a_4\,\xi^3 \;+\; \cdots\right) \\ &\qquad\qquad +\; \left(\frac{\lambda}{\alpha}-1\right)\left(a_0 \;+\; a_1\,\xi \;+\; a_2\,\xi^2 \;+\; a_3\,\xi^3 \;+\; \cdots\right) \;=\; 0 \end{aligned}$$

is the power series form of Hermite's equation, completing steps 3 and 4.

10–59. Find the coefficient of each power of ξ in the power series form of Hermite's equation then develop a recursion relation summarizing all coefficients.

Steps 5 and 6 in the power series solution road map follow.

$$\begin{aligned} &1\cdot 2a_2 \;+\; 2\cdot 3a_3\,\xi \;+\; 3\cdot 4a_4\,\xi^2 \;+\; 4\cdot 5a_5\,\xi^3 \;+\; \cdots \\ &\qquad -\; 2\xi\,a_1 \;-\; 2\xi\,2a_2\,\xi \;-\; 2\xi\,3a_3\,\xi^2 \;-\; 2\xi\,4a_4\,\xi^3 \;-\; \cdots \\ &\qquad\qquad +\; \left(\frac{\lambda}{\alpha}-1\right)a_0 \;+\; \left(\frac{\lambda}{\alpha}-1\right)a_1\,\xi \;+\; \left(\frac{\lambda}{\alpha}-1\right)a_2\,\xi^2 \;+\; \left(\frac{\lambda}{\alpha}-1\right)a_3\,\xi^3 \;+\; \cdots \;=\; 0 \\ \Rightarrow\quad &1\cdot 2a_2 \;+\; 2\cdot 3a_3\,\xi \;+\; 3\cdot 4a_4\,\xi^2 \;+\; 4\cdot 5a_5\,\xi^3 \;+\; \cdots \\ &\qquad -2\,a_1\,\xi \;-\; 2\cdot 2a_2\,\xi^2 \;-\; 2\cdot 3a_3\,\xi^3 \;-\; 2\cdot 4a_4\,\xi^4 \;-\; \cdots \\ &\qquad\qquad +\; \left(\frac{\lambda}{\alpha}-1\right)a_0 \;+\; \left(\frac{\lambda}{\alpha}-1\right)a_1\,\xi \;+\; \left(\frac{\lambda}{\alpha}-1\right)a_2\,\xi^2 \;+\; \left(\frac{\lambda}{\alpha}-1\right)a_3\,\xi^3 \;+\; \cdots \;=\; 0\,. \end{aligned}$$

Examining each power of ξ reveals

$$\begin{aligned} &\text{coefficient of } \xi^0: && 1\cdot 2a_2 \;+\; \left(\frac{\lambda}{\alpha}-1\right)a_0 \\ &\text{coefficient of } \xi^1: && 2\cdot 3a_3 \;+\; \left(\frac{\lambda}{\alpha}-1-2\right)a_1 \\ &\text{coefficient of } \xi^2: && 3\cdot 4a_4 \;+\; \left(\frac{\lambda}{\alpha}-1-2\cdot 2\right)a_2 \\ &\text{coefficient of } \xi^3: && 4\cdot 5a_5 \;+\; \left(\frac{\lambda}{\alpha}-1-2\cdot 3\right)a_3 \\ &\qquad\vdots && \qquad\vdots \end{aligned}$$

The pattern is $\quad (n+1)(n+2)\,a_{n+2} \;+\; \left(\dfrac{\lambda}{\alpha}-1-2\cdot n\right)a_n \qquad \text{for} \quad n \;=\; 0,\; 1,\; 2,\; 3, \ldots$

Each coefficient must vanish individually, or $\quad (n+1)(n+2)\,a_{n+2} \;+\; \left(\dfrac{\lambda}{\alpha}-1-2\cdot n\right)a_n \;=\; 0$

$$\Rightarrow \qquad a_{n+2} \;=\; -\,\frac{\left(\lambda/\alpha-1-2\cdot n\right)}{(n+1)(n+2)}\,a_n \qquad \text{for} \;\; n \;=\; 0,\; 1,\; 2,\; 3,\; \ldots\,.$$

is the recursion relation that completes step 6.

Postscript: The statement that says each coefficient must vanish individually is

$$(n+1)\,(n+2)\,a_{n+2} \;+\; \left(\frac{\lambda}{\alpha} - 1 - 2\cdot n\right) a_n \;=\; 0\,.$$

Notice that because the subscripts of the coefficients differ by two, the recursion relation will actually yield two series, one for $a_{n\,\mathrm{even}}$ and a second for $a_{n\,\mathrm{odd}}$, that can be generated separately.

10–60. Find the eigenenergies of the SHO from the recursion relation.

The eigenfunctions do not approach zero at $|\,x\,| \gg 0$ quickly enough to be normalizable if the power series does not terminate[5]. The numerator of the recursion relation will be zero for special values of λ and α and the series will terminate $\quad\Rightarrow\quad \lambda/\alpha \;-\; 1 \;-\; 2n \;=\; 0$ for such values.

$$\frac{\lambda}{\alpha} \;-\; 1 \;-\; 2n \;=\; 0 \qquad\Rightarrow\qquad \lambda_n \;=\; \big(2n+1\big)\,\alpha\,.$$

Also

$$\lambda \;=\; \frac{2mE}{\hbar^2} \qquad \text{and} \qquad \alpha^2 \;=\; \frac{mk}{\hbar^2}$$

from problem 10–53,

$$\Rightarrow \qquad \frac{2mE_n}{\hbar^2} \;=\; \big(2n+1\big)\,\frac{\sqrt{mk}}{\hbar}$$

$$\Rightarrow \qquad E_n \;=\; \big(2n+1\big)\,\frac{1}{\hbar}\,\frac{\hbar^2}{2m}\sqrt{mk}$$

$$\Rightarrow \qquad E_n \;=\; \left(n+\frac{1}{2}\right)\hbar\,\sqrt{\frac{k}{m}}\,, \qquad \text{or} \qquad E_n \;=\; \left(n+\frac{1}{2}\right)\hbar\omega\,.$$

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[5] Gasiorowicz *Quantum Physics* (John Wiley & Sons, New York, 1974), pp 101–105.

Exercises The Three-dimensional SHO

Guidance for problems 10–61 through 10–64 is given following the statement of problem 10–64.

10–61. Consider the three-dimensional SHO with the potential $V(r) = \frac{1}{2}m\omega^2 r^2$. Separate the three-dimensional, time-dependent Schrodinger equation into time and spatial variables in Cartesian coordinates, and then solve the time-dependent portion of the separated equation. Discuss the meaning of the differential equation dependent only on time.

10–62. Solve the time-independent Schrodinger equation in Cartesian coordinates by separating spatial variables. Find the eigenenergies and the degree of degeneracy for a three-dimensional SHO in the arbitrary excited state n.

10–63. Solve the time-independent Schrodinger equation in spherical coordinates in three dimensions for the SHO. Separate radial and angular dependence. Solve the radial equation using a power series solution. Find the eigenenergies for an arbitrary excited state.

10–64. Compare your solutions for the Cartesian and spherical models by showing that the eigenenergies and total degeneracy are the same. Relate the eigenstates expressed in Cartesian coordinates and the eigenstates expressed in spherical coordinates.

We are going to address these four problems as one problem with 21 parts. This set of exercises is designed to guide you through two different differential equation solutions to the three-dimensional harmonic oscillator problem, namely the solution in Cartesian coordinates which is precisely like solving the one-dimensional problem three times, and the solution in spherical coordinates which involves a separation of the radial and angular degrees of freedom which is very similar to our solution of the hydrogen atom—specifically, there is an effective radial potential governing the radial dependence, and spherical harmonics govern the angular dependence. This problem contains several important pedagogical issues:

(1) You should be able to separate the time and space dependence of the wave function. You should understand how the energy eigenvalues emerge as the separation constant during this separation of time and space, and how this separation of variables leads from the time-dependent Schrodinger equation to the time-independent Schrodinger equation.

As we saw for the one-dimensional harmonic oscillator, only special values of the separation constant terminate the power series—these special solutions to the time-independent Schrodinger equation are the "stationary states". When you solve the time-independent Schrodinger equation to get the stationary states, remember that there are only a few special values of the separation constant (the energy eigenvalues) that produce these very special time and space separated stationary solutions. For an arbitrary energy, you cannot separate the

wave function into a single function of space times a single function of time! In fact, there are infinitely many linear combinations of the stationary states with any given expectation value of the energy. However, you can always uniquely separate any given initial state (which will always have a definite expectation value of its energy E at $t = 0$) into a sum of the stationary states times their respective time dependences. Of course, that's why we spent so much time expanding the initial $t = 0$ wave function in terms of the energy eigenstates...

(2) You should be able to separate three-dimensional problems in Cartesian coordinates or in spherical coordinates. The $3D$ SHO is one of the few problems that is so easily soluble in both coordinate systems, and it gives us a good chance to compare the two approaches.

(3) You should be able to make the separated differential equation dimensionless. Once you have a dimensionless equation, you should be able to solve it in the asymptotic limit. Then you should be able to separate the asymptotic behavior. Finally, you must be able to solve for the dimensionless asymptotic-behavior-removed stationary state wave functions. Of course, the point is that by making the equation dimensionless, and by removing the asymptotic behavior, you will find a complete set of finite polynomials that solve your problem. The special values of the separation constant that terminate these otherwise infinite series solutions are the dimensionless energy eigenvalues. And, of course, you must be able to use the recursion relations you obtain to deduce the polynomials and the corresponding energy eigenvalues.

(4) Finally, you should realize that no matter what set of coordinates you use to solve the problem, you must get the same answer! For this problem your answers will look very different, but there is nevertheless a fairly simple way to relate them to each other: linear combinations of the Cartesian stationary states are the energy eigenfunctions of the radial and angular momentum description, and, of course, linear combinations of the radial and angular momentum stationary states are the energy eigenfunctions of the Cartesian description...

10 – 61. Separating Variables for the 3d SHO

(a) Write down the time-dependent Schrodinger equation in the position space representation using $V(r) = \frac{1}{2}m\omega^2 r^2$. Then separate the time and space dependence of this equation using separable product eigenfunctions of the form $\Psi_n(\vec{\mathbf{r}}, t) = \psi_n(\vec{\mathbf{r}})\, g_n(t)$.

(b) Use $r^2 = x^2 + y^2 + z^2$ and the Cartesian form of the Laplacian to express the time-dependent Schrodinger equation in Cartesian coordinates. Then separate the time and space dependence using separable product eigenfunctions of the form $\Psi_n(x, y, z, t) = \psi_n(x, y, z)\, g_n(t)$. The resulting time dependent $g_n(t)$ must be the same as part (a).

Parts (a) and (b) illustrate how the time-independent Schrodinger equation can be constructed from the time-dependent Schrodinger equation in a position space representation. The time-independent Schrodinger equation only applies to the stationary states—all wave functions obey the time-dependent Schrodinger equation, but only the stationary states obey the time-independent Schrodinger equation!

(c) Show that the time-dependent functions are given by $g_n(t) = e^{-iE_n t/\hbar}$ by solving the differential equation that you obtained for $g_n(t)$ when you separated the time and space dependence. This is the differential equation version of the origin of the exponential phase describing time-dependence of the stationary states!

10 – 62. The 3d SHO in Cartesian Coordinates

(d) Express your time-independent Schrodinger equation in Cartesian coordinates, *i.e.,* in terms of x, y, z, p_x, p_y, and p_z, and then separate the x, y, and z dependence of this equation with eigenfunctions of the form $\psi_n(\vec{\mathbf{r}}) = \psi_n(x,y,z) = f(x)\,g(y)\,h(z)$. This is a little trickier than parts (a) and (b) since we considered only two degrees of freedom but have three degrees of freedom and a constant term here. Consider the Hamiltonian for the SHO

$$\mathcal{H} = \mathcal{H}_x + \mathcal{H}_y + \mathcal{H}_z = \left(\frac{\mathcal{P}_x^2}{2m} + \frac{1}{2}m\omega^2 x^2\right) + \left(\frac{\mathcal{P}_y^2}{2m} + \frac{1}{2}m\omega^2 y^2\right) + \left(\frac{\mathcal{P}_z^2}{2m} + \frac{1}{2}m\omega^2 z^2\right)$$

and you should be able to conclude what the separation constants must be. The final form of your separated equations for $f(x)$, $g(y)$, and $h(z)$ are time-independent Schrodinger equations for the one-dimensional SHO.

(e) Show that the eigenenergies for the three-dimensional harmonic oscillator are just the sum of the eigenenergies for the three separated directions, *i.e.,* show that

$$E_n = E(n_x, n_y, n_z) = \left(n + \frac{3}{2}\right)\hbar\omega, \qquad \text{where} \qquad n = n_x + n_y + n_z\,.$$

(f) Make a table of all possible combinations of the component and total quantum numbers for the ground state and for the first three excited states. Show that the degeneracy of the n-th state is $d(n) = \frac{1}{2}(n+1)(n+2)$ and list n_x, n_y, and n_z. This can be tricky. You may want to use form 1.2.2.1 in the *Handbook of Mathematical Formulas and Integrals* by Jeffrey,

$$\sum_{\mathrm{k}=0}^{m-1}(a+kd) = \frac{m}{2}\Big[2a + (m-1)\,d\Big]\,.$$

10 – 63. The 3d SHO in Spherical Coordinates

(g) Express your time-independent Schrodinger equation in spherical coordinates, *i.e.,* in terms of r, θ, and ϕ. Use the Laplacian in spherical coordinates,

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,.$$

Separate the radial dependence and the angular dependence of this equation using product eigenfunctions consisting of radial wave functions times the spherical harmonics, *i.e.,*

$$\psi_{klm}(\vec{\mathbf{r}}) = \psi_{klm}(r,\theta,\phi) = R_{kl}(r)\,Y_{lm}(\theta,\phi)\,.$$

The subscripts are important but not particularly useful at this point so just use $\psi = RY$. Spherical harmonics are another family of orthogonal polynomials dependent only on polar and azimuthal angle for the moment. We will discuss the spherical harmonics fully in chapter 12. Use $l(l+1)$ as the separation constant. The reason for this choice should become clear in chapters 12 and 13.

(h) Show that your separated radial equation has the form

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r \;+\; \frac{1}{2}m\omega^2 r^2 \;+\; \frac{l(l+1)\hbar^2}{2mr^2} \right] R_{kl}(r) \;=\; E_{kl}\,R_{kl}(r)\,.$$

Again, the subscripts will become important but since we have placed little emphasis on their meaning, they are largely cosmetic at this point.

(i) Set $R_{kl}(r) = r^{-1}u_{kl}(r)$ and $\epsilon_{kl} = 2mE_{kl}/\hbar^2$ to obtain the corresponding dimensionless energy version of the time-independent Schrodinger equation

$$\left[\frac{d^2}{dr^2} \;-\; \beta^4 r^2 \;-\; \frac{l(l+1)}{r^2} \;+\; \epsilon_{kl} \right] u_{kl}(r) \;=\; 0\,, \qquad \text{where} \qquad \beta \;=\; \sqrt{\frac{m\omega}{\hbar}}\,.$$

(j) Show that at large r, your asymptotic differential equation becomes

$$\left[\frac{d^2}{dr^2} \;-\; \beta^4 r^2 \right] u_{kl}(r) \;=\; 0\,.$$

Solve this asymptotic differential equation to obtain the asymptotic solutions $e^{\beta^2 r^2/2}$ and $e^{-\beta^2 r^2/2}$. Discard the solution that diverges at infinity since the wave function must go to zero at infinity. It is likely easiest to "guess" a proposed solution and differentiate to show that it is, in fact, a solution. See problem 10–55.

(k) Separate variables again to remove the Gaussian asymptotic behavior by substituting

$$u_{kl}(r) \;=\; e^{-\beta^2 r^2/2}\,y_{kl}(r)$$

into the differential equation for u_{kl} to obtain the corresponding differential equation for y_{kl},

$$\left[\frac{d^2}{dr^2} \;-\; 2\beta^2 r\frac{d}{dr} \;+\; \epsilon_{kl} \;-\; \beta^2 \;-\; \frac{l(l+1)}{r^2} \right] y_{kl}(r) \;=\; 0\,.$$

Again, it is good that you see the subscripts, but they are still cosmetic at this point.

(l) Now substitute the power series $y_{kl}(r) \;=\; r^s \sum a_q\, r^q$ into the differential equation to obtain the recursion relation for the coefficients. See problems 10–58 and 10–59.

(m) Show that $\left[\, s(s-1) \;-\; l(l+1) \,\right] a_0 \;=\; 0\,,$ and that this requires $s = l+1$ so that $a_0 \neq 0\,.$

(n) Show that $\left[\, s\,(s+1) \;-\; l\,(l+1) \;+\; 2s \,\right] a_1 \;=\; 0\,,$ and that this requires $a_1 \;=\; 0\,.$

(o) Show that for the coefficient of the r^{q+s} term to be equal to zero we must have

$$\left[\, (q \,+\, s \,+\, 2)(q \,+\, s \,+\, 1) \;-\; l\,(l\,+\,1) \,\right] a_{q+2} \;+\; \left[\, \epsilon_{kl} \;-\; \beta^2 \;-\; 2\beta^2\,(q \,+\, s) \,\right] a_q \;=\; 0$$

or equivalently, after using $s \;=\; l + 1\,,$ that

$$\left[\, (q \,+\, 2)(q \,+\, 2l \,+\, 3) \,\right] a_{q+2} \;=\; \left[\, (2q \,+\, 2l \,+\, 3)\,\beta^2 \;-\; \epsilon_{kl} \,\right] a_q\,.$$

(p) Show that all the coefficients with odd subscripts q are zero.

(q) Explain why the interesting values of the separation constants are those that terminate the series. Replace q with the index k to reflect the result of part (p) denoting only even integers can be used as indices. Then show that the series terminates when $\epsilon_{kl} \;=\; (2k + 2l + 3)\,\beta^2$ where k and l are non-negative integers.

(r) Show that the eigenenergies are given by

$$E_{kl} \;=\; \left(k + l + \frac{3}{2}\right)\hbar\omega \;=\; \left(n + \frac{3}{2}\right)\hbar\omega\,.$$

(s) Show that the allowed values of $\{k, l\}$ for a given n depend on whether n is even or odd and are given by

For n even: $\{k, l\} \;=\; \{0, n\},\ \{2, n-2\},\ \ldots\,,\ \{n-2, 2\},\ \{n, 0\}\,.$

For n odd: $\{k, l\} \;=\; \{0, n\},\ \{2, n-2\},\ \ldots\,,\ \{n-3, 3\},\ \{n-1, 1\}\,.$

10 – 64. Comparison of the Cartesian and Spherical Solutions

(t) Show that when the $2l + 1$ degeneracy of the angular momentum states is included, the total degeneracy of each state of the three-dimensional harmonic oscillator described in spherical coordinates is exactly the same as the degeneracy that you already calculated in Cartesian coordinates, $g\,(n) \;=\; \frac{1}{2}\,(n+1)(n+2)\,.$ Use the formula for a finite arithmetic progression given in part (f). You must cast these sums into the same form where the index starts at zero and is consecutive. The forms that are comparable to the given finite arithmetic sum are

$$\sum_{l\,\text{even}}^{n}(2l+1) \;=\; \sum_{i}^{n/2}(4i+1) \qquad \text{and} \qquad \sum_{l\,\text{odd}}^{n}(2l+1) \;=\; \sum_{i}^{(n-1)/2}(4i+3)\,.$$

We would like to have you show that you can form a linear combination of the Cartesian stationary states to produce one of the spherical stationary states and vice versa, but we will not ask that here because we have not developed spherical harmonics sufficiently to create the spherical stationary states. Please be assured that the Cartesian stationary states are simply a linear combination of the spherical stationary states and vice versa. Not surprisingly, likely the easiest way to show this is using Dirac notation. . .

Chapter 11

The Finite Square Well

Like chapter 9, this chapter concerns primarily potential energy functions that are piecewise constant. These problems are also usually addressed using the position space, time-independent form of the Schrodinger equation, which is just a convenient form of the Schrodinger postulate. The wave function and its first derivative must be the same on both sides of a boundary. Chapter 9 addresses primarily scattering states, this chapter addresses primarily bound states.

Equating the wave function and its first derivative at boundaries is a process that can be somewhat long and tedious. The finite square well problem is no exception. The finite square well is further complicated by the fact that an algebraic solution does not exist; only numerical (to predetermined precision) or graphical solutions are possible.

All potential energy wells have at least one bound state, regardless of how shallow or thin. Deeper and wider wells will have more bound states, though a finite number. The infinite square well, with infinite bound states, is a limiting case of a finite square well. The impenetrable walls of an infinite square do not allow barrier penetration, though barrier penetration was evident for scattering states and the SHO potential well, and is anticipated for all potential energy functions except the infinite square well. The concepts obtained in this chapter apply generally to potential energy wells that do not have precisely square corners, meaning the qualitative features of (1) at least one bound state and (2) a finite number of bound states extend to finite wells of any shape.

11–1. Show that a complex number divided by its conjugate has modulus 1 .

Problems 11–1 and 11–2 are math problems used in the development of the finite square well. The Euler equation

$$e^{i\theta} \;=\; \cos\theta + i\,\sin\theta \qquad \Rightarrow \qquad a + bi \;=\; r\,e^{i\theta}$$

where $r = \sqrt{a^2+b^2}$ and $\theta = \tan^{-1}\dfrac{b}{a}$.

For a complex number, r is obtained

$$r = \left|\, a+bi \,\right| = \sqrt{(a+bi)\,(a-bi)} = \sqrt{a^2+b^2}$$

and modulus 1 means $\left|\, a+bi \,\right| = 1$ or $r = 1$.

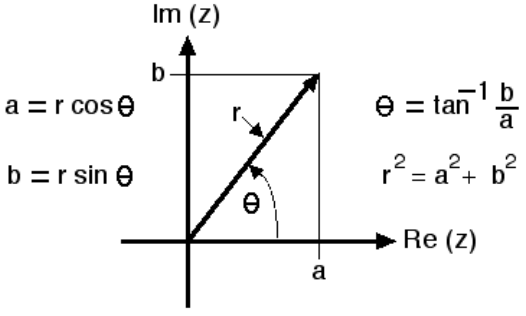

Figure 11–1. The complex number $z = a + bi$.

$$\frac{a+bi}{a-bi} \;=\; \frac{a+bi}{a-bi}\,\frac{a+bi}{a+bi} \;=\; \frac{a^2+2iab-b^2}{a^2+b^2} \;=\; \frac{a^2-b^2}{a^2+b^2} + \frac{2ab}{a^2+b^2}\,i$$

so the real part of $\dfrac{a+bi}{a-bi}$ is $\dfrac{a^2-b^2}{a^2+b^2}$ and the imaginary part is $\dfrac{2ab}{a^2+b^2}$. The modulus is the

square root of the sum of the squares of the real and imaginary parts, or

$$\left| \frac{a+bi}{a-bi} \right| = \left[\left(\frac{a^2-b^2}{a^2+b^2} \right)^2 + \left(\frac{2ab}{a^2+b^2} \right)^2 \right]^{1/2}$$
$$= \left[\frac{a^4 - 2a^2b^2 + b^4 + 4a^2b^2}{a^4 + 2a^2b^2 + b^4} \right]^{1/2}$$
$$= \left[\frac{a^4 + 2a^2b^2 + b^4}{a^4 + 2a^2b^2 + b^4} \right]^{1/2} = \sqrt{1} = 1 .$$

11–2. Obtain the phase of a complex number divided by its conjugate.

For a complex number $a+bi = r(\cos\theta + i\sin\theta) = re^{i\theta}$, the phase is $\theta = \tan^{-1}\left(\frac{b}{a}\right)$.

For a complex number $a+bi = re^{i\theta}$, the conjugate is $a-bi = re^{-i\theta}$, so

$$\frac{a+bi}{a-bi} = \frac{re^{i\theta}}{re^{-i\theta}} = e^{2i\theta} = e^{i\,2\tan^{-1}(b/a)}$$

and thus the phase of $\frac{a+bi}{a-bi}$ is $2\tan^{-1}\left(\frac{b}{a}\right)$.

Postscript: Notice that this is a second proof that the modulus of a complex number divided by its conjugate is 1 because

$$\frac{a+bi}{a-bi} = e^{2i\theta} = 1 \cdot e^{2i\theta}$$

shows that $r = 1$.

11–3. Apply the boundary conditions for the wave function and its first derivative to the rectangular well

$$V(x) = \begin{cases} -V_0, & \text{for } -a < x < a, \\ 0, & \text{for } |x| > a \end{cases}$$

for $-V_0 < E < 0$ to show that

$$\left(\frac{\kappa + ik}{\kappa - ik} \right)^2 = e^{-4ika} .$$

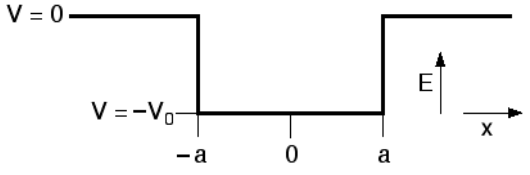

Figure 11–2. Finite square well.

Notice that though the vertical extent of the potential energy well is limited, the horizontal extent is infinite. Notice also that zero is placed in the center of the well which is consistent with our treatment of the infinite square well, most barriers, and the simple harmonic oscillator.

The first step is to define the geometry as seen in figure 11–3. The next step is to write the wave function for $-V_0 < E < 0$ which is

$$\psi(x) = \begin{cases} A\,e^{\kappa x} + B\,e^{-\kappa x} & \text{for} \quad x < -a\,, \\ C\,e^{ikx} + D\,e^{-ikx} & \text{for} \quad -a < x < a\,, \\ F\,e^{\kappa x} + G\,e^{-\kappa x} & \text{for} \quad x > a\,, \end{cases}$$

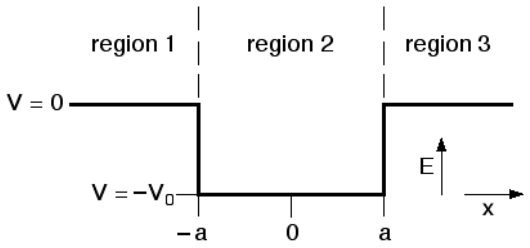

Figure 11–3. Regions for finite square well.

where $\kappa = \sqrt{-2mE}\,/\,\hbar$ and

$k = \sqrt{2m\,(V_0 - (-E))}\,/\,\hbar = \sqrt{2m\,(V_0 + E)}\,/\,\hbar\,.$

Notice that for $E < 0$ the wavenumbers are real in regions 1 and 3 so that the wave functions indicate exponential decay, thus non-zero probability density outside the well, which is barrier penetration. "Wave" behavior is apparent only inside the well.

That the wave function must be bounded means $B = 0$ in region 1 (because $x < 0$ makes $B\,e^{-\kappa x}$ an increasing exponential) and $F = 0$ in region 3, so

$$\psi(x) = \begin{cases} A\,e^{\kappa x} & \text{for} \quad x < -a\,, \\ C\,e^{ikx} + D\,e^{-ikx} & \text{for} \quad -a < x < a\,, \\ G\,e^{-\kappa x} & \text{for} \quad x > a\,. \end{cases}$$

Continuity of the wave function means

$$A\,e^{-\kappa a} = C\,e^{-ika} + D\,e^{ika} \tag{1}$$

$$C\,e^{ika} + D\,e^{-ika} = G\,e^{-\kappa a} \tag{2}$$

at the boundaries. Continuity of the first derivative means

$$A\kappa\,e^{-\kappa a} = Cik\,e^{-ika} - Dik\,e^{ika} \tag{3}$$

$$Cik\,e^{ika} - Dik\,e^{-ika} = -G\kappa\,e^{-\kappa a}\,. \tag{4}$$

Notice that there are four equations and four coefficients. This means that all four coefficients can be eliminated to arrive at a relationship that is dependent only on the wavenumbers and the well width. The strategy is to solve for C, D, and G in terms of A, substitute appropriately, then divide the resulting equation by A.

Multiply equation (1) by ik,

$$Aik\,e^{-\kappa a} = Cik\,e^{-ika} + Dik\,e^{ika}$$

and add to equation (3) to obtain

$$A\,(\kappa + ik)e^{-\kappa a} = 2Cik\,e^{-ika} \quad \Rightarrow \quad C = A\,\frac{\kappa + ik}{2ik}\,e^{-\kappa a + ika}\,.$$

Multiply equation (1) by $-ik$,

$$-Aik\,e^{-\kappa a} = -Cik\,e^{-ika} - Dik\,e^{ika}$$

and add to equation (3),

$$A\left(\kappa - ik\right)e^{-\kappa a} \;=\; -2Dik\,e^{ika} \qquad \Rightarrow \qquad D \;=\; -A\,\frac{\kappa - ik}{2ik}\,e^{-\kappa a - ika}\,.$$

Substitute these expressions for C and D into equation (2),

$$A\,\frac{\kappa + ik}{2ik}\,e^{-\kappa a + ika}\,e^{ika} \;-\; A\,\frac{\kappa - ik}{2ik}\,e^{-\kappa a - ika}\,e^{-ika} \;=\; G\,e^{-\kappa a}$$

$$\Rightarrow \qquad A\left[\frac{\kappa + ik}{2ik}\,e^{2ika} \;-\; \frac{\kappa - ik}{2ik}\,e^{-2ika}\right] \;=\; G\,.$$

Substituting the same expressions for C and D into equation (4),

$$A\,\frac{\kappa + ik}{2ik}\,e^{-\kappa a + ika}(ik)\,e^{ika} \;+\; A\,\frac{\kappa - ik}{2ik}\,e^{-\kappa a - ika}(ik)\,e^{-ika} \;=\; -G\kappa\,e^{-\kappa a}$$

$$\Rightarrow \qquad -A\left[\frac{\kappa + ik}{2\kappa}\,e^{2ika} \;+\; \frac{\kappa - ik}{2\kappa}\,e^{-2ika}\right] \;=\; G\,.$$

Equating the two expressions for G,

$$A\left[\frac{\kappa + ik}{2ik}\,e^{2ika} \;-\; \frac{\kappa - ik}{2ik}\,e^{-2ika}\right] \;=\; -A\left[\frac{\kappa + ik}{2\kappa}\,e^{2ika} \;+\; \frac{\kappa - ik}{2\kappa}\,e^{-2ika}\right]$$

$$\Rightarrow \qquad \frac{\kappa + ik}{2ik}\,e^{4ika} \;-\; \frac{\kappa - ik}{2ik} \;=\; -\frac{\kappa + ik}{2\kappa}\,e^{4ika} \;-\; \frac{\kappa - ik}{2\kappa}$$

$$\Rightarrow \qquad \left(\frac{\kappa + ik}{2ik} \;+\; \frac{\kappa + ik}{2\kappa}\right)e^{4ika} \;=\; \frac{\kappa - ik}{2ik} \;-\; \frac{\kappa - ik}{2\kappa}$$

$$\Rightarrow \qquad \left(\frac{1}{2ik} \;+\; \frac{1}{2\kappa}\right)\left(\kappa + ik\right)e^{4ika} \;=\; \left(\frac{1}{2ik} \;-\; \frac{1}{2\kappa}\right)\left(\kappa - ik\right)$$

$$\Rightarrow \qquad \left(\frac{\kappa + ik}{2ik\kappa}\right)\left(\kappa + ik\right)e^{4ika} \;=\; \left(\frac{\kappa - ik}{2ik\kappa}\right)\left(\kappa - ik\right)$$

$$\Rightarrow \qquad \left(\kappa + ik\right)^2 e^{4ika} \;=\; \left(\kappa - ik\right)^2 \qquad \Rightarrow \qquad \left(\frac{\kappa + ik}{\kappa - ik}\right)^2 \;=\; e^{-4ika}$$

which is a relationship containing only wave numbers and the width of the well.

11–4. Analyze both possible cases for $\left(\dfrac{\kappa + ik}{\kappa - ik}\right)^2 \;=\; e^{-4ika}$.

This relationship is quadratic in $\dfrac{\kappa + ik}{\kappa - ik}$, thus either

$$\frac{\kappa + ik}{\kappa - ik} \;=\; e^{-2ika} \qquad \text{or} \qquad \frac{\kappa + ik}{\kappa - ik} \;=\; -e^{-2ika}$$

after taking a square root of both sides. The left side of both cases is a complex number divided by its conjugate so the results of problems 11–1 and 11–2 will be useful.

We are going to define $k_0^2 = k^2 + \kappa^2$. Realize that

$$k_0 = \sqrt{k^2+\kappa^2} = \sqrt{\frac{2m\left(E+V_0\right)}{\hbar^2} + \left(-\frac{2mE}{\hbar^2}\right)} = \sqrt{\frac{2mV_0}{\hbar^2}} = \frac{\sqrt{2mV_0}}{\hbar}$$

so k_0 is a convenient constant that serves to encode the depth of the well.

If $\dfrac{\kappa+ik}{\kappa-ik} = e^{-2ika}$, the phase is

$$2\tan^{-1}\left(\frac{k}{\kappa}\right) = -2ka \quad \Rightarrow \quad \tan(-ka) = \frac{k}{\kappa} \quad \Rightarrow \quad -\tan(ka) = \frac{k}{\kappa} \quad \Rightarrow \quad \tan(ka) = -\frac{k}{\kappa}$$

which means $\tan(ka) < 0$ because the definitions require wavenumbers that are positive. The constant k_0 encodes the depth of the well. Consider

$$\frac{k_0^2}{k^2} = \frac{k^2+\kappa^2}{k^2} = 1 + \frac{\kappa^2}{k^2} = 1 + \frac{1}{\tan^2(ka)} = \frac{\tan^2(ka)+1}{\tan^2(ka)} = \frac{\sec^2(ka)}{\tan^2(ka)} = \frac{1}{\sin^2(ka)}$$

$$\Rightarrow \quad \sin^2(ka) = \frac{k^2}{k_0^2} \quad \Rightarrow \quad \left|\sin(ka)\right| = \frac{k}{k_0} \qquad \text{for} \qquad \tan(ka) < 0\,.$$

If $\dfrac{\kappa+ik}{\kappa-ik} = -e^{-2ika}$, the phase is more involved. $e^{i\pi} = \cos(\pi) + i\sin(\pi) = -1$, so

$$\frac{\kappa+ik}{\kappa-ik} = -e^{-2ika} = e^{i\pi}\,e^{-2ika} = e^{i(-2ka+\pi)}$$

so using the result of problem 11–2 the phase is

$$2\tan^{-1}\left(\frac{k}{\kappa}\right) = -2ka+\pi \quad \Rightarrow \quad \frac{k}{\kappa} = \tan\left(-ka+\frac{\pi}{2}\right) = -\tan\left(ka-\frac{\pi}{2}\right) = \cot(ka)$$

$$\Rightarrow \quad \frac{1}{\tan(ka)} = \frac{k}{\kappa} \quad \Rightarrow \quad \tan(ka) = \frac{\kappa}{k}$$

which means that $\tan(ka) > 0$. Then

$$\frac{k_0^2}{k^2} = \frac{k^2+\kappa^2}{k^2} = 1 + \frac{\kappa^2}{k^2} = 1 + \tan^2(ka) = \sec^2(ka) = \frac{1}{\cos^2(ka)}$$

$$\Rightarrow \quad \cos^2(ka) = \left(\frac{k}{k_0}\right)^2 \quad \Rightarrow \quad \left|\cos(ka)\right| = \frac{k}{k_0} \qquad \text{for} \qquad \tan(ka) > 0\,.$$

11–5. Create a graphical solution from the results of the previous problem.

The pertinent results of the last problem are

$$\left| \cos(ka) \right| = \frac{k}{k_0} \quad \text{for} \quad \tan(ka) > 0 \quad \text{and} \quad \left| \sin(ka) \right| = \frac{k}{k_0} \quad \text{for} \quad \tan(ka) < 0 \,.$$

The two equations are transcendental, meaning that an exact algebraic solution is not possible. Only numerical or a graphical solutions are possible. The graphical solution is illustrative. The final compilation of arcs and lines and the overall interpretation can be perceived as formidable, so the graph will be built in steps starting with a cosine curve.

The lowest energy solution is from $\left| \cos(ka) \right| = \frac{k}{k_0}$ for $\tan(ka) > 0$, so the cosine curve is examined first. Figure 11–4 is a cosine curve as a function of k. The wavenumber encodes the energy, an energy lower than the bottom of the well is not possible, so the cosine curve and those that follow all start at $k = 0$. Figure 11–5 shows the absolute value of the same cosine

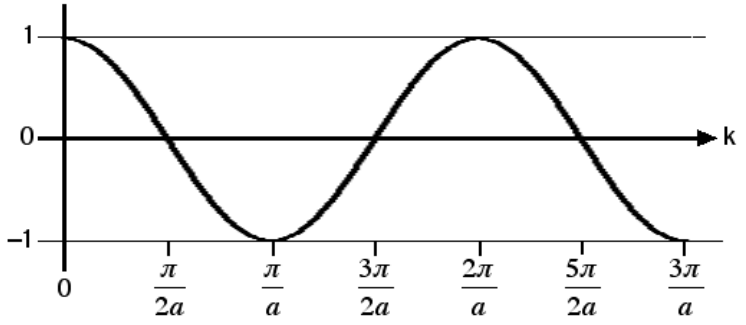

Figure 11–4. Cosine (ka).

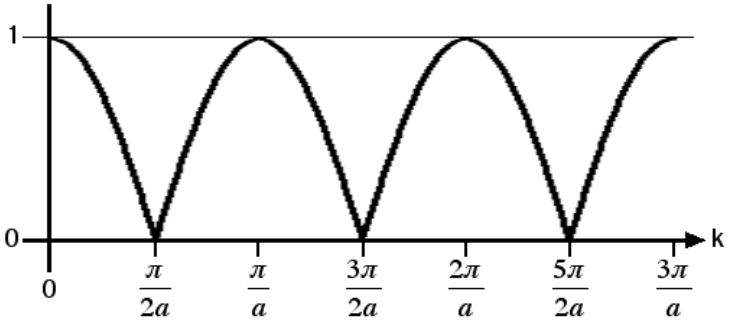

Figure 11–5. | Cosine (ka) |.

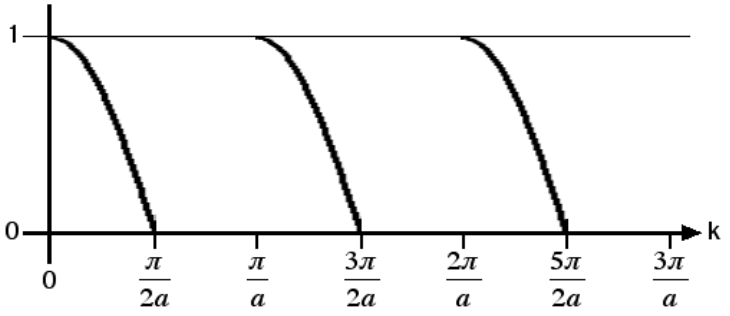

Figure 11–6. | Cosine (ka) | and tangent (ka) > 0 .

curve. Figure 11–6 shows the absolute value of this cosine subject to the condition $\tan(ka) > 0$. The sine curve is the same as the cosine curve shifted to the right by $\pi/2$, thus the absolute value of the sine curve looks the same as figure 11–5 shifted to the right by $\pi/2$. The absolute value of

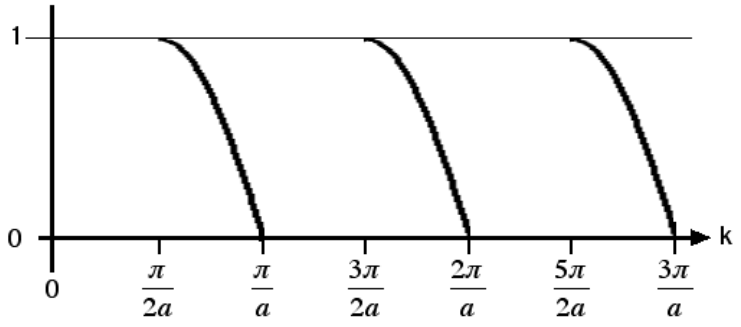

Figure 11–7. $\left|\text{Sine}\,(ka)\right|$ and tangent $(ka) < 0$.

the sine curve subject to the condition $\tan(ka) < 0$ is seen in figure 11–7. Solutions address both the absolute value of the cosine and sine of ka subject to different conditions on $\tan(ka)$, so figures 11–6 and 11–7 are consolidated in figure 11–8.

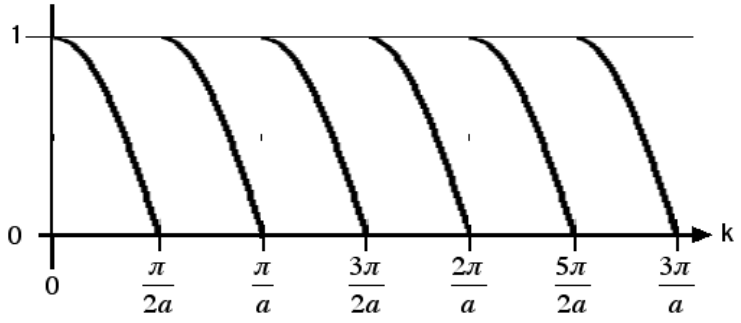

Figure 11–8. $\left|\text{Cosine}\,(ka)\right|$ and $\left|\text{sine}\,(ka)\right|$ with tangent (ka) conditions.

Both equations indicate that the absolute value of the cosine and sine of ka are equal to $\dfrac{k}{k_0}$, which is linear in k and has slope $1/k_0$. An overall graphical solution is shown in figure 11–9.

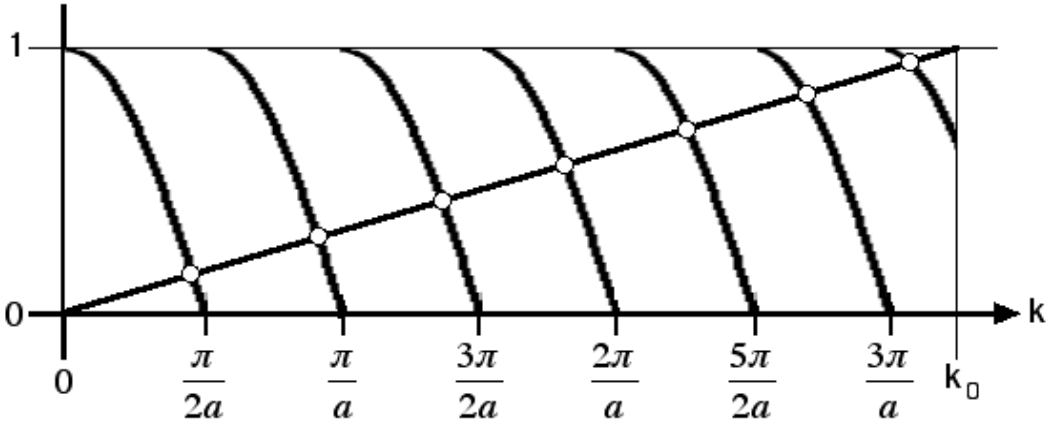

Figure 11–9. Overall graphical solution to the finite square well.

The open circles are the intersections of the trigonometric and linear curves so represent the wavenumbers of the bound states of a finite square well.

The right side of the constructive rectangle is at $k = k_0$ since the maximum of both trigonometric equations is $1 = \dfrac{k}{k_0} \Leftrightarrow k = k_0$, and there are no other solutions for a given k_0. Recall that k_0 encodes the depth of the well,

$$k_0 = \frac{\sqrt{2mV_0}}{\hbar}$$

so $k = k_0 \Leftrightarrow E = 0$ relative to the well, which is at the top of the well, so is not bound.

Figure 11–9 indicates seven bound states for the given k_0. Notice that the line k/k_0 is from $k = 0$ to $k = k_0$, from lower left to upper right along the diagonal of the bounding rectangle.

Postscript: Our definition of a finite square well is that the top of the well is $E = 0$, the bottom of the well is at $-V_0$, and the well is of width $2a$. Other definitions are possible. Many authors use $V = 0$ as the bottom of the well, $V = V_0$ at the top of the well, and a well width of a placing 0 in the center or at the left edge.

Also, figure 11–9 is not unique. Graphical solutions to the finite square well can made using tangents, cotangents, and/or a wide variety of parameters that encode the wavenumbers.

11–6. Show graphically that a finite square well must have at least one bound state.

This problem is a primary reason to examine the finite square well. Any potential energy well, no matter how shallow or thin, must have at least one bound state.

The well has $-V_0 < 0$ using our conventions. If $V_0 = 0$, a well does not exist. The left edge of the bounding rectangle is at $k = 0$, and the right side is at $k_0 > 0$ for an existing well.

Should $0 < k_0 < \pi/2a$, a figure analogous to figure 11–9 is seen at the right. The line k/k_0 is from $k = 0$ to $k = k_0$, from lower left to upper right along the diagonal of the bounding rectangle, but with steeper slope than in figure 11–9 because k_0 is smaller. The first branch of the $\left|\ \text{cosine}\ (ka)\ \right|$ curve will intersect this line regardless of steepness of the line k/k_0. The slope of $1/k_0$ cannot become purely vertical because that would require $V_0 = 0$, meaning that a potential energy well does not exist. Thus, figure 11–10 graphically shows that a finite square well must have at least one bound state.

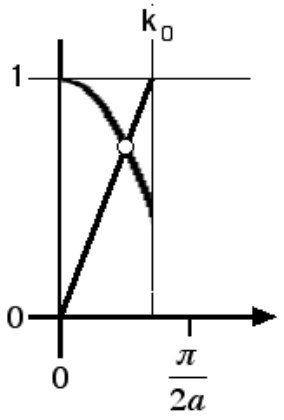

Figure 11–10. Finite square well, $0 < k_0 < \pi/2a$.

11–7. Estimate the energy of a particle in a finite square well with exactly one bound state.

There is an assumption and two approximations in this reduction. The assumption is that $k = k_0/2$, which looks slightly low for figure 11–10, but choosing the center of the range of possible bound wavenumbers seems reasonable. It is the usual assumption for this problem which will be closer as $k_0 \to 0$. The series form of a cosine is

$$\cos(x) = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots \approx 1 - \frac{x^2}{2}$$

for small x. The binomial series is

$$(1 \pm x)^\alpha = 1 \pm \alpha x + \frac{\alpha(\alpha-1)x^2}{2!} \pm \frac{\alpha(\alpha-1)(\alpha-2)x^3}{3!} + \cdots \approx 1 \pm \alpha x$$

again for $x \ll 1$. The first cosine branch is the only one involved for a well with exactly one bound state, per figure 11–10. An additional unusual technique in this problem is that though k appears twice in the first equation, the assumption $k = k_0/2$ is used only once within the cosine term, allowing a solution for the energy in question.

$\cos(ka) = \dfrac{k}{k_0}$ for a particle in a potential well with exactly one bound state, and $k \approx \dfrac{k_0}{2}$

$$\Rightarrow \quad \cos\left(\frac{k_0 a}{2}\right) \approx 1 - \frac{1}{2!}\left(\frac{k_0 a}{2}\right)^2 = 1 - \frac{k_0^2 a^2}{8} = \frac{k}{k_0}$$

and in terms of energy this is

$$1 - \frac{\left(\sqrt{2mV_0}/\hbar\right)^2 a^2}{8} = \frac{\sqrt{2m(E+V_0)}/\hbar}{\sqrt{2mV_0}/\hbar}$$

$$\Rightarrow \quad 1 - \frac{mV_0 a^2}{4\hbar^2} = \sqrt{\frac{E+V_0}{V_0}}$$

$$\Rightarrow \quad \left(1 - \frac{mV_0 a^2}{4\hbar^2}\right)^2 = \frac{E+V_0}{V_0}$$

and applying the approximation for a binomial series to the left side, this is

$$1 - \frac{mV_0 a^2}{2\hbar^2} = \frac{E}{V_0} + 1 \quad \Rightarrow \quad E = -\frac{mV_0^2 a^2}{2\hbar^2}.$$

Postscript: Briefly review figure 11–2. With width on the horizontal and the depth of the well on the vertical, the product $2a\,V_0$ is analogous to the area of our well. The above result indicates the energy of a single bound state is proportional to the square of this area analog.

11–8. How does the number of bound states vary as a finite square well of width $2a$ is deepened?

The constant $k_0 = \sqrt{2mV_0}/\hbar$ encodes the depth of the well. Review figure 11–10 for one bound state. As the well is deepened, the constant k_0 moves to the right. What happens as the constant k_0 moves past successive graduations of $n\pi/2a$, evolving toward figure 11–9, as V_0 gets larger?

$$\begin{aligned}
0 < k_0 < \frac{\pi}{2a} \quad &\Rightarrow \quad \text{1 bound state} \\
\frac{\pi}{2a} < k_0 < \frac{2\pi}{2a} \quad &\Rightarrow \quad \text{2 bound states} \\
\frac{2\pi}{2a} < k_0 < \frac{3\pi}{2a} \quad &\Rightarrow \quad \text{3 bound states} \\
&\vdots \\
\frac{6\pi}{2a} < k_0 < \frac{7\pi}{2a} \quad &\Rightarrow \quad \text{7 bound states, like figure 11–9, and} \\
&\vdots \\
\frac{(n-1)\pi}{2a} < k_0 < \frac{n\pi}{2a} \quad &\Rightarrow \quad n \text{ bound states}
\end{aligned}$$

thus, the deeper the well the larger the number of bound states for a given well width.

11–9. Obtain the lowest eigenenergies for a very deep finite potential energy well of width $2a$.

A very deep well is indicated by a large V_0 which means a large k_0. Picture a graph like figure 11–9 for large k_0. The line k/k_0 approaches the horizontal axis as k_0 is increased. Thus, the lowest eigenenergies are approximately at

$$k = \frac{n\pi}{2a}.$$

$$k = \frac{n\pi}{2a} \quad \Rightarrow \quad \frac{\sqrt{2m(E+V_0)}}{\hbar} = \frac{n\pi}{2a} \quad \Rightarrow \quad \frac{2m(E+V_0)}{\hbar^2} = \frac{n^2\pi^2}{4a^2}$$

$$\Rightarrow \quad E = n^2\frac{\pi^2\hbar^2}{8ma^2} - V_0.$$

Postscript: The eigenenergies of the infinite square well of chapter 8 are

$$E = n^2\frac{\pi^2\hbar^2}{8ma^2}$$

which is the same as a very deep finite square well with $V_0 = 0$ as it was defined for the infinite square well. The infinite square well is a limiting case of a very deep finite square well.

Placing the top of the finite square well at $E = 0$ and the bottom at $-V_0$ has the advantage of making the energy for bound states negative. This convention is used for many physical systems so that a negative energy is an indicator of a bound state. Placing the bottom of the infinite square well at $V_0 = 0$ as done in chapter 8 allows the picture of a free particle within the well, and is more mathematically accessible than placing $V_0 = -\infty$.

11–10. Sketch the three eigenfunctions of a particle in a finite square well with three bound states.

A limiting case of a finite square well is the infinite square well of chapter 8 so the eigenfunctions of the finite square well must converge to

$$\psi_n(x) = \begin{cases} \dfrac{1}{\sqrt{a}} \cos\left(\dfrac{n\pi}{2a}\, x\right), & n \text{ odd}, \\ \dfrac{1}{\sqrt{a}} \sin\left(\dfrac{n\pi}{2a}\, x\right), & n \text{ even}, \end{cases}$$

for large n per problem 8–2. Half of a finite square well resembles the step function of problem 9–1, or if the step does not extend to $x = \infty$, the barrier function of problem 9–3. Within the barrier (or the step), exponential decay of the wave function is expected. This is barrier penetration. In fact, we expect the wave function to exhibit exponential decay in any classically forbidden region. Thus, we expect cosine-like and sine-like behavior inside the well and exponential decay in the classically forbidden region.

Each eigenfunction is a cosine or a sine with exponential decay near and past the edges. The energy levels for a finite square well should be slightly closer than $n^2\, E_{\text{ground}}$ as they are in the infinite square well. Figure 11–9 shows seven bound states. The line k/k_0 intersects each successive cosine or sine branch slightly closer to the $n\pi/2a$ graduation than the last. As the constant k_0 is moved to the right, meaning the well is being made deeper, the slope of k/k_0 decreases until at $V_0 \to \infty \;\Rightarrow\; 1/k_0 \to 0$, and the energy level spacing converges to $n^2\, E_{\text{ground}}$. For all n,,

$$\frac{(n-1)\pi}{2a} < k < \frac{n\pi}{2a} \quad \Rightarrow \quad \frac{(n-1)^2\pi^2\hbar^2}{8ma^2} - V_0 < E < \frac{n^2\pi^2\hbar^2}{8ma^2} - V_0$$

so approximate $n^2\, E_{\text{ground}}$ spacing of energy levels is anticipated.

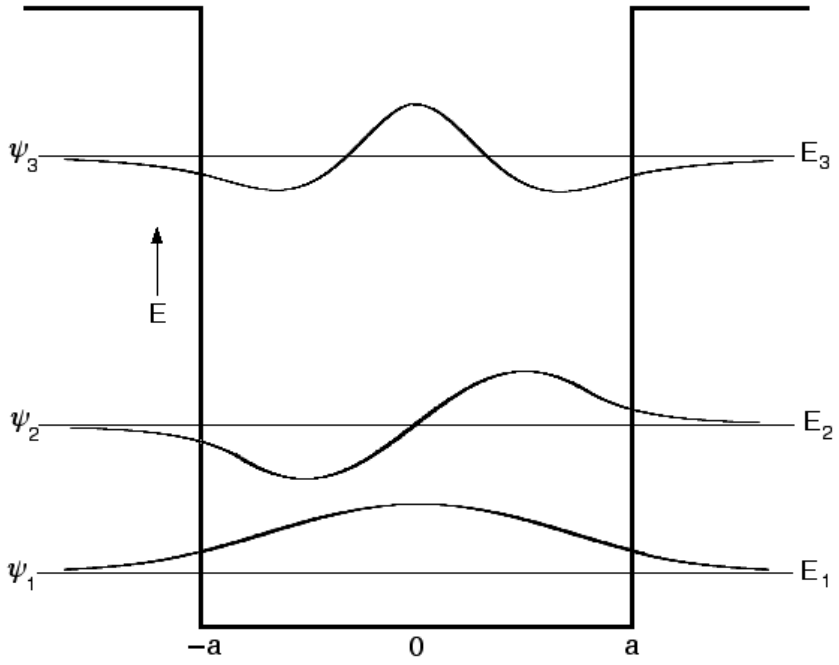

Figure 11–11. Eigenfunctions for a finite square well of depth V_0 with three bound states.

Exercises

11–11. Show that $z = a + bi$

$$\Rightarrow \qquad \frac{2a}{a+bi} \;=\; 2\,\cos(\theta)\,e^{-i\theta}\,.$$

Analogous to problems 11–1 and 11–2 using the same interpretation of Euler's equation. Find the modulus which is r in $re^{i\theta}$, then establish that the phase is the inverse tangent of $-b/a$ so the argument of the exponential is negative.

11–12. Consider a finite square well of width $2a$ possessing exactly one bound state.

(a) Find the maximum depth of the well.

(b) Compare the result of part (a) to the ground state eigenenergy of the infinite square well

$$E_n \;=\; n^2\frac{\pi^2\hbar^2}{8ma^2} \qquad \Rightarrow \qquad E_{\text{ground}} \;=\; \frac{\pi^2\hbar^2}{8ma^2}\,.$$

(c) Can the single bound state eigenenergy be at the part (a) maximum depth?

(d) Calculate the maximum V_0 for an electron in this finite square well for $a = 0.5$ Å

(e) Calculate the eigenenergy for the well of part (d) ($a = 0.5$ Å, maximum V_0) using the estimate of problem 11–7,

$$E \;=\; -\frac{mV_0^2a^2}{2\hbar^2}\,.$$

(f) Where does the part (e) answer place a bound electron above the floor of the well ($a = 0.5$ Å, maximum V_0) to the nearest percent?

The intent of this exercise is to provide some perspective for a finite square well possessing one bound state. Examine figures 11-10 and 11–9. The depth of the well is encoded in the constant k_0. Should k_0 be larger than $\pi/2a$, there will be two or more bound states. Thus, $\pi/2a$ is the maximum wavenumber for one bound state. You should find the part (b) comparison the same for $n = 1$ in an infinite square well. Examine figure 11–10 for part (c) which is asking only for a qualitative answer. We use $hc = 1.24 \times 10^4\, eV \cdot$ Å and the electron mass $= 0.511\ MeV/c^2$ for parts (d) and (e) rather than convert from CGS or MKS units. The diameter of a small atom is on the order of one Angstrom. You should find that the bound state eigenenergy is closer to the floor of the well than the top in part (f).

11–13. (a) Does the number of bound states vary as a finite square well of depth V_0 is widened?

(b) Does the number of bound states vary as the product $V_0\,a$ is increased?

Answer qualitatively concerning the number of the eigenenergies. Examine figure 11-9. That the depth of the well is fixed means V_0 is a constant which means that k_0 is a constant. How would figure 11–9 evolve if k_0 remained in the same location but a got bigger? It is commonly stated that there are increasing bound states as a finite well gets deeper. The width of the well is often overlooked. The number of bound states of a finite well must also increase with width.

The area analog $V_0\,a$ mentioned in the postscript to problem 11-7 may be viewed as the expression most pertinent to the number of bound states rather than just the depth or just the width individually. Your answers should be a sentence or two for each part.

Some use a well of width a with 0 at the left edge so that the area analog is $V_0\,a$. Our well is of width $2a$ with 0 in the center to be consistent with our treatment of the infinite square well, barriers, and other topics. The area analog for our well is actually $2V_0\,a$, however, the number of bound states in a finite square well is proportional to the product $V_0\,a$ in either case.

11–14. Calculate the number of possible bound states for an electron in a finite square well of $a = 6$ Å and $V_0 = 100\,eV$.

Problem 11–8 indicates bound states at $k_0 < n\pi/2a$ for which the given information allows a solution for n. The answer must be an integer. When a graduation of $n\pi/2a$ is included in the constructive rectangle bounded on the right by k_0, another bound state is allowed.

11–15. (a) Calculate the eigenenergy for the bound state of a delta function potential

$$V(x) = -V_0\,a\,\delta(x) \qquad \text{given} \qquad E < 0\,.$$

(b) Compare your answer to the estimate of problem 11–7,

$$E = -\frac{mV_0^2a^2}{2\hbar^2}\,.$$

(c) Find and sketch the associated normalized wave function.

This exercise develops another limiting case for a finite square well. It intends that you apply the boundary value conditions of the wave function and its first derivative at boundaries. Delta functions can lead to relatively direct solutions, for instance, there is only one boundary so there are only two (instead of three or more) regions.

The units of a delta function depend on the space in which it is employed. The potential given is in one spatial dimension, for which a delta function is defined

$$\int_{-\infty}^{\infty}\delta(x)\,dx = \begin{cases} 1 & \text{if } x = 0\,, \\ 0 & \text{if } x \neq 0\,, \end{cases}$$

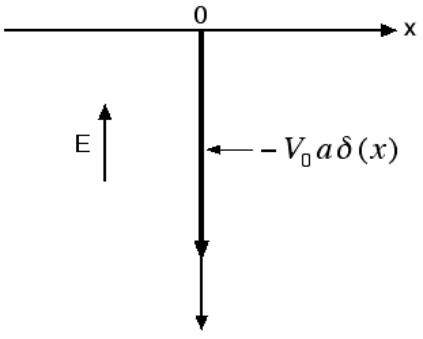

Figure 11–12. Negative delta function potential.

the differential dx has units of length, so the delta function must have units of inverse length in position space. Thus, the potential written $V(x) = -V_0\, a\, \delta(x)$ is dimensionally consistent while $-\alpha\, \delta(x)$ may be less clear because it leaves units as an implied portion of the constant α.

First, write the wave function for two regions, for instance,

$$\begin{aligned} \psi_1(x) &= A\, e^{\kappa x} + B\, e^{-\kappa x}, \quad x < 0 \\ \psi_2(x) &= C\, e^{\kappa x} + D\, e^{-\kappa x}, \quad x > 0 \end{aligned}$$

where $\kappa = \sqrt{-2mE}/\hbar$. The coefficients of two of the four terms must be zero because the associated exponential factors are not normalizable.

The delta function is a discontinuity. The value of the discontinuity in the first derivative was found in problem 9–7,

$$\Delta\left(\psi'(x)\right) = \frac{2m}{\hbar^2} \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} V(x)\, \psi(x)\, dx,$$

which allows you to write an equation for the first derivatives (see problem 9–8). Together with the condition of continuity of the wave function, all coefficients can be eliminated allowing solution for the part (b) energy. The part (b) comparison may be surprising. Normalize the wave function and prepare a sketch for part (c). The normalization condition is

$$\int_{-\infty}^{0} \left| N_1\, \psi(x) \right|^2 dx + \int_{0}^{\infty} \left| N_2\, \psi(x) \right|^2 dx = 1$$

avoiding the discontinuity, and you should conclude that the two integrals must be identical so the normalization constant can be obtained by doubling the integral from zero to infinity. Use

$$\int_0^{\infty} e^{-bx}\, dx = \frac{1}{b}.$$

Notice that part (a) asks for "the eigenenergy" in the singular. The delta function potential well has exactly one allowed bound energy state. This fact reinforces the statement that **all potential energy wells have at least one bound state**.

Chapter 12

Orbital Angular Momentum

Angular momentum comes in three flavors, orbital angular momentum, spin, and total angular momentum, which is the vector sum of orbital angular momentum and spin. This chapter is primarily about orbital angular momentum.

Classical orbital angular momentum is a vector quantity denoted $\vec{L} = \vec{r}\ \text{X}\ \vec{p}$. A common mnemonic to calculate the components is

$$\vec{L} = \begin{vmatrix} \widehat{i} & \widehat{j} & \widehat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} = \big(yp_z - zp_y\big)\widehat{i} + \big(zp_x - xp_z\big)\widehat{j} + \big(xp_y - yp_x\big)\widehat{k}$$
$$= L_x\widehat{i} + L_y\widehat{j} + L_z\widehat{k}\,.$$

Let's focus on one component of angular momentum, say $L_x = yp_z - zp_y$. On the right side of the equation are two components of position and two components of linear momentum. Quantum mechanically, all four quantities are dynamic variables which are operators. The components of quantum mechanical orbital angular momentum do not commute. Thus, we are forced to seek another operator, like $\mathcal{L}^2$ that does commute with the component operators, to obtain a complete set of commuting observables. As with the SHO, raising and lowering operators will be useful. Unlike all other systems encountered where one quantum number uniquely identifies the state, two quantum numbers are required to uniquely identify the quantum state of orbital angular momentum because two operators are required for the complete set of commuting observables.

The first part of this chapter is dominated by arguments from linear algebra and commutator algebra. The middle portion is calculus-based arguments in position space. Problems concerning angular momentum often use, some practically require, spherical polar coordinates. The special functions known as **spherical harmonics** are of particular importance in the description of quantum mechanical orbital angular momentum in position space. The final portion of this chapter revisits material from the first six chapters demonstrating its utility in $\mathbb{C}^3$ and applying the Heisenberg uncertainty relations to non-commuting operators.

The next chapter is the quantum mechanical description of the hydrogen atom. The electron orbits the proton, and defining the proton as the origin in a spherical polar coordinate description, the three parameters to consider are azimuthal angle, polar angle, and radial distance from the origin. The azimuthal angle and polar angle portions to the quantum mechanical description of the hydrogen atom are addressed largely in this chapter.

12–1. What are the component orbital angular momentum operators in position space?

Since the product of two operators is an operator, and the difference of operators is another operator, we expect the components of angular momentum to be operators. Quantum mechanically,

$$\mathcal{L}_x = \mathcal{Y}\mathcal{P}_z - \mathcal{Z}\mathcal{P}_y, \qquad \mathcal{L}_y = \mathcal{Z}\mathcal{P}_x - \mathcal{X}\mathcal{P}_z, \qquad \mathcal{L}_z = \mathcal{X}\mathcal{P}_y - \mathcal{Y}\mathcal{P}_x\,. \tag{1}$$

These are the component operators. Angular momentum is the vector sum of the components. The sum of operators is another operator, so angular momentum is an operator. We have not encountered an operator like this though it is comparable to a vector sum of operators.

Equation (1) is in abstract Hilbert space and is devoid of a representation. In position space

$$\mathcal{X} \;\rightarrow\; x, \qquad \mathcal{Y} \;\rightarrow\; y, \qquad \text{and} \qquad \mathcal{Z} \;\rightarrow\; z, \qquad \text{and}$$

$$\mathcal{P}_x \;\rightarrow\; -i\hbar\frac{\partial}{\partial x}, \qquad \mathcal{P}_y \;\rightarrow\; -i\hbar\frac{\partial}{\partial y}, \qquad \text{and} \qquad \mathcal{P}_z \;\rightarrow\; -i\hbar\frac{\partial}{\partial z}.$$

Equation (1) in position space would then be written

$$\mathcal{L}_x \;=\; -i\hbar y\frac{\partial}{\partial z} \;+\; i\hbar z\frac{\partial}{\partial y}\,, \qquad \mathcal{L}_y \;=\; -i\hbar z\frac{\partial}{\partial x} \;+\; i\hbar x\frac{\partial}{\partial z}\,, \qquad \mathcal{L}_z \;=\; -i\hbar x\frac{\partial}{\partial y} \;+\; i\hbar y\frac{\partial}{\partial x}\,. \quad (2)$$

Postscript: The operator nature of the components promise challenges, because unlike their classical analogs which are scalars, the component angular momentum operators do not commute.

The orbital angular momentum operator is conventionally written just $\mathcal{L}$, and the component nature of quantum mechanical angular momentum is only implied and not explicitly written.

12–2. Show that the components of angular momentum do not commute in position space.

Let the commutator of any two components, say $\big[\mathcal{L}_x, \mathcal{L}_y\big]$, act on any function. Pick a simple function like x, to show $\big[\mathcal{L}_x, \mathcal{L}_y\big] \neq 0$.

$$\big[\mathcal{L}_x, \mathcal{L}_y\big]x \;=\; \big(\mathcal{L}_x\,\mathcal{L}_y - \mathcal{L}_y\,\mathcal{L}_x\big)x$$

$$\rightarrow\; \left(-i\hbar y\frac{\partial}{\partial z} + i\hbar z\frac{\partial}{\partial y}\right)\left(-i\hbar z\frac{\partial}{\partial x} + i\hbar x\frac{\partial}{\partial z}\right)x \;-\; \left(-i\hbar z\frac{\partial}{\partial x} + i\hbar x\frac{\partial}{\partial z}\right)\left(-i\hbar y\frac{\partial}{\partial z} + i\hbar z\frac{\partial}{\partial y}\right)x$$

$$= \left(-i\hbar y\frac{\partial}{\partial z} + i\hbar z\frac{\partial}{\partial y}\right)\big(-i\hbar z\big) \;-\; \left(-i\hbar z\frac{\partial}{\partial x} + i\hbar x\frac{\partial}{\partial z}\right)(0)$$

$$= \Big(\big(-i\hbar\big)^2 y\Big) \;=\; -\hbar^2 y \neq 0,$$

therefore $\mathcal{L}_x$ and $\mathcal{L}_y$ do not commute. The other components of angular momentum can be shown not to commute similarly.

12–3. Represent equation (1) in the momentum basis.

In momentum space, the operators are

$$\mathcal{X} \;\rightarrow\; i\hbar\frac{\partial}{\partial p_x}, \qquad \mathcal{Y} \;\rightarrow\; i\hbar\frac{\partial}{\partial p_y}, \qquad \text{and} \qquad \mathcal{Z} \;\rightarrow\; i\hbar\frac{\partial}{\partial p_z}, \qquad \text{and}$$

$$\mathcal{P}_x \;\rightarrow\; p_x\,, \qquad \mathcal{P}_y \;\rightarrow\; p_y\,, \qquad \text{and} \qquad \mathcal{P}_z \;\rightarrow\; p_z\,.$$

Equation (1) in momentum space would be written

$$\mathcal{L}_x \;=\; i\hbar\frac{\partial}{\partial p_y}\,p_z \;-\; i\hbar\frac{\partial}{\partial p_z}\,p_y\,, \qquad \mathcal{L}_y \;=\; i\hbar\frac{\partial}{\partial p_z}\,p_x \;-\; i\hbar\frac{\partial}{\partial p_x}\,p_z\,, \qquad \mathcal{L}_z \;=\; i\hbar\frac{\partial}{\partial p_x}\,p_y \;-\; i\hbar\frac{\partial}{\partial p_y}\,p_x\,.$$

12–4. Develop the canonical commutation relations in three dimensions.

In one dimension, the fundamental canonical commutator is $\left[\,\mathcal{X},\,\mathcal{P}_x\,\right] \;=\; i\hbar\,.$ In position space,

$$\begin{aligned}\left[\,\mathcal{X},\,\mathcal{P}_x\,\right] f(x) \;&=\; \left(\mathcal{X}\,\mathcal{P}_x \;-\; \mathcal{P}_x\,\mathcal{X}\right) f(x) \;\rightarrow\; x\left(-i\hbar\frac{d}{dx}\right) f(x) \;-\; \left(-i\hbar\frac{d}{dx}\right) x\,f(x) \\ &=\; -i\hbar x f'(x) \;-\; (-i\hbar)\;f(x) \;-\; -i\hbar x\,f'(x) \\ &=\; -i\hbar\cancel{x f'(x)} \;+\; i\hbar\,f(x) \;+\; i\hbar\cancel{x f'(x)} \;=\; i\hbar\,f(x)\end{aligned}$$

where the terms that sum to zero have been struck. Orbital angular momentum generally requires three dimensions.

The generalization to three dimensions is

$$\left[\,\mathcal{X}_i,\,\mathcal{X}_j\,\right] \;=\; 0\,, \tag{3}$$

meaning any position component commutes with any other position component including itself,

$$\left[\,\mathcal{P}_i,\,\mathcal{P}_j\,\right] \;=\; 0\,, \tag{4}$$

which means any linear momentum component commutes with any other linear momentum component including itself, and

$$\left[\,\mathcal{X}_i,\,\mathcal{P}_j\,\right] \;=\; i\hbar\,\delta_{i,j}\,. \tag{5}$$

The meaning of this equation requires some discussion. This means a position component will commute with an unlike component of linear momentum,

$$\left[\,\mathcal{X},\,\mathcal{P}_y\,\right] \;=\; \left[\,\mathcal{X},\,\mathcal{P}_z\,\right] \;=\; \left[\,\mathcal{Y},\mathcal{P}_x\,\right] \;=\; \left[\,\mathcal{Y},\,\mathcal{P}_z\,\right] \;=\; \left[\,\mathcal{Z},\,\mathcal{P}_x\,\right] \;=\; \left[\,\mathcal{Z},\,\mathcal{P}_y\,\right] \;=\; 0\,,$$

but a position component and a like component of linear momentum are canonical commutators,

$$\left[\,\mathcal{X},\,\mathcal{P}_x\,\right] \;=\; \left[\,\mathcal{Y},\,\mathcal{P}_y\,\right] \;=\; \left[\,\mathcal{Z},\,\mathcal{P}_z\,\right] \;=\; i\hbar\,.$$

Postscript: Much depends on commutator algebra. The derivations of equations (3), (4), and (5) are left as exercises. The solutions to these exercises are modeled by the prescript to this problem. The differences are the three dimensional cases require partial derivatives, and the function needs to be more general, for instance $f \;=\; f\,(x,y,z)\,.$

12–5. Show that for any operators $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$,

$$\big[\mathcal{A},\,\mathcal{B}\mathcal{C}\big] \;=\; \big[\mathcal{A},\,\mathcal{B}\big]\,\mathcal{C} \;+\; \mathcal{B}\,\big[\mathcal{A},\,\mathcal{C}\big]\,,$$

In order to use equations (3) through (5), we need to develop some relations for commutators in excess of those discussed earlier. For any operators $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$, the relations below, some of which we have used previously, may be a useful list.

$$\begin{aligned}
\big[\mathcal{A},\,\mathcal{A}\big] &= 0 \\
\big[\mathcal{A},\,\mathcal{B}\big] &= -\big[\mathcal{B},\,\mathcal{A}\big] \\
\big[\mathcal{A},\,c\big] &= 0, \qquad \text{for any scalar } c, \\
\big[\mathcal{A},\,c\mathcal{B}\big] &= c\,\big[\mathcal{A},\,\mathcal{B}\big], \qquad \text{for any scalar } c, \\
\big[\mathcal{A}+\mathcal{B},\,\mathcal{C}\big] &= \big[\mathcal{A},\,\mathcal{C}\big] \;+\; \big[\mathcal{B},\,\mathcal{C}\big] \\
\big[\mathcal{A},\,\mathcal{B}\mathcal{C}\big] &= \big[\mathcal{A},\,\mathcal{B}\big]\,\mathcal{C} \;+\; \mathcal{B}\,\big[\mathcal{A},\,\mathcal{C}\big] \qquad (6)
\end{aligned}$$

$$\Big[\mathcal{A},\,\big[\mathcal{B},\,\mathcal{C}\big]\Big] \;+\; \Big[\mathcal{B},\,\big[\mathcal{C},\,\mathcal{A}\big]\Big] \;+\; \Big[\mathcal{C},\,\big[\mathcal{A},\,\mathcal{B}\big]\Big] \;=\; 0\,.$$

Equation (6) is a relation we want to develop further.

$$\begin{aligned}
\big[\mathcal{A},\,\mathcal{B}\mathcal{C}\big] &= \mathcal{A}\mathcal{B}\mathcal{C} \;-\; \mathcal{B}\mathcal{C}\mathcal{A} \\
&= \mathcal{A}\mathcal{B}\mathcal{C} \;-\; \mathcal{B}\mathcal{A}\mathcal{C} \;+\; \mathcal{B}\mathcal{A}\mathcal{C} \;-\; \mathcal{B}\mathcal{C}\mathcal{A} \\
&= \big(\mathcal{A}\mathcal{B} \;-\; \mathcal{B}\mathcal{A}\big)\,\mathcal{C} \;+\; \mathcal{B}\,\big(\mathcal{A}\mathcal{C} \;-\; \mathcal{C}\mathcal{A}\big) \\
&= \big[\mathcal{A},\,\mathcal{B}\big]\,\mathcal{C} \;+\; \mathcal{B}\,\big[\mathcal{A},\,\mathcal{C}\big]\,,
\end{aligned}$$

where we have added zero, in the form $-\mathcal{B}\mathcal{A}\mathcal{C} \;+\; \mathcal{B}\mathcal{A}\mathcal{C}$, in the second line.

Postscript: You may have encountered relations similar to these in classical mechanics where the brackets are Poisson brackets. We are interested in quantum mechanical commutators and there are two important differences. Classical mechanics is concerned with quantities which are intrinsically real and are of finite dimension. Quantum mechanics is concerned with quantities which are intrinsically complex and are generally of infinite dimension.

12–6. Develop a relation for $\big[\mathcal{A}\mathcal{B},\,\mathcal{C}\big]$ in terms of commutators of individual operators.

The double operator in equation (6) is the second operator in the commutator. This problem develops a similar relation where the double operator is the first operator in the commutator.

$$\begin{aligned}
\big[\mathcal{A}\mathcal{B},\,\mathcal{C}\big] &= \mathcal{A}\mathcal{B}\mathcal{C} \;-\; \mathcal{C}\mathcal{A}\mathcal{B} \\
&= \mathcal{A}\mathcal{B}\mathcal{C} \;-\; \mathcal{A}\mathcal{C}\mathcal{B} \;+\; \mathcal{A}\mathcal{C}\mathcal{B} \;-\; \mathcal{C}\mathcal{A}\mathcal{B} \\
&= \mathcal{A}\,\big(\mathcal{B}\mathcal{C} \;-\; \mathcal{C}\mathcal{B}\big) \;+\; \big(\mathcal{A}\mathcal{C} \;-\; \mathcal{C}\mathcal{A}\big)\,\mathcal{B} \\
&= \mathcal{A}\,\big[\mathcal{B},\,\mathcal{C}\big] \;+\; \big[\mathcal{A},\,\mathcal{C}\big]\,\mathcal{B}.
\end{aligned}$$

where zero in the form $-\mathcal{A}\mathcal{C}\mathcal{B} \;+\; \mathcal{A}\mathcal{C}\mathcal{B}$ is added in the second line.

12–7. Develop a relation for $\big[\,\mathcal{A}\,\mathcal{B},\,\mathcal{C}\,\mathcal{D}\,\big]$ in terms of commutators of individual operators.

Problems 12–5, 12–6, and 12–7 are intended to build some familiarity with commutator algebra, but are really motivated to reach the result of problem 12–8. Here the results of the last two problems are used to arrive at a third relation that will be useful in problem 12–8.

Using the result of problem 12–5,

$$\big[\,\mathcal{A}\,\mathcal{B},\,\mathcal{C}\,\mathcal{D}\,\big] \;=\; \big[\,\mathcal{A}\,\mathcal{B},\,\mathcal{C}\,\big]\,\mathcal{D} \;+\; \mathcal{C}\,\big[\,\mathcal{A}\,\mathcal{B},\,\mathcal{D}\,\big]\,,$$

and then using the result of problem 12–6 on both of the commutators on the right,

$$\begin{aligned}\big[\,\mathcal{A}\,\mathcal{B},\,\mathcal{C}\,\mathcal{D}\,\big] \;&=\; \Big(\mathcal{A}\,\big[\,\mathcal{B},\,\mathcal{C}\,\big] + \big[\,\mathcal{A},\,\mathcal{C}\,\big]\,\mathcal{B}\Big)\,\mathcal{D} \;+\; \mathcal{C}\,\Big(\mathcal{A}\,\big[\,\mathcal{B},\,\mathcal{D}\,\big] + \big[\,\mathcal{A},\,\mathcal{D}\,\big]\,\mathcal{B}\Big) \\ &=\; \mathcal{A}\,\big[\,\mathcal{B},\,\mathcal{C}\,\big]\,\mathcal{D} \;+\; \big[\,\mathcal{A},\,\mathcal{C}\,\big]\,\mathcal{B}\,\mathcal{D} \;+\; \mathcal{C}\,\mathcal{A}\,\big[\,\mathcal{B},\,\mathcal{D}\,\big] \;+\; \mathcal{C}\,\big[\,\mathcal{A},\,\mathcal{D}\,\big]\,\mathcal{B}\,,\end{aligned}$$

which is the desired result.

12–8. Show $\big[\,\mathcal{L}_x,\,\mathcal{L}_y\,\big] \;=\; i\hbar\,\mathcal{L}_z$.

Given the relations of equations (3) through (5) and the thus far developed commutator algebra, it follows that

$$\big[\,\mathcal{L}_x,\,\mathcal{L}_y\,\big] \;=\; i\hbar\,\mathcal{L}_z, \qquad \big[\,\mathcal{L}_y,\,\mathcal{L}_z\,\big] \;=\; i\hbar\,\mathcal{L}_x, \qquad \text{and} \qquad \big[\,\mathcal{L}_z,\,\mathcal{L}_x\,\big] \;=\; i\hbar\,\mathcal{L}_y. \tag{7}$$

These are known as the **orbital angular momentum commutation relations**, or more commonly just the **angular momentum commutation relations**.

$$\begin{aligned}\big[\,\mathcal{L}_x,\,\mathcal{L}_y\,\big] \;&=\; \big[\,\mathcal{Y}\,\mathcal{P}_z - \mathcal{Z}\,\mathcal{P}_y,\;\mathcal{Z}\,\mathcal{P}_x - \mathcal{X}\,\mathcal{P}_z\,\big] \\ &=\; \Big(\mathcal{Y}\,\mathcal{P}_z - \mathcal{Z}\,\mathcal{P}_y\Big)\Big(\mathcal{Z}\,\mathcal{P}_x - \mathcal{X}\,\mathcal{P}_z\Big) \;-\; \Big(\mathcal{Z}\,\mathcal{P}_x - \mathcal{X}\,\mathcal{P}_z\Big)\Big(\mathcal{Y}\,\mathcal{P}_z - \mathcal{Z}\,\mathcal{P}_y\Big)\end{aligned}$$

$$= \;\mathcal{Y}\,\mathcal{P}_z\mathcal{Z}\,\mathcal{P}_x - \mathcal{Y}\,\mathcal{P}_z\mathcal{X}\,\mathcal{P}_z - \mathcal{Z}\,\mathcal{P}_y\mathcal{Z}\,\mathcal{P}_x + \mathcal{Z}\,\mathcal{P}_y\mathcal{X}\,\mathcal{P}_z - \mathcal{Z}\,\mathcal{P}_x\mathcal{Y}\,\mathcal{P}_z + \mathcal{Z}\,\mathcal{P}_x\mathcal{Z}\,\mathcal{P}_y + \mathcal{X}\,\mathcal{P}_z\mathcal{Y}\,\mathcal{P}_z - \mathcal{X}\,\mathcal{P}_z\mathcal{Z}\,\mathcal{P}_y$$

$$\begin{aligned}= \;&\Big(\mathcal{Y}\,\mathcal{P}_z\mathcal{Z}\,\mathcal{P}_x - \mathcal{Z}\,\mathcal{P}_x\mathcal{Y}\,\mathcal{P}_z\Big) \;+\; \Big(\mathcal{Z}\,\mathcal{P}_y\mathcal{X}\,\mathcal{P}_z - \mathcal{X}\,\mathcal{P}_z\mathcal{Z}\,\mathcal{P}_y\Big) \\ &\qquad\qquad +\; \Big(\mathcal{Z}\,\mathcal{P}_x\mathcal{Z}\,\mathcal{P}_y - \mathcal{Z}\,\mathcal{P}_y\mathcal{Z}\,\mathcal{P}_x\Big) \;+\; \Big(\mathcal{X}\,\mathcal{P}_z\mathcal{Y}\,\mathcal{P}_z - \mathcal{Y}\,\mathcal{P}_z\mathcal{X}\,\mathcal{P}_z\Big) \\ &=\; \big[\,\mathcal{Y}\,\mathcal{P}_z,\;\mathcal{Z}\,\mathcal{P}_x\,\big] \;+\; \big[\,\mathcal{Z}\,\mathcal{P}_y,\;\mathcal{X}\,\mathcal{P}_z\,\big] \;+\; \big[\,\mathcal{Z}\,\mathcal{P}_x,\;\mathcal{Z}\,\mathcal{P}_y\,\big] \;+\; \big[\,\mathcal{X}\,\mathcal{P}_z,\;\mathcal{Y}\,\mathcal{P}_z\,\big].\end{aligned}$$

Now applying the result of problem 12–7, the plan is to express these commutators in terms of individual operators, and then evaluate those using the commutation relations of equations (3) through (5). In problem 12–7, one commutator of the products of two operators turns into four commutators. Since we start with four commutators of the products of two operators, we are going to get 16 commutators in terms of individual operators. The good news is 14 of them are zero from equations (3), (4), and (5), so will be struck.

$$
\begin{aligned}
\big[\,\mathcal{L}_x,\,\mathcal{L}_y\,\big] \;&=\; \mathcal{Y}\,\big[\,\mathcal{P}_z,\,\mathcal{Z}\,\big]\,\mathcal{P}_x \;+\; \big[\,\mathcal{Y},\cancel{\mathcal{Z}}\,\big]\,\mathcal{P}_z\,\mathcal{P}_x \;+\; \mathcal{Z}\,\mathcal{Y}\,\big[\,\mathcal{P}_z,\cancel{\mathcal{P}_x}\,\big] \;+\; \mathcal{Z}\,\big[\,\mathcal{Y},\cancel{\mathcal{P}_x}\,\big]\,\mathcal{P}_z \\
&+\; \mathcal{Z}\,\big[\,\mathcal{P}_y,\cancel{\mathcal{X}}\,\big]\,\mathcal{P}_z \;+\; \big[\,\mathcal{Z},\cancel{\mathcal{X}}\,\big]\,\mathcal{P}_y\,\mathcal{P}_z \;+\; \mathcal{X}\,\mathcal{Z}\,\big[\,\mathcal{P}_y,\cancel{\mathcal{P}_z}\,\big] \;+\; \mathcal{X}\,\big[\,\mathcal{Z},\,\mathcal{P}_z\,\big]\,\mathcal{P}_y \\
&+\; \mathcal{Z}\,\big[\,\mathcal{P}_x,\cancel{\mathcal{Z}}\,\big]\,\mathcal{P}_y \;+\; \big[\,\mathcal{Z},\cancel{\mathcal{Z}}\,\big]\,\mathcal{P}_x\,\mathcal{P}_y \;+\; \mathcal{Z}\,\mathcal{Z}\,\big[\,\mathcal{P}_x,\cancel{\mathcal{P}_y}\,\big] \;+\; \mathcal{Z}\,\big[\,\mathcal{Z},\cancel{\mathcal{P}_y}\,\big]\,\mathcal{P}_x \\
&+\; \mathcal{X}\,\big[\,\mathcal{P}_z,\cancel{\mathcal{Y}}\,\big]\,\mathcal{P}_z \;+\; \big[\,\mathcal{X},\cancel{\mathcal{Y}}\,\big]\,\mathcal{P}_z\,\mathcal{P}_z \;+\; \mathcal{Y}\,\mathcal{X}\,\big[\,\mathcal{P}_z,\cancel{\mathcal{P}_z}\,\big] \;+\; \mathcal{Y}\,\big[\,\mathcal{X},\cancel{\mathcal{P}_z}\,\big]\,\mathcal{P}_z \\
&=\; \mathcal{Y}\,\big[\,\mathcal{P}_z,\,\mathcal{Z}\,\big]\,\mathcal{P}_x \;+\; \mathcal{X}\,\big[\,\mathcal{Z},\,\mathcal{P}_z\,\big]\,\mathcal{P}_y \\
&=\; \mathcal{Y}\big(-i\hbar\big)\mathcal{P}_x \;+\; \mathcal{X}\big(i\hbar\big)\mathcal{P}_y \\
&=\; i\hbar\big(\mathcal{X}\,\mathcal{P}_y - \mathcal{Y}\,\mathcal{P}_x\big) \;=\; i\hbar\mathcal{L}_z.
\end{aligned}
$$

Postscript: The other two relations, $\big[\,\mathcal{L}_y,\,\mathcal{L}_z\,\big] = i\hbar\,\mathcal{L}_x$ and $\big[\,\mathcal{L}_z,\,\mathcal{L}_x\,\big] = i\hbar\,\mathcal{L}_y$ can be calculated using similar procedures.

The operators $\mathcal{L}_x$, $\mathcal{L}_y$, and $\mathcal{L}_z$ are abstract operators in an infinite dimensional Hilbert space. Practical calculations can be accomplished in the much simpler subspace $\mathbb{C}^3$. In other words, we want 3 X 3 matrix operators that satisfy the angular momentum commutation relations. The component angular momentum operators do not commute meaning that we can diagonalize one, but only one. The most popular choice is to diagonalize $\mathcal{L}_z$. So, **in the $\underline{\mathcal{L}_z}$ basis**

$$
\mathcal{L}_x \;\to\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar\,, \qquad \mathcal{L}_y \;\to\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar\,, \qquad \mathcal{L}_z \;\to\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\hbar\,. \tag{8}
$$

In a basis which makes $\mathcal{L}_x$ or $\mathcal{L}_y$ diagonal, the angular momentum matrix operators are different than those seen in relations (8). This is the most popular representation of these matrix operators.

12–9. Show $\big[\,\mathcal{L}_x,\,\mathcal{L}_y\,\big] = i\hbar\,\mathcal{L}_z$ using relations (8).

$$
\big[\,\mathcal{L}_x,\,\mathcal{L}_y\,\big] \;\to\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar \;-\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar
$$

$$
=\; \frac{\hbar^2}{2}\begin{pmatrix} i & 0 & -i \\ 0 & -i+i & 0 \\ i & 0 & -i \end{pmatrix} \;-\; \frac{\hbar^2}{2}\begin{pmatrix} -i & 0 & -i \\ 0 & i-i & 0 \\ i & 0 & i \end{pmatrix} \;=\; \frac{\hbar^2}{2}\begin{pmatrix} i+i & 0 & -i+i \\ 0 & 0 & 0 \\ i-i & 0 & -i-i \end{pmatrix}
$$

$$
=\; \frac{\hbar^2}{2}\begin{pmatrix} 2i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2i \end{pmatrix} \;=\; i\hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\hbar \;\to\; i\hbar\,\mathcal{L}_z\,.
$$

12–10. Define $\mathcal{L}^2 = \mathcal{L}_x^2 + \mathcal{L}_y^2 + \mathcal{L}_z^2$. Show $\mathcal{L}^2 = 2\hbar^2\mathcal{I}$.

The component angular momentum operators do not commute. The sum of the squares of the component angular momentum operators, $\mathcal{L}_x^2 + \mathcal{L}_y^2 + \mathcal{L}_z^2$, does commute with the component angular momentum operators. This sum is denoted $\mathcal{L}^2$ for convenience. Also conveniently,

$$\mathcal{L}^2 = 2\hbar^2\mathcal{I} \rightarrow 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{9}$$

in $\mathbb{C}^3$. This is a simply an exercise in matrix arithmetic.

$$\mathcal{L}^2 = \mathcal{L}_x^2 + \mathcal{L}_y^2 + \mathcal{L}_z^2$$

$$\rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \hbar \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \hbar + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \hbar \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \hbar$$
$$+ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \hbar$$

$$= \frac{1}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1+1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \hbar^2 + \frac{1}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1+1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \hbar^2 + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \hbar^2$$

$$= \begin{pmatrix} 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{pmatrix} \hbar^2 + \begin{pmatrix} 1/2 & 0 & -1/2 \\ 0 & 1 & 0 \\ -1/2 & 0 & 1/2 \end{pmatrix} \hbar^2 + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \hbar^2$$

$$= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \hbar^2 + \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \hbar^2 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \hbar^2 = 2\hbar^2\mathcal{I}.$$

Postscript: The Hamiltonian for a spherically symmetric potential commutes with $\mathcal{L}^2$ and the three component angular momentum operators. So $\mathcal{H}$, $\mathcal{L}^2$, and one of the three component angular momentum operators, conventionally $\mathcal{L}_z$, is a complete set of commuting observables for a spherically symmetric potential.

We will use a Hamiltonian with a Coulomb potential for the hydrogen atom. The Coulomb potential is rotationally invariant, or spherically symmetric. We have indicated $\mathcal{H}$, $\mathcal{L}^2$, and $\mathcal{L}_z$ form a complete set of commuting observables for such a system. You may be familiar with the principal quantum number n, the angular momentum quantum number l, and the magnetic quantum number m for hydrogen from other studies. We will find there is a correspondence

between these two sets of three quantities, which is n comes from application of $\mathcal{H}$, l comes from application of $\mathcal{L}^2$, and m comes from application of $\mathcal{L}_z$. A significant portion of the reason to address angular momentum now is for use in the next chapter on the hydrogen atom.

12–11. Show that $\mathcal{L}^2$ commutes with $\mathcal{L}_y$ in $\mathbb{C}^3$.

This is a partial proof that $\mathcal{L}^2$ commutes with $\mathcal{L}_x$, $\mathcal{L}_y$, and $\mathcal{L}_z$.

$$\big[\,\mathcal{L}^2,\,\mathcal{L}_y\,\big] \;\to\; \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \hbar^2 \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \hbar \;-\; \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \hbar \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \hbar^2$$

$$= \frac{\hbar^3}{\sqrt{2}} \begin{pmatrix} 0 & -2i & 0 \\ 2i & 0 & -2i \\ 0 & 2i & 0 \end{pmatrix} \;-\; \frac{\hbar^3}{\sqrt{2}} \begin{pmatrix} 0 & -2i & 0 \\ 2i & 0 & -2i \\ 0 & 2i & 0 \end{pmatrix} \;=\; 0$$

Postscript: The fact that $\mathcal{L}^2$ commutes with component operators of orbital angular momentum is of fundamental physical importance in creating a complete set of commuting observables for the hydrogen atom (and other systems with spherical symmetry if you want).

Mathematically, we expect the identity operator and a scalar multiple of the identity operator, like $\mathcal{L}^2 = 2\hbar^2\mathcal{I}$, to commute with any other operator in the same space.

12–12. Show $\mathcal{L}_x^2 + \mathcal{L}_y^2 \neq \big(\mathcal{L}_x + i\mathcal{L}_y\big)\big(\mathcal{L}_x - i\mathcal{L}_y\big)$.

We are going to address angular momentum, like the SHO, from both a linear algebra and a differential equation perspective. We are going to assume rotational invariance, or spherical symmetry, for the hydrogen atom so will have $\mathcal{H}$, $\mathcal{L}^2$, and $\mathcal{L}_z$ as a complete set of commuting observables. The linear algebra arguments will be first, working only with the components and $\mathcal{L}^2$. The Hamiltonian for a Coulomb potential is added in the next chapter.

The four angular momentum operators are related as

$$\mathcal{L}^2 \;=\; \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; \mathcal{L}_z^2 \quad\Rightarrow\quad \mathcal{L}^2 \;-\; \mathcal{L}_z^2 \;=\; \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2.$$

The sum of the two components $\mathcal{L}_x^2 + \mathcal{L}_y^2$ would appear to factor

$$\big(\mathcal{L}_x + i\mathcal{L}_y\big)\big(\mathcal{L}_x - i\mathcal{L}_y\big), \tag{10}$$

and they would if the factors were scalars, but they are operators which do not commute, so this is not actually factoring. Just like the SHO, the sometimes named **factorization method** is useful for the development of arguments using linear algebra. Also like the SHO, raising and lowering operators will be useful.

$$\begin{aligned}
\big(\mathcal{L}_x + i\mathcal{L}_y\big)\big(\mathcal{L}_x - i\mathcal{L}_y\big) &= \mathcal{L}_x^2 \;-\; i\mathcal{L}_x\mathcal{L}_y \;+\; i\mathcal{L}_y\mathcal{L}_x \;+\; \mathcal{L}_y^2 \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;-\; i\big(\mathcal{L}_x\mathcal{L}_y - \mathcal{L}_y\mathcal{L}_x\big) \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;-\; i\big[\mathcal{L}_x,\, \mathcal{L}_y\big] \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;-\; i\big(i\hbar\mathcal{L}_z\big) \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; \hbar\mathcal{L}_z \qquad (11) \\
&\neq \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2
\end{aligned}$$

Postscript: The expression in the next to last line is a significant intermediate result, and we will have reason to refer to it.

Like the SHO, the idea is to take advantage of the angular momentum commutation relations from equation (7). We will use the notation

$$\mathcal{L}_+ \;=\; \mathcal{L}_x \;+\; i\mathcal{L}_y \qquad \text{and} \qquad \mathcal{L}_- \;=\; \mathcal{L}_x \;-\; i\mathcal{L}_y\,. \qquad (12)$$

The operator $\mathcal{L}_+$ is known as the **raising operator** and the operator $\mathcal{L}_-$ is known as the **lowering operator**. They are commonly denoted together as $\mathcal{L}_\pm$ and are called the **ladder operators** for orbital angular momentum.

12–13. Show that $\mathcal{L}_-\mathcal{L}_+ \;=\; \mathcal{L}^2 \;-\; \mathcal{L}_z^2 \;-\; \hbar\mathcal{L}_z\,.$

The intent is to develop this operator that we will need later in a calculation similar to the last.

$$\begin{aligned}
\mathcal{L}_-\mathcal{L}_+ &= \big(\mathcal{L}_x - i\mathcal{L}_y\big)\big(\mathcal{L}_x + i\mathcal{L}_y\big) \\
&= \mathcal{L}_x^2 \;+\; i\mathcal{L}_x\mathcal{L}_y \;-\; i\mathcal{L}_y\mathcal{L}_x \;+\; \mathcal{L}_y^2 \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; i\big(\mathcal{L}_x\mathcal{L}_y - \mathcal{L}_y\mathcal{L}_x\big) \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; i\big[\mathcal{L}_x,\, \mathcal{L}_y\big] \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; i\big(i\hbar\mathcal{L}_z\big) \\
&= \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;-\; \hbar\mathcal{L}_z \\
\mathcal{L}^2 \;=\; \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; \mathcal{L}_z^2 \quad &\Rightarrow \quad \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;=\; \mathcal{L}^2 \;-\; \mathcal{L}_z^2 \\
\Rightarrow \quad \mathcal{L}_-\mathcal{L}_+ \;&=\; \mathcal{L}^2 \;-\; \mathcal{L}_z^2 \;-\; \hbar\mathcal{L}_z\,.
\end{aligned}$$

12–14. Show that $\big[\mathcal{L}^2,\, \mathcal{L}_+\big] \;=\; 0\,.$

Problems 12–14 and 12–15 develop the commutators for $\mathcal{L}_\pm$. In general,

$$\big[\mathcal{L}^2,\, \mathcal{L}_\pm\big] \;=\; 0\,. \qquad (13)$$

$$\big[\mathcal{L}^2,\, \mathcal{L}_+\big] \;=\; \big[\mathcal{L}^2,\, \mathcal{L}_x + i\mathcal{L}_y\big] \;=\; \big[\mathcal{L}^2,\, \mathcal{L}_x\big] \;+\; i\big[\mathcal{L}^2,\, \mathcal{L}_y\big] \;=\; 0 \;+\; i(0) \;=\; 0.$$

12–15. Show that $\big[\mathcal{L}_z,\, \mathcal{L}_+\big] \;=\; \hbar\, \mathcal{L}_+ \,.$

This problem uses the expression in equation (11) from problem 12–12. In general,

$$\big[\mathcal{L}_z,\, \mathcal{L}_\pm\big] \;=\; \pm\hbar\, \mathcal{L}_\pm \,. \tag{14}$$

$$\big[\mathcal{L}_z,\, \mathcal{L}_+\big] \;=\; \big[\mathcal{L}_z,\, \mathcal{L}_x + i\mathcal{L}_y\big] \;=\; \big[\mathcal{L}_z,\, \mathcal{L}_x\big] + i\big[\mathcal{L}_z,\, \mathcal{L}_y\big] \;=\; i\hbar\mathcal{L}_y + i\big(-i\hbar\mathcal{L}_x\big) \;=\; \hbar\big(\mathcal{L}_x + i\mathcal{L}_y\big) \;=\; \hbar\mathcal{L}_+ \,.$$

Postscript: The linear algebra arguments that follow rely heavily on equation 14.

12–16. Show $\mathcal{L}^2$ and $\mathcal{L}_z$ commute using commutator algebra.

Remember that all operators commute with themselves and powers of themselves. The reduction uses the result of problem 12–6 and the angular momentum commutation relations.

$$\begin{aligned}
\big[\mathcal{L}^2,\, \mathcal{L}_z\big] \;&=\; \big[\mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; \mathcal{L}_z^2,\; \mathcal{L}_z\big] \\
&=\; \big[\mathcal{L}_x^2,\, \mathcal{L}_z\big] \;+\; \big[\mathcal{L}_y^2,\, \mathcal{L}_z\big] \;+\; \cancel{\big[\mathcal{L}_z^2,\, \mathcal{L}_z\big]} \\
&=\; \big[\mathcal{L}_x\, \mathcal{L}_x,\, \mathcal{L}_z\big] \;+\; \big[\mathcal{L}_y\, \mathcal{L}_y,\, \mathcal{L}_z\big] \\
&=\; \mathcal{L}_x\big[\mathcal{L}_x,\, \mathcal{L}_z\big] \;+\; \big[\mathcal{L}_x,\, \mathcal{L}_z\big]\mathcal{L}_x \;+\; \mathcal{L}_y\big[\mathcal{L}_y,\, \mathcal{L}_z\big] \;+\; \big[\mathcal{L}_y,\, \mathcal{L}_z\big]\mathcal{L}_y \\
&=\; \mathcal{L}_x\big(-i\hbar\mathcal{L}_y\big) \;+\; \big(-i\hbar\mathcal{L}_y\big)\mathcal{L}_x \;+\; \mathcal{L}_y\big(i\hbar\mathcal{L}_x\big) \;+\; \big(i\hbar\mathcal{L}_x\big)\mathcal{L}_y \\
&=\; \big(-i\hbar\mathcal{L}_x\, \mathcal{L}_y + i\hbar\mathcal{L}_x\, \mathcal{L}_y\big) \;+\; \big(-i\hbar\mathcal{L}_y\, \mathcal{L}_x + i\hbar\mathcal{L}_y\, \mathcal{L}_x\big) \;=\; 0 \,.
\end{aligned}$$

Postscript: That $\mathcal{L}^2$ and $\mathcal{L}_z$ commute means they share a common eigenbasis.

Prelude: The next six problems are really one problem broken into a sequence of smaller parts. The intent is to show

$$\mathcal{L}^2\,|\,l,\, m>\;=\; \hbar^2\, l(l+1)\,|\,l,\, m>, \qquad l \;\geq\; 0 \tag{15}$$

$$\mathcal{L}_z\,|\,l,\, m>\;=\; m\hbar\,|\,l,\, m>, \qquad -l \;\leq\; m \;\leq\; l \tag{16}$$

using eigenvector/eigenvalue arguments. The general eigenvector/eigenvalue problem is

$$\mathcal{A}\,|\,v>\;=\; \alpha\,|\,v>\,, \tag{17}$$

where $|\,v>$ is the eigenvector and α is the eigenvalue of the operator $\mathcal{A}$. Equation (15) and (16) are comparable to equation (17) for the eigenvector $|\,l,\, m>$, where the eigenvalue of $\mathcal{L}^2$ is $\hbar^2\, l(l+1)$ and the eigenvalue of $\mathcal{L}_z$ is $m\hbar$.

Here is an outline of the process. We know that $\mathcal{L}^2$ and $\mathcal{L}_z$ share a common eigenbasis, but they will likely have different eigenvalues when they operate on the same basis vector, thus

an index is needed for each operator. The first unknown index is the eigenvalue for $\mathcal{L}^2$, where we will use the symbol α for the eigenvalue. The second non-specific index is the eigenvalue for $\mathcal{L}_z$, denoted by the symbol β. Two indices are necessary to represent the eigenvalues of the two commuting operators. The generic eigenvector/eigenvalue equations for $\mathcal{L}^2$ and $\mathcal{L}_z$ are

$$\mathcal{L}^2 \,|\, \alpha, \beta> \;=\; \alpha \,|\, \alpha, \beta>,$$

$$\mathcal{L}_z \,|\, \alpha, \beta> \;=\; \beta \,|\, \alpha, \beta> \;.$$

The intent of problems 12–17 to 12–22 is to show $\alpha = \hbar^2 \, l(l+1)$ and $\beta = m\hbar$ while discovering the meaning of the quantum numbers l and m.

12–17. Show that $\mathcal{L}_+ \,|\, \alpha, \beta>$ is an eigenvector of $\mathcal{L}_z$ with eigenvalue $\beta + \hbar$.

From problem 12–15

$$\big[\mathcal{L}_z, \mathcal{L}_+\big] \;=\; \mathcal{L}_z \mathcal{L}_+ \;-\; \mathcal{L}_+ \mathcal{L}_z \;=\; \hbar \mathcal{L}_+$$

$$\Rightarrow \qquad \mathcal{L}_z \mathcal{L}_+ \;=\; \mathcal{L}_+ \mathcal{L}_z \;+\; \hbar \mathcal{L}_+.$$

Combine this with the generic eigenvector/eigenvalue statement $\mathcal{L}_z \,|\, \alpha, \beta> \;=\; \beta \,|\, \alpha, \beta>$. Remember from chapter 1 that the product of an operator and a vector is a vector.

$$\begin{aligned}
\mathcal{L}_z \mathcal{L}_+ \,|\, \alpha, \beta> \;&=\; \big(\mathcal{L}_+ \mathcal{L}_z + \hbar \mathcal{L}_+\big) \,|\, \alpha, \beta> \\
&=\; \mathcal{L}_+ \mathcal{L}_z \,|\, \alpha, \beta> \;+\; \hbar \mathcal{L}_+ \,|\, \alpha, \beta> \\
&=\; \mathcal{L}_+ \beta \,|\, \alpha, \beta> \;+\; \hbar \mathcal{L}_+ \,|\, \alpha, \beta> \\
&=\; \big(\beta + \hbar\big) \mathcal{L}_+ \,|\, \alpha, \beta> \;.
\end{aligned}$$

Summarizing,

$$\mathcal{L}_z\big(\mathcal{L}_+ \,|\, \alpha, \beta>\big) \;=\; \big(\beta + \hbar\big)\big(\mathcal{L}_+ \,|\, \alpha, \beta>\big),$$

which means $\mathcal{L}_+ \,|\, \alpha, \beta>$ is itself an eigenvector of $\mathcal{L}_z$ with eigenvalue $\big(\beta + \hbar\big)$.

Postscript: The effect of $\mathcal{L}_+$ is to increase the eigenvalue of $\mathcal{L}_z$ by the amount $\hbar$, so it is called the **raising operator**. A better name would be the raising operator for $\mathcal{L}_z$, but the convention is simply to call it the raising operator.

Similarly, $\mathcal{L}_- \,|\, \alpha, \beta>$ is itself an eigenvector of $\mathcal{L}_z$ with eigenvalue $\big(\beta - \hbar\big)$. The effect of $\mathcal{L}_-$ is to decrease the eigenvalue by the amount $\hbar$, so it is called the **lowering operator**. Again, the convention is to refer to the lowering operator without reference to $\mathcal{L}_z$.

12–18. Show $|\,\alpha,\,\beta>$ is an eigenvector of $\mathcal{L}^2$.

Problem 12–14 showed $\mathcal{L}^2$ and $\mathcal{L}_+$ commute, that is

$$\big[\mathcal{L}^2,\,\mathcal{L}_+\big] \;=\; \mathcal{L}^2\,\mathcal{L}_+ \;-\; \mathcal{L}_+\,\mathcal{L}^2 \;=\; 0$$

$$\Rightarrow \quad \mathcal{L}^2\,\mathcal{L}_+ \;=\; \mathcal{L}_+\,\mathcal{L}^2.$$

Combine this with $\mathcal{L}^2\,|\,\alpha,\,\beta> \;=\; \alpha\,|\,\alpha,\,\beta>$.

$$\mathcal{L}^2\,\mathcal{L}_+\,|\,\alpha,\,\beta> \;=\; \mathcal{L}_+\,\mathcal{L}^2\,|\,\alpha,\,\beta> \;=\; \mathcal{L}_+\,\alpha\,|\,\alpha,\,\beta> \;=\; \alpha\,\mathcal{L}_+\,|\,\alpha,\,\beta>,$$

or summarizing

$$\mathcal{L}^2\big(\mathcal{L}_+\,|\,\alpha,\,\beta>\big) \;=\; \alpha\big(\mathcal{L}_+\,|\,\alpha,\,\beta>\big),$$

so $\mathcal{L}_+\,|\,\alpha,\,\beta>$ is itself an eigenvector of $\mathcal{L}^2$ with eigenvalue α.

Postscript: Similarly, $\mathcal{L}_-\,|\,\alpha,\,\beta>$ is itself an eigenvector of $\mathcal{L}^2$ with eigenvalue α.

It is important that $\mathcal{L}_+\,|\,\alpha,\,\beta>$ is itself an eigenvector of $\mathcal{L}^2$, but notice that the raising/lowering operator does not affect the eigenvalue of $\mathcal{L}^2$. The eigenvalue of $\mathcal{L}^2$ acting on an eigenstate or a combination of the raising/lowering operator and an eigenstate is α.

12–19. Establish a relation between α and β using the generic eigenvector/eigenvalue equations.

Recalling the definition of the square of the angular momentum operator,

$$\mathcal{L}^2 \;=\; \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; \mathcal{L}_z^2 \quad \Rightarrow \quad \mathcal{L}^2 \;-\; \mathcal{L}_z^2 \;=\; \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2\,.$$

The left side of the last equation conveniently contains only $\mathcal{L}$ and $\mathcal{L}_z$. The fact that the right side is the sum of the squares of two Hermitian operators is pertinent. The sum of the squares of the eigenvalues, corresponding to operations by $\mathcal{L}_x^2$ and $\mathcal{L}_y^2$ must be non–negative. In mathematical vernacular, the sum of $\mathcal{L}_x^2$ and $\mathcal{L}_y^2$ is positive definite.

$$\begin{aligned}
\big(\mathcal{L}^2 - \mathcal{L}_z^2\big)\,|\,\alpha,\,\beta> \;&=\; \mathcal{L}^2\,|\,\alpha,\,\beta> \;-\; \mathcal{L}_z^2\,|\,\alpha,\,\beta> \\
&=\; \alpha\,|\,\alpha,\,\beta> \;-\; \mathcal{L}_z\beta\,|\,\alpha,\,\beta> \\
&=\; \alpha\,|\,\alpha,\,\beta> \;-\; \beta^2\,|\,\alpha,\,\beta> \\
&=\; \big(\alpha - \beta^2\big)\,|\,\alpha,\,\beta>\,.
\end{aligned}$$

Forming an adjoint eigenstate and a braket,

$$\begin{aligned}
<\alpha,\beta\,|\,\mathcal{L}^2 - \mathcal{L}_z^2\,|\,\alpha,\,\beta> \;&=\; <\alpha,\beta\,|\,\alpha \;-\; \beta^2\,|\,\alpha,\,\beta> \\
&=\; \big(\alpha - \beta^2\big)\,<\alpha,\beta\,|\,\alpha,\,\beta> \\
&=\; \alpha \;-\; \beta^2
\end{aligned}$$

using orthonormality of eigenstates $<\alpha,\beta\,|\,\alpha,\beta> \;=\; 1$. Since $\mathcal{L}^2 - \mathcal{L}_z^2 \;=\; \mathcal{L}_x^2 + \mathcal{L}_y^2$,

$$<\alpha,\beta\,|\,\mathcal{L}^2 - \mathcal{L}_z^2\,|\,\alpha,\beta> \;=\; <\alpha,\beta\,|\,\mathcal{L}_x^2 + \mathcal{L}_y^2\,|\,\alpha,\beta> \;\geq\; 0\,.$$

$$\text{Thus} \qquad <\alpha,\beta\,|\,\mathcal{L}^2 - \mathcal{L}_z^2\,|\,\alpha,\beta> \;=\; \alpha \;-\; \beta^2 \;\geq\; 0 \qquad \text{or} \qquad \alpha \;\geq\; \beta^2\,.$$

Postscript: Again, the difference $\alpha - \beta^2$ is non–negative since the braket can be expressed as a sum of $\mathcal{L}_x^2$ and $\mathcal{L}_y^2$. Both $\mathcal{L}_x$ and $\mathcal{L}_y$ are Hermitian, so their eigenvalues are real scalars. The sum of the squares of two real scalars is non-negative, *i.e.*, $a^2 + b^2 \;\geq\; 0$ for all a and $b \in \mathbb{R}$.

The condition $\alpha \geq \beta^2$ means β is bounded for a given value of α. Therefore, there is an eigenstate $|\,\alpha,\beta_{\max}>$ which cannot be raised, and another eigenstate $|\,\alpha,\beta_{\min}>$ which cannot be lowered. In other words, the ladder for the z component of angular momentum has a bottom, like the SHO, and a top, unlike the SHO.

12–20. Solve for $\beta_{\max}$ in terms of $\beta_{\min}$.

We found $\mathcal{L}_-\mathcal{L}_+ \;=\; \mathcal{L}^2 - \mathcal{L}_z^2 - \hbar\mathcal{L}_z$ in problem 12–13. Notice in the expression $\mathcal{L}_-\mathcal{L}_+\,|\,\alpha,\beta>$ that the raising operator acts on the eigenket first. So, if we let $\mathcal{L}_-\mathcal{L}_+$ act on the eigenket at the top of the ladder, $|\,\alpha,\beta_{\max}>$, we necessarily obtain the zero vector. Similarly, $\mathcal{L}_+\mathcal{L}_-$ acting on $|\,\alpha,\beta_{\min}>$ yields a zero vector, just like the lowering operator acting on the bottom of the SHO ladder. Together, these will yield relations that allow us to solve for $\beta_{\max}$ in terms of $\beta_{\min}$.

$$\begin{aligned}
&\mathcal{L}_-\mathcal{L}_+\,|\,\alpha,\beta_{\max}> \;=\; \vec{0}\\
&\quad\Rightarrow\quad \left(\mathcal{L}^2 - \mathcal{L}_z^2 - \hbar\mathcal{L}_z\right)|\,\alpha,\beta_{\max}> \;=\; 0\\
&\quad\Rightarrow\quad \mathcal{L}^2\,|\,\alpha,\beta_{\max}> \;-\; \mathcal{L}_z^2\,|\,\alpha,\beta_{\max}> \;-\; \hbar\mathcal{L}_z\,|\,\alpha,\beta_{\max}> \;=\; 0\\
&\quad\Rightarrow\quad \alpha\,|\,\alpha,\beta_{\max}> \;-\; \beta_{\max}^2\,|\,\alpha,\beta_{\max}> \;-\; \hbar\,\beta_{\max}\,|\,\alpha,\beta_{\max}> \;=\; 0\\
&\quad\Rightarrow\quad \left(\alpha - \beta_{\max}^2 - \hbar\,\beta_{\max}\right)|\,\alpha,\beta_{\max}> \;=\; 0\\
&\quad\Rightarrow\quad \alpha \;-\; \beta_{\max}^2 \;-\; \hbar\,\beta_{\max} \;=\; 0 \qquad \text{because} \qquad |\,\alpha,\beta_{\max}> \;\neq 0 \qquad \text{for an existing system}\\
&\quad\Rightarrow\quad \alpha \;=\; \beta_{\max}^2 \;+\; \hbar\,\beta_{\max}.
\end{aligned}$$

Similarly, $\mathcal{L}_+\mathcal{L}_-\,|\,\alpha,\beta_{\min}> \;=\; \vec{0} \;\;\Rightarrow\;\; \alpha \;=\; \beta_{\min}^2 \;-\; \hbar\,\beta_{\min}$. Equating these relations for α,

$$\beta_{\max}^2 \;+\; \hbar\beta_{\max} \;=\; \beta_{\min}^2 \;-\; \hbar\beta_{\min} \quad\Rightarrow\quad \beta_{\max}^2 \;+\; \hbar\beta_{\max} \;-\; \beta_{\min}^2 \;+\; \hbar\beta_{\min} \;=\; 0$$

which is quadratic in $\beta_{\max}$. The quadratic formula yields

$$\begin{aligned}
\beta_{\max} \;&=\; -\frac{1}{2}\hbar \;\pm\; \frac{1}{2}\sqrt{\hbar^2 - 4(-\beta_{\min}^2 + \hbar\,\beta_{\min})}\\
&=\; -\frac{1}{2}\hbar \;\pm\; \frac{1}{2}\sqrt{4\beta_{\min}^2 - 4\hbar\,\beta_{\min} + \hbar^2}\\
&=\; -\frac{1}{2}\hbar \;\pm\; \frac{1}{2}\sqrt{(2\beta_{\min} - \hbar)^2}\\
&=\; -\frac{1}{2}\hbar \;\pm\; \frac{1}{2}(2\beta_{\min} - \hbar)\\
\Rightarrow\quad \beta_{\max} \;&=\; -\beta_{\min} \qquad \text{and} \qquad \beta_{\max} \;=\; \beta_{\min} \;-\; \hbar\,.
\end{aligned}$$

12–21. Express the eigenvalues of $\mathcal{L}^2$ using the orbital angular momentum quantum number l.

The relation

$$\alpha \;=\; \beta_{\max}^2 \;+\; \hbar\,\beta_{\max}$$

was developed in the last problem. Examine the figure at the right. Unlike the SHO for which the bottom of the ladder is $n = 0$, the z-component of orbital angular momentum quantum number $l = 0$ is the center quantum number, where l is simply an integer index. Then up one step is $l = 1$, down one step is $l = -1$, up two steps is $l = 2$, down two steps is $l = -2$, and so on.

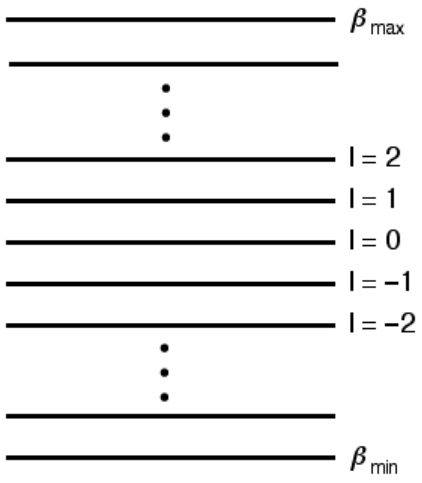

Figure 12–1. Z–component of orbital angular momentum quantum number ladder.

$\beta_{\max} = -\beta_{\min}$ from the last problem. The second solution, $\beta_{\max} = \beta_{\min} - \hbar$, is discarded because there cannot be an eigenstate below the bottom of the ladder. Thus, $\beta_{\max} - \beta_{\min} = 2\beta_{\max}$ because there are l steps above $l = 0$ and l steps below $l = 0$. The raising and lowering operators indicated the steps for the z-component operator are separated by $\hbar$ in problem 12–17, so

$$2\beta_{max} \;=\; 2\hbar l \quad\Rightarrow\quad \beta_{\max} \;=\; \hbar l\,, \qquad \text{so}$$

$$\alpha \;=\; \beta_{\max}^2 \;+\; \hbar\,\beta_{\max} \quad\Rightarrow\quad \alpha \;=\; \big(\hbar l\big)^2 \;+\; \hbar\,\big(\hbar l\big) \;=\; \hbar^2 l^2 + \hbar^2 l \qquad \text{or}$$

$$\alpha \;=\; \hbar^2 l\big(\,l + 1\,\big)$$

which is the conventional expression for the eigenvalues of $\mathcal{L}^2$ in terms of the orbital angular momentum quantum number l.

Postscript: Remember that l is simply an integer index used to label the rungs of the z-component ladder. The z-component ladder has negative values, however, l is strictly non-negative because $\alpha \geq \beta^2$ from problem 12–19, and β^2 is strictly non-negative.

The vector sum of the orbital angular momentum and **spin angular momentum**, using quantum number s, is **total angular momentum**, denoted by quantum number j. Spin and total angular momenta are discussed in Quantum Mechanics II.

12–22. Express the eigenvalues of $\mathcal{L}_z$ in terms of the magnetic quantum number m.

Figure 12–1 is motivated by

$$\mathcal{L}_z\big(\mathcal{L}_+\,|\,\alpha,\,\beta>\big) \;=\; \big(\beta + \hbar\big)\big(\mathcal{L}_+\,|\,\alpha,\,\beta>\big)\,, \qquad \beta_{\max} \;=\; l\hbar\,, \quad \text{and} \qquad \beta_{\min} \;=\; -l\hbar\,,$$

and the fact that an eigenstate having a z-component of angular momentum that is zero is physically required. We shall use the above equation, the known top of the ladder, and the known bottom of the ladder to find the value of the generic eigenvalue of $\mathcal{L}_z$ previously labeled β.

Starting on the eigenstate with the z-component of angular momentum $\beta_{\min} = -l\hbar$,

$$\mathcal{L}_z\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar >\big) \;=\; (-l\hbar + \hbar)\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar >\big)\,.$$

Operating on this eigenstate,

$$\mathcal{L}_z\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar + \hbar >\big) \;=\; \big(-l\hbar + \hbar + \hbar\big)\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar + \hbar >\big) \;=\; \big(-l\hbar + 2\hbar\big)\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar + \hbar >\big),$$

then

$$\mathcal{L}_z\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar + 2\hbar >\big) \;=\; \big(-l\hbar + 2\hbar + \hbar\big)\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar + 2\hbar >\big) \;=\; \big(-l\hbar + 3\hbar\big)\big(\mathcal{L}_+ \,|\, \alpha,\, -l\hbar + 2\hbar >\big)\,.$$

The eigenvalue increase by one unit of $\hbar$ for each successive application of the $\mathcal{L}_z\,\mathcal{L}_+$ operator. An eigenstate having a z-component of angular momentum that is zero is physically required. Thus, we have eigenvalues which climb from $-l\hbar$ to $l\hbar$ in integral increments of $\hbar$. The eigenvalue of the z-component of orbital angular momentum is just an integer times $\hbar$, from minimum to maximum values. The symbol conventionally used to denote this integer is m, so

$$\mathcal{L}_z \,|\, \alpha,\, \beta > \;=\; m\hbar \,|\, \alpha,\, \beta >, \qquad -l \,\le\, m \,\le\, l$$

is the eigenvalue/eigenvector equation for the z-component of angular momentum. Picture figure 12–1 with the rungs separated by $\hbar$ and m as the integer index.

Postscript: Early quantum effects were seen in various sorts of spectra. The effects of the $\mathcal{L}_z$ operator were seen as spectral splitting only when the sample being observed was immersed in a magnetic field, thus, the name "magnetic quantum number."

The magnetic quantum number m is occasionally denoted m_l, indicating that it is bounded by the orbital angular momentum quantum number.

Using l within the ket to denote the state of orbital angular momentum, realizing $\hbar^2 l\,\big(l{+}1\big)$ is the actual eigenvalue of $\mathcal{L}^2$, and m as the ket's second index to denote the state of the z-component of angular momentum, realizing the eigenvalue of $\mathcal{L}_z$ is actually $m\hbar$, the eigenvalue/eigenvector equations for $\mathcal{L}^2$ and $\mathcal{L}_z$ are

$$\mathcal{L}^2 \,|\, l,\, m > \;=\; \hbar^2\, l(l+1) \,|\, l,\, m >, \qquad l \;\ge\; 0$$

$$\mathcal{L}_z \,|\, l,\, m > \;=\; m\hbar \,|\, l,\, m >, \qquad -l \,\le\, m \,\le\, l$$

which are the conventional forms of the eigenvalue/eigenvector equations for $\mathcal{L}^2$ and $\mathcal{L}_z$.

Again, l and m are not eigenvalues of $\mathcal{L}^2$ and $\mathcal{L}_z$. The eigenvalues are $\hbar^2\, l\,(\,l+1\,)$ and $m\,\hbar$ where l and m are simply integer indices used to easily compute the actual eigenvalues. Should an eigenstate be denoted by using the eigenvalues in the ket, it would look like $|\,\hbar^2\, l\,(\,l{+}1\,),\; m\,\hbar >$, however, $|\,l,\, m >$ is more economical, identifies the eigenstate uniquely, and is preferred, just as $|\,n>$ is preferred for the SHO rather than $|\,\big(n + \frac{1}{2}\big)\,\hbar\,\omega >$.

12–23. (a) What are the possible results of a measurement of $\mathcal{L}^2$?

(b) A measurement of $\mathcal{L}^2$ yields $6\,\hbar^2$. What are the possible results of a measurement of $\mathcal{L}_z$?

(c) A measurement of $\mathcal{L}_z$ yields $2\,\hbar$. What are the possible results of a measurement of $\mathcal{L}^2$?

The only possible results of a measurement are the eigenvalues, which are $\hbar^2\, l\,(\,l+1\,)$ for $\mathcal{L}^2$ and $m\,\hbar$ for $\mathcal{L}_z$ per the eigenvalue postulate. The orbital angular momentum quantum number is non-negative and integral, *i.e.*, $l = 0,\ 1,\ 2,\ 3, \ldots$, and is unbounded. The magnetic quantum number may be positive, negative, or zero; is integral, but is bounded between $-l$ and l.

(a) $\hbar^2\, l\,(\,l+1\,) = 0\,,\ 2\hbar^2\,,\ 6\hbar^2\,,\ 12\hbar^2\,,\ 20\hbar^2\,, \ldots$

(b) $\hbar^2\, l\,(\,l+1\,) = 6\hbar^2 \quad \Rightarrow \quad l = 2 \quad \Rightarrow \quad m = -2,\ -1,\ 0,\ 1,\ 2 \quad \Rightarrow \quad -2\hbar,\ -\hbar,\ 0,\ \hbar,\ 2\hbar$ are possible results of a measurement of $\mathcal{L}_z$.

(c) $m\hbar = 2\hbar \quad \Rightarrow \quad l \geq 2 \quad \Rightarrow \quad 6\hbar^2\,,\ 12\hbar^2\,,\ 20\hbar^2, \ldots$ are possible results of a measurement of $\mathcal{L}^2$, though 0 and $2\hbar^2$ are not possible.

12–24. For the eigenstate $|\,l,\, m> \;=\; |\,3,\, m>$, what measurements are possible for $\mathcal{L}^2$ and $\mathcal{L}_z$?

The only measurements that are possible are the eigenvalues.

The eigenvalue of $\mathcal{L}^2$ is $\hbar^2\, l(l+1) \;=\; \hbar^2\, 3(3+1) \;=\; 12\hbar^2$.

For $l = 3$, the possible eigenvalues of $\mathcal{L}_z$ can range from $-3\hbar$ to $3\hbar$ in increments of $\hbar$. Explicitly, the measurements that are possible for $\mathcal{L}_z$ for the eigenstate $|\,3, m>$ are $-3\hbar,\ -2\hbar,\ -\hbar,\ 0,\ \hbar,\ 2\hbar,$ or $3\hbar$.

12–25. What are the eigenvalues of the raising operator $\mathcal{L}_+$?

Problems 12–17 to 12–22 developed much of the mathematics for this problem. Use the facts that $\mathcal{L}_+\,|\,l, m>$ is an eigenstate of $\mathcal{L}_z$ increasing the eigenvalue by $\hbar$ to obtain a symbol for the eigenvalue of $\mathcal{L}_+$, then form a braket. We also know $\mathcal{L}_-\mathcal{L}_+ \;=\; \alpha \;-\; \beta^2 \;-\; \hbar\beta$ for which α and β are now known, which will allow us to solve for the eigenvalues of $\mathcal{L}_+$.

The fact $\mathcal{L}_+\,|\,l, m>$ is an eigenstate of $\mathcal{L}_z$ can be written

$$\mathcal{L}_z\mathcal{L}_+\,|\,l,\, m> \;=\; \big(m\hbar + \hbar\big)\mathcal{L}_+\,|\,l,\, m> \;.$$

The effect of $\mathcal{L}_z$ operating on the ket $|\,l,\, m+1>$ is

$$\mathcal{L}_z\,|\,l,\, m+1> \;=\; \big(m\hbar + \hbar\big)\,|\,l,\, m+1> \qquad \text{which together}$$

$$\Rightarrow \qquad \mathcal{L}_+\,|\,l, m> \;\propto\; |\,l,\, m+1>$$

Let γ be a proportionality constant. Then

$$\mathcal{L}_+ \,|\, l, m> \;=\; \gamma \,|\, l, m+1>$$

is the eigenvalue/eigenvector equation for the raising operator, where γ is evidently the eigenvalue, and the eigenvector is raised by one element of quantization in the z-component. This means if the z-component of the state on which the raising operator acts is $m\hbar$, the new state has a z-component of $m\hbar + \hbar = (m+1)\hbar$, and thus the index $m+1$ is used in the new eigenket. The adjoint of the last equation is

$$< l, m \,|\, \mathcal{L}_+^\dagger \;=\; < l, m+1 \,|\, \gamma^* \quad \Rightarrow \quad < l, m \,|\, \mathcal{L}_- \;=\; < l, m+1 \,|\, \gamma^*$$

because $\mathcal{L}_+^\dagger \;=\; \mathcal{L}_-$. Forming a braket,

$$< l, m \,|\, \mathcal{L}_-\mathcal{L}_+ \,|\, l, m> \;=\; < l, m+1 \,|\, \gamma^*\gamma \,|\, l, m+1> .$$

Though we did it only for $\beta_{\max}$, the maximum eigenvalue of $\mathcal{L}_z$, the algebra remains the same for any β, any eigenvalue of $\mathcal{L}_z$, so

$$\mathcal{L}_-\mathcal{L}_+ \;=\; \alpha \;-\; \beta^2 \;-\; \hbar\beta \;=\; \hbar^2\, l(l+1) \;-\; m^2\hbar^2 \;-\; m\hbar^2 .$$

Using this in the braket,

$$\begin{aligned} < l, m \,|\, \hbar^2\Big(l(l+1) - m^2 - m\Big) \,|\, l, m> \;&=\; < l, m+1 \,|\, \gamma^*\gamma \,|\, l, m+1> \\ \Rightarrow \quad \hbar^2\Big(l(l+1) - m(m+1)\Big) <l, m \,|\, l, m> \;&=\; |\,\gamma^*\gamma\,| \;<l, m+1 \,|\, l, m+1> \\ \Rightarrow \quad \hbar^2\Big(l(l+1) - m(m+1)\Big) \;&=\; |\,\gamma\,|^{\,2} \end{aligned}$$

$$\Rightarrow \quad \gamma \;=\; \sqrt{l(l+1) - m(m+1)}\,\hbar,$$

where we used the orthonormality of eigenstates. The eigenvalue/eigenvector equation is then

$$\mathcal{L}_+ \,|\, l, m> \;=\; \sqrt{l(l+1) - m(m+1)}\,\hbar \,|\, l, m+1> .$$

Postscript: Were we to do the similar calculation for $\mathcal{L}_-$, we find

$$\mathcal{L}_- \,|\, l, m> \;= \sqrt{l(l+1) - m(m-1)}\,\hbar \,|\, l, m-1> .$$

These are often expressed as one relation,

$$\mathcal{L}_\pm \,|\, l, m> \;=\; \sqrt{l(l+1) - m(m \pm 1)}\,\hbar \,|\, l, m \pm 1> .$$

12–26. What are the final states when (a) $\mathcal{L}_+$ and (b) $\mathcal{L}_-$ operate on the eigenstate $|\,2,-1>$?

This is a numerical application of the previous result.

$$\begin{aligned}
\text{(a)}\qquad \mathcal{L}_+\,|\,2,-1> &= \sqrt{2(2+1)-(-1)((-1)+1)}\,\hbar\,|\,2,-1+1> \\
&= \sqrt{2(3)-(-1)(0)}\,\hbar\,|\,2,0> \\
&= \sqrt{6}\,\hbar\,|\,2,0>\ .
\end{aligned}$$

$$\begin{aligned}
\text{(b)}\qquad \mathcal{L}_-\,|\,2,-1> &= \sqrt{2(2+1)-(-1)((-1)-1)}\,\hbar\,|\,2,-1-1> \\
&= \sqrt{2(3)-(-1)(-2)}\,\hbar\,|\,2,-2> \;=\; \sqrt{6-2}\,\hbar\,|\,2,-2> \;=\; \sqrt{4}\,\hbar\,|\,2,-2> \\
&= 2\hbar\,|\,2,-2>\,.
\end{aligned}$$

The next six problems are intended to apply calculations developed previously and the postulates of quantum mechanics to eigenstates of orbital angular momentum. Problems 12–27 through 12–32 all refer to the linear combination of two eigenstates for the $t=0$ state vector

$$|\,\psi(t=0)> \;=\; A\big(\,|\,2,1> \;+\; 3\,|\,1,-1>\,\big) \tag{18}$$

12–27. Normalize the state vector of equation (18).

This normalization is done twice. The first calculation is done in a two dimensional subspace. The second calculation is more general and done solely in abstract Dirac notation.

There are two eigenstates, so we can work in a two dimensional subspace. We can model the first eigenstate $\begin{pmatrix}1\\0\end{pmatrix}$ and the second $\begin{pmatrix}0\\1\end{pmatrix}$. Then the state vector can be written

$$|\,\psi(0)> \;=\; A\left[\begin{pmatrix}1\\0\end{pmatrix} \;+\; 3\begin{pmatrix}0\\1\end{pmatrix}\right] \;=\; A\begin{pmatrix}1\\3\end{pmatrix}\,.$$

Another way to look at it is the state vector is two dimensional with one part the first eigenstate and three parts the second eigenstate. Proceeding with the normalization,

$$\big(1,\,3\big)\,A^*A\begin{pmatrix}1\\3\end{pmatrix} \;=\; |\,A\,|^{\,2}\big(1+9\big) \;=\; 10\,|\,A\,|^{\,2} \;=\; 1$$

$$\Rightarrow\quad A \;=\; \frac{1}{\sqrt{10}}\qquad\Rightarrow\qquad |\,\psi(0)> \;=\; \frac{1}{\sqrt{10}}\begin{pmatrix}1\\3\end{pmatrix} \;=\; \frac{1}{\sqrt{10}}\big(\,|\,2,1> + 3\,|\,1,-1>\,\big)\,.$$

In abstract Dirac notation,

$$<\psi\,|\,\psi> \;=\; \big(\,<2,1\,|\,+3<1,-1\,|\,\big)A^*A\big(\,|\,2,1> + 3\,|\,1,-1>\,\big) \;=\; 1$$

$$\Rightarrow \quad \big(<2,\,1\,|\,2,\,1> + 3 <2,\,1\,|\,1,\,-1> \,+\, 3 <1,\,-1\,|\,2,\,1> \,+\, 9 <1,\,-1\,|\,1,\,-1> \big)\,|\,A\,|^{\,2} \;=\; 1$$

$$\Rightarrow \quad \big(1 + 0 + 0 + 9\cdot 1\big)\,|\,A\,|^{\,2} \;=\; 1 \quad \Rightarrow \quad 10\,|\,A\,|^{\,2} \;=\; 1 \quad \Rightarrow \quad A \;=\; \frac{1}{\sqrt{10}}$$

yielding the same normalization constant, and thus the same state vector, as above.

Postscript: Recognizing the orthonormality of eigenstates is required in the second calculation.

12–28. What are the possibilities and probabilities of a measurement of $\mathcal{L}^2$?

Apply the postulates. "What are the possibilities?" and "What are the probabilities?" are likely the two most fundamental questions for any application of quantum mechanics.

The possibilities are the eigenvalues. There are two eigenstates, each with its own eigenvalue. If we measure and put the system into the first eigenstate, we measure the state corresponding to the quantum number $l = 2$, which has the eigenvalue $\hbar^2\, l(l+1) \;=\; \hbar^2\, 2\,(2+1) \;=\; 6\hbar^2$. If we measure and place the state vector into the second eigenstate corresponding to the quantum number $l = 1$, the eigenvalue measured is $\hbar^2\, l(l+1) \;=\; \hbar^2\, 1(1+1) \;=\; 2\hbar^2$.

Since the state function is now normalized,

$$P\big(\mathcal{L}^2 \;=\; 6\hbar^2\big) \;=\; |\,<\psi_{2,1}|\psi>\,|^{\,2} = \left|\,\big(1,\;0\big)\,\frac{1}{\sqrt{10}}\begin{pmatrix}1\\3\end{pmatrix}\right|^2 = \;\frac{1}{10}\,|\,1+0\,|^{\,2} = \;\frac{1}{10}\,.$$

$$P\big(\mathcal{L}^2 \;=\; 2\hbar^2\big) \;=\; |\,<\psi_{1,-1}|\psi>\,|^{\,2} = \left|\,\big(0,\;1\big)\,\frac{1}{\sqrt{10}}\begin{pmatrix}1\\3\end{pmatrix}\right|^2 = \;\frac{1}{10}\,|\,0+3\,|^{\,2} = \;\frac{9}{10}\,.$$

12–29. What are the possibilities and probabilities of a measurement of $\mathcal{L}_z$?

The possible results of a measurement of $\mathcal{L}_z$ are $m = 1 \;\Rightarrow\; \hbar$ is the first eigenvalue, and $m = -1 \;\Rightarrow\; -\hbar$ is the second possible eigenvalue. Using exactly the same math,

$$P\big(\mathcal{L}_z = \hbar\big) \;=\; \frac{1}{10}\,, \qquad\qquad P\big(\mathcal{L}_z = -\hbar\big) \;=\; \frac{9}{10}\,.$$

12–30. What is the expectation value of $\mathcal{L}^2$?

$$<\mathcal{L}^2> \;=\; \sum P(\alpha_i)\,\alpha_i \;=\; \frac{1}{10}\,6\hbar^2 \;+\; \frac{9}{10}\,2\hbar^2 \;=\; \frac{6}{10}\,\hbar^2 \;+\; \frac{18}{10}\,\hbar^2 \;=\; \frac{24}{10}\,\hbar^2 \;=\; 2.4\,\hbar^2\,.$$

12–31. What is the uncertainty of $\mathcal{L}^2$?

$$\triangle\,\mathcal{L}^2 = \;\sqrt{\sum P(\alpha_i)\big(\alpha_i - <\mathcal{L}^2>\big)^2} \;=\; \left[\,\frac{1}{10}\,\big(6\hbar^2 - 2.4\hbar^2\big)^2 \;+\; \frac{9}{10}\,\big(2\hbar^2 - 2.4\hbar^2\big)^2\,\right]^{1/2}$$

$$=\; \hbar^2\left[\,\frac{1}{10}\,\big(3.6\big)^2 \;+\; \frac{9}{10}\,\big(-0.4\big)^2\,\right]^{1/2} \;=\; \hbar^2\big[\,1.296 \;+\; 0.144\,\big]^{1/2} = \;\hbar^2\sqrt{1.44} \;=\; 1.2\,\hbar^2\,.$$

12–32. What is the time dependent state vector?

$$\begin{aligned}
|\psi(t)> &= \sum |\, j><j\,|\,\psi(0)>\, e^{-iE_j t/\hbar} \\
&= \begin{pmatrix}1\\0\end{pmatrix}(1,\ 0)\frac{1}{\sqrt{10}}\begin{pmatrix}1\\3\end{pmatrix} e^{-iE_1 t/\hbar} \ +\ \begin{pmatrix}0\\1\end{pmatrix}(0,\ 1)\frac{1}{\sqrt{10}}\begin{pmatrix}1\\3\end{pmatrix} e^{-iE_2 t/\hbar} \\
&= \frac{1}{\sqrt{10}}\begin{pmatrix}1\\0\end{pmatrix} e^{-iE_1 t/\hbar} \ +\ \frac{3}{\sqrt{10}}\begin{pmatrix}0\\1\end{pmatrix} e^{-iE_2 t/\hbar} \\
&= \frac{1}{\sqrt{10}}\,|\,2,\,1>\, e^{-iE_1 t/\hbar} \ +\ \frac{3}{\sqrt{10}}\,|\,1,\,-1>\, e^{-iE_2 t/\hbar}
\end{aligned}$$

which is as far as we can go with the given information. We need an energy operator, a Hamiltonian, encoding the potential energy function of a specific system to obtain non-generic E_i.

The central portion of this chapter uses calculus-based arguments to describe quantum mechanical orbital angular momentum. Special functions become focal. The special functions used in our development are families of solutions to differential equations.

The conservation of angular momentum, or rotational invariance, implies circular or spherical symmetry. We want to examine spherical symmetry, because spherical symmetry is often a reasonable assumption for simple physical systems. We will assume a hydrogen atom is spherically symmetric, for instance. Remember in spherical coordinates,

$$\begin{aligned}
x &= r\sin\theta\cos\phi, & r &= \left(x^2+y^2+z^2\right)^{1/2} \\
y &= r\sin\theta\sin\phi, & \theta &= \tan^{-1}\left(\sqrt{x^2+y^2}/z\right) \\
z &= r\cos\theta, & \phi &= \tan^{-1}\left(y/x\right).
\end{aligned}$$

From these it follows that position space representations in spherical coordinates are

$$\begin{aligned}
\mathcal{L}_x &\rightarrow i\hbar\left(\sin\phi\,\frac{\partial}{\partial\theta} \ +\ \cos\phi\,\cot\theta\,\frac{\partial}{\partial\phi}\right), \\
\mathcal{L}_y &\rightarrow i\hbar\left(-\cos\phi\,\frac{\partial}{\partial\theta} \ +\ \sin\phi\,\cot\theta\,\frac{\partial}{\partial\phi}\right), \\
\mathcal{L}_z &\rightarrow -i\hbar\frac{\partial}{\partial\phi}, \qquad (19) \\
\mathcal{L}^2 &\rightarrow -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} \ +\ \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} \ +\ \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \qquad (20) \\
\mathcal{L}_\pm &\rightarrow \pm\,\hbar\,e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \ \pm\ i\cot\theta\frac{\partial}{\partial\phi}\right). \qquad (21)
\end{aligned}$$

12–33. Derive equation (19).

All five of the above representations are addressed in problems or exercises.

From equation (2),

$$\mathcal{L}_z \;\rightarrow\; i\hbar\left(-x\,\frac{\partial}{\partial y} \;+\; y\,\frac{\partial}{\partial x}\right).$$

Developing partial differentials from the relation between azimuthal angle and position coordinates,

$$\phi \;=\; \tan^{-1}(y/x) \qquad \Rightarrow \qquad y \;=\; x\,\tan\phi$$

$$\Rightarrow \qquad \frac{\partial y}{\partial\phi} \;=\; x\,\partial\big(\tan\phi\big) \;=\; x\,\sec^2\phi \;=\; \frac{x}{\cos^2\phi}$$

$$\Rightarrow \qquad \partial y \;=\; \frac{x\,\partial\phi}{\cos^2\phi}\,.$$

The same relation gives us

$$x \;=\; \frac{y}{\tan\phi} \;=\; y\,\frac{\cos\phi}{\sin\phi} \;=\; y\,\cos\phi\,\sin^{-1}\phi$$

$$\Rightarrow \qquad \frac{\partial x}{\partial\phi} \;=\; y\big(-\sin\phi\,\sin^{-1}\phi \;+\; \cos\phi\,(-1)\,\sin^{-2}\phi\cos\phi\big)$$

$$=\; -y\left(1+\frac{\cos^2\phi}{\sin^2\phi}\right) \;=\; -y\left(\frac{\sin^2\phi+\cos^2\phi}{\sin^2\phi}\right) \;=\; -\frac{y}{\sin^2\phi}$$

$$\Rightarrow \qquad \partial x \;=\; -\frac{y\,\partial\phi}{\sin^2\phi}\,.$$

Using the partial differentials in the Cartesian formulation,

$$\mathcal{L}_z \;=\; i\hbar\left(-x\,\cos^2\phi\frac{\partial}{x\,\partial\phi} \;+\; y\left(-\sin^2\phi\frac{\partial}{y\,\partial\phi}\right)\right)$$

$$=\; -i\hbar\big(\cos^2\phi+\sin^2\phi\big)\frac{\partial}{\partial\phi} \;=\; -i\hbar\frac{\partial}{\partial\phi}\,.$$

12–34. Obtain $\mathcal{L}_+$ given the spherical coordinate representations of $\mathcal{L}_x$ and $\mathcal{L}_y$.

$$\begin{aligned}
\mathcal{L}_+ \;&=\; \mathcal{L}_x \;+\; i\mathcal{L}_y \\
&\rightarrow\; i\hbar\left(\sin\phi\,\frac{\partial}{\partial\theta}+\cos\phi\,\cot\theta\,\frac{\partial}{\partial\phi}\right) \;+\; i\left[i\hbar\left(-\cos\phi\,\frac{\partial}{\partial\theta}+\sin\phi\,\cot\theta\,\frac{\partial}{\partial\phi}\right)\right] \\
&=\; \hbar\left[i\sin\phi\,\frac{\partial}{\partial\theta} \;+\; i\cos\phi\,\cot\theta\,\frac{\partial}{\partial\phi} \;+\; \cos\phi\,\frac{\partial}{\partial\theta} \;-\; \sin\phi\,\cot\theta\,\frac{\partial}{\partial\phi}\right] \\
&=\; \hbar\left[(\cos\phi+i\sin\phi)\,\frac{\partial}{\partial\theta} \;+\; (i\cos\phi-\sin\phi)\,\cot\theta\,\frac{\partial}{\partial\phi}\right] \\
&=\; \hbar\left[(\cos\phi+i\sin\phi)\,\frac{\partial}{\partial\theta} \;+\; i\,(\cos\phi+i\sin\phi)\,\cot\theta\,\frac{\partial}{\partial\phi}\right] \\
&=\; \hbar\left[\big(e^{i\phi}\big)\,\frac{\partial}{\partial\theta} \;+\; i\,\big(e^{i\phi}\big)\,\cot\theta\,\frac{\partial}{\partial\phi}\right] \;=\; \hbar\,e^{i\phi}\left(\frac{\partial}{\partial\theta} \;+\; i\,\cot\theta\frac{\partial}{\partial\phi}\right).
\end{aligned}$$

Postscript: Notice that the position space representations of all angular momentum operators in spherical coordinates are functions of angle only, $f = f(\theta, \phi)$. Length or distance from an origin in terms of spatial variables such as x, y, z, or r is not addressed.

12–35. What are spherical harmonics?

The **Laplace equation**

$$\nabla^2 f = 0 \quad \Leftrightarrow \quad \left(\frac{\partial^2}{\partial^2 x} + \frac{\partial^2}{\partial^2 y} + \frac{\partial^2}{\partial^2 z} \right) f = 0 \qquad \text{or}$$

$$\frac{\partial^2 f}{\partial r^2} + \frac{2}{r} \frac{\partial f}{\partial r} + \frac{1}{r^2} \left(\frac{\partial^2 f}{\partial \theta^2} + \cot\theta \frac{\partial f}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \right) = 0$$

in spherical coordinates. All solutions to Laplace's equation are known as **harmonic functions**. Remember that the first derivative of a function is related to slope, and that the second derivative is related to curvature, thus Laplace's equation is useful in many applications involving curves and spherical symmetry. The portion of the Laplace equation in spherical coordinates involving only angular derivatives is the **Legendrian**. A function $f(\theta, \phi)$ that satisfies

$$\frac{\partial^2 f}{\partial \theta^2} + \cot\theta \frac{\partial f}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} = 0$$

is a perfect sphere. The function satisfying the equation $\nabla^2 f + \lambda f = 0$ can be used to describe a non-perfect sphere. When $\lambda = l(l+1)$, it is the **Legendre equation** having the solutions known as **Legendre polynomials**. The reason to write the constant λ as $l(l+1)$ is that the solutions can be expressed in terms of non-negative integers, equivalent to polar periodicity. Problems having spherical symmetry with azimuthal dependence require the **associated Legendre equation** where

$$\lambda = l\left(l+1\right) - \frac{m^2}{\sin^2 \theta}$$

which is satisfied by the infinite set of functions known as **associated Legendre polynomials**. Again, the reason to write it this way is that it describes azimuthal periodicity when m is an integer. Notice that the associated Legendre equation reduces to the Legendre equation when $m = 0$. **Spherical harmonics** are closely related to associated Legendre polynomials. The first few spherical harmonics are listed in table 12–1.

$$
\begin{aligned}
Y_{0,0}(\theta,\phi) &= \frac{1}{4\pi} & Y_{2,0}(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}\big(3\cos^2\theta - 1\big) \\
Y_{1,\pm1}(\theta,\phi) &= \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi} & Y_{3,\pm3}(\theta,\phi) &= \sqrt{\frac{35}{64\pi}}\sin^3\theta\, e^{\pm 3i\phi} \\
Y_{1,0}(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta & Y_{3,\pm2}(\theta,\phi) &= \sqrt{\frac{105}{32\pi}}\sin^2\theta\,\cos\theta\, e^{\pm 2i\phi} \\
Y_{2,\pm2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{\pm 2i\phi} & Y_{3,\pm1}(\theta,\phi) &= \sqrt{\frac{21}{64\pi}}\sin\theta\,\Big(5\cos^2\theta - 1\Big)e^{\pm i\phi} \\
Y_{2,\pm1}(\theta,\phi) &= \sqrt{\frac{15}{8\pi}}\sin\theta\,\cos\theta\, e^{\pm i\phi} & Y_{3,0}(\theta,\phi) &= \sqrt{\frac{7}{16\pi}}\Big(5\cos^3\theta - 3\cos\theta\Big)
\end{aligned}
$$

Table $12-1$. The First Sixteen Spherical Harmonic Functions.

Nodal lines of some spherical harmonics are illustrated in figure 12–2. The sphere is static when $l=0\,,\ m=0\,.$ If struck on the top, the upper hemisphere may compress and the lower expand, and if allowed to oscillate, each hemisphere may alternately contract or expand where the equator is a nodal line as depicted for $l=1\,,\ m=0\,.$ If struck on the left side, it may oscillate by hemispheres similarly around longitudinal lines as seen for $l=1\,,\ m=1\,.$ Another mode of vibration is that the top third may compress if the sphere is struck on the top, the middle third may expand as the lower third contracts where two lines of latitude are nodes per $l=2\,,\ m=0\,.$

It is common to refer to spherical harmonic functions without explicitly indicating that the arguments are polar and azimuthal angles, for instance $Y_{2,1}$ rather than $Y_{2,1}(\theta,\phi)\,.$ Notice, for instance, $Y_{2,1}$ and $Y_{2,-1}$ are exactly the same except for the sign of the argument of the exponential. This means that the drawings are the same for $-m$ and are comparable to striking the $l=1\,,\ m=1$ sphere on the right side, for example. The $-m$

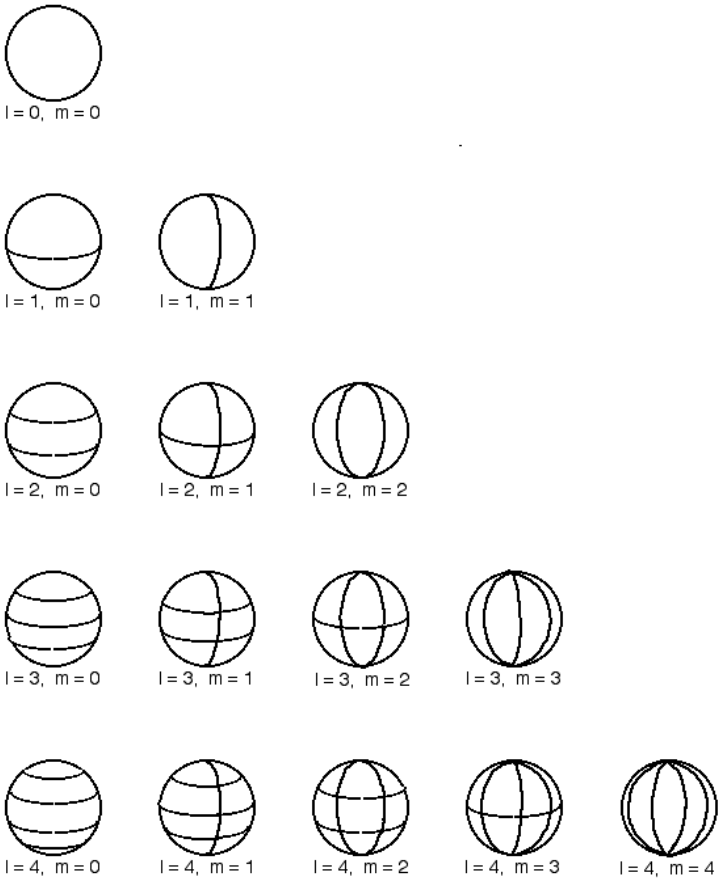

Figure 12–2. Nodal lines for spherical harmonics with non-negative $m\,.$

spherical harmonics simply swap areas of azimuthal compression and expansion relative to those with positive m where nodal lines are unaffected. Notice that when $m \neq 0$, the $Y_{l,m}$ and $Y_{l,-m}$ are adjoint functions. Some texts place a negative sign leading the spherical harmonic functions for which $m < 0$, which is a different choice of phase. We will use the convention denoted in table 12–1, where all spherical harmonics are positive. Used consistently, either choice is reasonable and both choices have advantages and disadvantages.

A taut string will vibrate when plucked with nodes at the ends. It can also have nodes at 1/2, 1/3, 1/4, ... of its length which are called harmonics. The idea here is the same for the more complex and three-dimensional geometry of a sphere. While it may be easiest to picture spherical harmonics as different modes of vibration on a sphere, our use is to describe the angular dependence of the possible wave functions of an electron in a spherically symmetric hydrogen atom. Spherical harmonics describe regions of higher and lower probabilities quantum mechanically rather than classical modes of vibrations.

Postscript: The strategy to describe the hydrogen atom is to separate the Schrodinger equation into radial and angular equations. The solutions to the radial equation can be expressed in terms of **associated Laguerre polynomials**, which will be introduced in the next chapter. The solutions to the angular equation are the spherical harmonic functions. Wave functions for an electron confined within a hydrogen atom are the product the radial and angular solutions. More explicitly, wave functions for an electron confined within a hydrogen atom are the product of **associated Laguerre functions** and spherical harmonics.

Spherical harmonics are orthogonal and complete. The spherical harmonics listed in table 12–1 are normalized so are orthonormal. They are also complete in the sense that angular space is spanned by an appropriate linear combination.

12–36. Derive $Y_{2,1}$ and $Y_{2,-1}$ using the generating function.

A generating function for spherical harmonics is

$$Y_{l,m}(\theta,\phi) \;=\; (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\, P_{l,m}(\cos\theta)\, e^{im\phi}, \qquad m \,\geq\, 0\,,$$

and

$$Y_{l,-m}(\theta,\phi) \;=\; Y^*_{l,m}(\theta,\phi), \qquad m \,<\, 0\,,$$

where the $P_{l,m}(\cos\theta)$ are associated Legendre polynomials. Associated Legendre polynomials can be generated from Legendre polynomials using

$$P_{l,m}(u) \;=\; (-1)^m \sqrt{(1-u^2)^m}\,\frac{d^m}{du^m}\,P_l(u)\,,$$

where the $P_l(u)$ are Legendre polynomials. Legendre polynomials can be generated using

$$P_l(u) \;=\; \frac{(-1)^l}{2^l l!}\,\frac{d^l}{du^l}(1-u^2)^l\,.$$

$$P_2(u) \;=\; \frac{(-1)^2}{2^2\cdot 2!}\,\frac{d^2}{du^2}(1-u^2)^2 \;=\; \frac{1}{4\cdot 2}\,\frac{d}{du}\Big[2(1-u^2)(-2u)\Big] \;=\; \frac{1}{2}\frac{d}{du}(u^3-u) \;=\; \frac{1}{2}(3u^2-1)$$

is the appropriate Legendre polynomial. The appropriate associated Legendre polynomial is

$$\begin{aligned} P_{2,1}(u) \;&=\; (-1)^1\sqrt{(1-u^2)^1}\,\frac{d^1}{du^1}\,P_2(u) \;=\; -\sqrt{(1-u^2)}\,\frac{d}{du}\frac{1}{2}(3u^2-1) \\ &=\; -\frac{1}{2}\sqrt{(1-u^2)}(6u) \;=\; -3u\sqrt{(1-u^2)}\,. \end{aligned}$$

The spherical harmonic in terms of this associated Legendre polynomial is

$$\begin{aligned} Y_{2,1}(\theta,\phi) \;&=\; (-1)^1\sqrt{\frac{(2\cdot 2+1)(2-1)!}{4\pi(2+1)!}}\,P_{2,1}(\cos\theta)\,e^{i(1)\phi} \\ &=\; -\sqrt{\frac{(5)(1)!}{4\pi(3)!}}\Big(-3\cos\theta\sqrt{(1-\cos^2\theta)}\Big)e^{i\phi} \\ &=\; 3\sqrt{\frac{5}{4\pi\cdot 3\cdot 2}}\cos\theta\,\sin\theta\,e^{i\phi} \;=\; \sqrt{\frac{3^2\cdot 5}{4\pi\cdot 3\cdot 2}}\cos\theta\,\sin\theta\,e^{i\phi} \\ &=\; \sqrt{\frac{15}{8\pi}}\cos\theta\,\sin\theta\,e^{i\phi}, \end{aligned}$$

which is identical to $Y_{2,1}$ in table 12–1. Then,

$$Y_{2,-1}(\theta,\phi) \;=\; Y^*_{2,1}(\theta,\phi) \qquad \Rightarrow \qquad Y_{2,-1}(\theta,\phi) \;=\; \sqrt{\frac{15}{8\pi}}\cos\theta\,\sin\theta\,e^{-i\phi},$$

also identical to the listing in table 12–1.

Postscript: Notice the generating function for spherical harmonics contains the restriction $m \geq 0$. Our strategy to obtain spherical harmonics with $m < 0$ is to find the corresponding $Y_{l,m}$, then to obtain $Y_{l,-m}$ by creating the adjoint. The advantage of this strategy is we do not need to consider associated Legendre polynomials with $m < 0$, though those also have meaning and can be obtained using

$$P_{l,-m}(u) \;=\; \frac{(l-m)!}{(l+m)!}\,P_{l,m}(u),$$

in our phase scheme.

Notice that all angular dependence is in the term $P_{l,m}(\cos\theta)\,e^{im\phi}$ in the generating function for the $Y_{l,m}$. Notice also that the expression underneath the radical consists entirely of constants or factors formed from the indices l and m, which is simply a normalization constant. The $Y_{l,m}$ listed in table 12–1 are properly normalized.

12–37. Show that $< Y_{1,1} \,|\, Y_{1,1} > \;=\; 1\,.$

Problems 12–37 and 12–38 provide some evidence that the spherical harmonics listed in table 12–1 are orthonormal. A general proof of orthogonality of Legendre polynomials is given in Byron and Fuller[1]. They then use that result to show that associated Legendre polynomials and spherical harmonics are orthogonal. Of course, if a system is orthogonal, it can be made orthonormal.

Having selected a representation, the appropriate form of integration for spherical angles is with respect to solid angle, $d\Omega \;=\; \sin\theta\, d\theta\, d\phi\,,$ and the normalization condition is

$$\int Y^*_{l,m}(\theta,\phi)\, Y_{l,m}(\theta,\phi)\, d\Omega \;=\; \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta \left|\, Y_{l,m}(\theta,\phi) \,\right|^2 \;=\; 1\,.$$

$$\begin{aligned}
< Y_{1,1} \,|\, Y_{1,1} > \;&=\; \int Y^*_{1,1}(\theta,\phi)\, Y_{1,1}(\theta,\phi)\, d\Omega \\
&=\; \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta \left|\, Y_{1,1}(\theta,\phi) \,\right|^2 \\
&=\; \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta \left(\sqrt{\frac{3}{8\pi}}\, \sin\theta\, e^{-i\phi} \right) \left(\sqrt{\frac{3}{8\pi}}\, \sin\theta\, e^{i\phi} \right) \\
&=\; \frac{3}{8\pi} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin^3\theta
\end{aligned}$$

Notice that since $e^{-i\phi} \cdot e^{i\phi} \;=\; e^0 \;=\; 1\,,$ the exponential dependence on ϕ vanishes. We are left with the product of two single integrals which can be evaluated at the same time, so

$$\begin{aligned}
< Y_{1,1} \,|\, Y_{1,1} > \;&=\; \frac{3}{8\pi} \Big[\, \phi \,\Big]_0^{2\pi} \left[-\frac{1}{3}\, \cos\theta \left(\sin^2\theta + 2 \right) \right]_0^{\pi} \\
&=\; \frac{3}{8\pi} \left[\, 2\pi - 0 \,\right] \left[-\frac{1}{3}\, \cos\pi \left(\sin^2\pi + 2 \right) \;+\; \frac{1}{3}\, \cos 0 \left(\sin^2 0 + 2 \right) \right] \\
&=\; \frac{3}{4} \left[-\frac{1}{3}\, (-1)\, (\,0 + 2\,) \;+\; \frac{1}{3}\, (\,1\,)\, (\,0 + 2\,) \right] \;=\; \frac{3}{4} \left[\frac{4}{3} \right] \;=\; 1\,.
\end{aligned}$$

12–38. Show that $< Y_{1,1} \,|\, Y_{2,0} > \;=\; 0\,.$

$$\begin{aligned}
< Y_{1,1} \,|\, Y_{2,0} > \;&=\; \int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta \left(\sqrt{\frac{3}{8\pi}}\, \sin\theta\, e^{-i\phi} \right) \left(\sqrt{\frac{5}{16\pi}}\, \left(3\cos^2 - 1 \right) \right) \\
&=\; \sqrt{\frac{15}{128\pi^2}} \int_0^{2\pi} d\phi\, e^{-i\phi} \int_0^{\pi} d\theta\, \sin^2\theta \left(3\cos^2 - 1 \right)
\end{aligned}$$

[1] Byron and Fuller *Mathematics of Classical and Quantum Physics* (Dover Publications, New York, 1992), pages 235–236.

Notice the form is constants times a definite integral in ϕ times a definite integral in θ. If either of the two integrals is zero, the product is zero. Focusing solely on the integral in ϕ,

$$\int_0^{2\pi} d\phi\, e^{-i\phi} \;=\; \int_0^{2\pi} d\phi \,\big(\, \cos\phi - i\sin\phi \,\big) \;=\; \int_0^{2\pi} d\phi\, \cos\phi \;-\; i\int_0^{2\pi} d\phi\, \sin\phi$$

$$=\; \sin\phi\,\Big|_0^{2\pi} - \; i\left(-\cos\phi\,\Big|_0^{2\pi}\right) \;=\; \sin 2\pi \;-\; \sin 0 \;+\; i\,\big(\cos 2\pi - \cos 0\,\big) \;=\; 0 \;-\; 0 \;+\; i\,\big(1-1\,\big) \;=\; 0\,.$$

Since the definite integral in ϕ is zero, the product is zero so $< Y_{1,1}\,|\,Y_{2,0} > \;=\; 0\,.$

Postscript: While not rising to the level of a proof, problems 12–37 and 12–38 are intended to show the plausibility of the spherical harmonics being orthonormal. Both problems seem to suggest that the integral in ϕ will require $< Y_{l,m}\,|\,Y_{l',m'} > \;=\; 0$ any time $m \neq m'$ as it did in problem 12–38. In fact, that is the case. The calculation where $m = m'$ but $l \neq l'$ is substantially more difficult. The literature supports that the spherical harmonics are orthonormal in any event.

The spherical harmonics are also complete in the sense angular space is spanned by an appropriate linear combination. While this statement is again supported by the literature, the proof is formidable. We shall say only that the starting point is the Weierstrass theorem of approximation of a continuous function by a sequence of polynomials that converge uniformly on an interval.

The integrals in ϕ and θ became separate in both problems 12–37 and 12–38. This fact suggests the two variables may be separable for all spherical harmonic functions. The next three problems exploit this idea in hybrid calculations combining calculus based arguments with earlier arguments from linear algebra.

12–39. Show that $Y_{l,m}(\theta,\phi) \;=\; A\big(\sin\theta\big)^l e^{im\phi}$ for $m = l\,.$

Spherical harmonics can be derived from the spherical coordinate form of the eigenvalue/eigenvector equation, $\mathcal{L}_z\,|\,l,\,m> \;=\; m\hbar\,|\,l,\,m>,$ and use of the raising operator for $|\,l,\,m> \rightarrow\; Y_{l,m}\,.$

The spherical coordinate system form of $\mathcal{L}_z$ and the functional forms of the eigenstates yields

$$-i\hbar\,\frac{\partial}{\partial\phi}\,Y_{l,m}(\theta,\phi) \;=\; m\hbar\; Y_{l,m}(\theta,\phi)\,.$$

We are going to assume the spherical harmonics are separable, that they can be expressed as a product of a function of θ and a second function of ϕ, as suggested by the last two problems, or

$$Y_{l,m}(\theta,\phi) \;=\; f_{l,m}(\theta)\; g_{l,m}(\phi)\,.$$

Remember that there is a top to the ladder for a given l. The top of the ladder is at $m = l\,.$ Acting on an eigenstate on the top of the ladder yields zero, meaning $\mathcal{L}_+\,|\,l,\,l> \;=\; 0\,.$ Using the spherical coordinate form of the raising operator, this equation can be developed to obtain the polar dependence $f_{l,m}(\theta)\,.$ The product of the azimuthal dependence and the polar dependence provides a solution to both partial differential equations that are posed in this development, so is itself a solution correct to within a normalization factor.

Using $Y_{l,m}(\theta,\phi) \;=\; f_{l,m}(\theta)\; g_{l,m}(\phi)$ in the differential equation built from the $\mathcal{L}_z$ operator

$$\begin{aligned}
-i\hbar\,\frac{\partial}{\partial\phi}\,f_{l,m}(\theta)\;g_{l,m}(\phi) \;&=\; m\hbar\,f_{l,m}(\theta)\;g_{l,m}(\phi) \\
\Rightarrow\quad -i\,f_{l,m}(\theta)\frac{\partial}{\partial\phi}\,g_{l,m}(\phi) \;&=\; m f_{l,m}(\theta)\;g_{l,m}(\phi) \\
\Rightarrow\quad -i\frac{\partial}{\partial\phi}\,g_{l,m}(\phi) \;&=\; m\,g_{l,m}(\phi) \\
\Rightarrow\quad \frac{\partial g_{l,m}(\phi)}{g_{l,m}(\phi)} \;&=\; im\,\partial\phi \\
\Rightarrow\quad \ln g_{l,m}(\phi) \;&=\; im\phi \\
\Rightarrow\quad g_{l,m}(\phi) \;&=\; e^{im\phi}.
\end{aligned}$$

Notice the exponential has no dependence on l, so we can write

$$g_m(\phi) \;=\; e^{im\phi}\,,$$

which is the azimuthal dependence.

Remember that there is a top and bottom to the ladder for a given l. The top of the ladder is at $m = l$. If we act on an eigenstate on the top of the ladder, we get zero, meaning

$$\mathcal{L}_+\,|\,l,\,l>\;=\;0\,.$$

Using the spherical coordinate forms of the raising operator and the separated eigenstate, this is

$$\hbar\,e^{i\phi}\left[\frac{\partial}{\partial\theta}\;+\;i\cot\theta\frac{\partial}{\partial\phi}\right]f_{l,l}(\theta)\,e^{il\phi}\;=\;0$$

$$\begin{aligned}
\Rightarrow\quad e^{il\phi}\frac{\partial}{\partial\theta}\,f_{l,l}(\theta)\;+\;i\,f_{l,l}(\theta)\,\cot\theta\big(il\big)e^{il\phi}\;&=\;0 \\
\Rightarrow\quad \frac{\partial}{\partial\theta}\,f_{l,l}(\theta)\;-\;l\,f_{l,l}(\theta)\cot\theta\;&=\;0\,.
\end{aligned}$$

The solution to this is $f_{l,l}(\theta) \;=\; A\big(\sin\theta\big)^l$. To see that it is a solution,

$$\frac{\partial}{\partial\theta}\,f_{l,l}(\theta) \;=\; \frac{\partial}{\partial\theta}A\big(\sin\theta\big)^l \;=\; A\,l\,\big(\sin\theta\big)^{l-1}\cos\theta,$$

and substituting this in the last differential equation,

$$A\,l\,\big(\sin\theta\big)^{l-1}\cos\theta\;-\;l\left[A\big(\sin\theta\big)^l\right]\frac{\cos\theta}{\sin\theta} \;=\; A\,l\,\big(\sin\theta\big)^{l-1}\left[\cos\theta\;-\;\sin\theta\frac{\cos\theta}{\sin\theta}\right] \;=\; 0\,.$$

So the unnormalized form of the $m = l$ spherical harmonics is

$$Y_{l,m}(\theta,\phi) \;=\; A\big(\sin\theta\big)^l e^{im\phi}\,.$$

Postscript: The ket $|\,l,\,m>$ is an eigenstate of the commuting operators $\mathcal{L}^2$ and $\mathcal{L}_z$, but it is an abstract eigenstate. That $|\,l,\,m>$ is abstract is irrelevant for the eigenvalues, since eigenvalues are properties of the operators. We can form an inner product with an abstract vector to obtain a representation. Using a guided choice, the angles of spherical coordinate system will yield an appropriate representation. Just as $<x\,|\,\psi> \;=\; \psi\,(x)\,,$

$$<\theta,\,\phi\,|\,l,\,m> \;=\; Y_{l,m}(\theta,\phi)\,,$$

where Y is chosen as the symbol conventionally used to represent the spherical harmonics.

12–40. Show $Y_{l,l} \;=\; A\big(\sin\theta\big)^{l} e^{im\phi}$ yields the $Y_{1,1}$ of table 12–1 when normalized.

This problem is evidence that the solution of the last problem is correct. Also, the probability postulate will eventually require that a state vector is normalized.

To normalize $Y_{1,1} \;=\; A\big(\sin\theta\big)^{1} e^{i(1)\phi} \;=\; A\sin\theta\, e^{i\phi}\,,$

$$1 \;=\; \int (Y_{1,1})^{*}\, Y_{1,1}\, d\Omega \;=\; \int A^{*}\sin\theta\, e^{-i\phi}\; A\sin\theta\, e^{i\phi}\, d\Omega$$

$$=\; |\,A\,|^{\,2} \int \sin^{2}\theta\, e^{0}\, d\Omega \;=\; |\,A\,|^{\,2} \int_{0}^{2\pi} d\phi \int_{0}^{\pi} d\theta\, \sin^{2}\theta\, \sin\theta$$

$$=\; |\,A\,|^{\,2} \int_{0}^{\pi} d\theta\, \sin^{3}\theta \int_{0}^{2\pi} d\phi \;=\; 2\pi\,|\,A\,|^{\,2} \int_{0}^{\pi} d\theta\, \sin^{3}\theta$$

$$=\; 2\pi\,|\,A\,|^{\,2} \left[-\frac{1}{3}\cos\theta\big(\sin^{2}\theta + 2\big)\right]_{0}^{\pi} \;=\; \frac{2\pi}{3}\,|\,A\,|^{\,2} \left[\cos\theta\big(\sin^{2}\theta + 2\big)\right]_{\pi}^{0}$$

$$=\; \frac{2\pi}{3}\,|\,A\,|^{\,2} \left[\cos(0)\Big(\cancel{\sin^{2}}(0) + 2\Big) \;-\; \cos(\pi)\Big(\cancel{\sin^{2}}(\pi) + 2\Big)\right]$$

$$=\; \frac{2\pi}{3}\,|\,A\,|^{\,2} \Big[(1)(2) \;-\; (-1)(2)\Big] \;=\; \frac{2\pi}{3}\,|\,A\,|^{\,2}[4]$$

$$\Rightarrow \quad \frac{8\pi}{3}\,|\,A\,|^{\,2} \;=\; 1 \quad \Rightarrow \quad A \;=\; \sqrt{\frac{3}{8\pi}} \quad \Rightarrow \quad Y_{1,1} \;=\; \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi},$$

which is identical to $Y_{1,1}$ in table 12–1.

12–41. Derive $Y_{1,0}$ from the result of the previous example.

Use the lowering operator in spherical coordinates on $Y_{1,1}$ to obtain $Y_{1,0}$.

A lowering operator acting on an abstract eigenstate is $\mathcal{L}_- \,|\, l, m > \;=\; B \,|\, l, m-1 >$, where B is the eigenvalue. Using the spherical angle representation on the eigenstate $Y_{1,1}$, this eigenvalue/eigenvector equation is

$$-\hbar\, e^{-i\phi} \left(\frac{\partial}{\partial\theta} \;-\; i \cot\theta \frac{\partial}{\partial\phi} \right) Y_{1,1} \;=\; B\, Y_{1,0}\,,$$

again, where B is the eigenvalue. Using the unnormalized form of $Y_{1,1}$, we have

$$\begin{aligned}
B\, Y_{1,0} \;&=\; -\hbar\, e^{-i\phi} \left(\frac{\partial}{\partial\theta} \;-\; i \cot\theta \frac{\partial}{\partial\phi} \right) A \,\sin\theta\, e^{i\phi} \\
&=\; -A\hbar\, e^{-i\phi} \left(e^{i\phi} \frac{\partial}{\partial\theta} \sin\theta \;-\; i \cot\theta \,\sin\theta \frac{\partial}{\partial\phi}\, e^{i\phi} \right) \\
&=\; -A\hbar\, e^{-i\phi} \left(e^{i\phi} \cos\theta \;-\; i \frac{\cos\theta}{\sin\theta} \,\sin\theta (i) e^{i\phi} \right) \\
&=\; -A\hbar \big(\cos\theta \;+\; \cos\theta \big) \;=\; -2A\hbar \big(\cos\theta \big) \qquad \Rightarrow \qquad Y_{1,0} \;=\; C \cos\theta\,,
\end{aligned}$$

where all constants have been combined to form C, which becomes simply a new symbol for the normalization constant. We normalize this using the same procedure as the previous example,

$$\begin{aligned}
1 \;&=\; \int C^* \cos\theta\, C \cos\theta\, d\Omega \;=\; |\, C \,|^{\,2} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \,\cos^2\theta \,\sin\theta \\
&=\; 2\pi \,|\, C \,|^{\,2} \int_0^{\pi} d\theta \,\cos^2\theta \,\sin\theta \;=\; 2\pi \,|\, C \,|^{\,2} \Big[-\frac{\cos^3\theta}{3} \Big]_0^{\pi} \;=\; \frac{2\pi}{3} \,|\, C \,|^{\,2} \Big[\cos^3\theta \Big]_{\pi}^{0} \\
&=\; \frac{2\pi}{3} \,|\, C \,|^{\,2} \Big[\cos^3(0) \;-\; \cos^3(\pi) \Big] \;=\; \frac{2\pi}{3} \,|\, C \,|^{\,2} \Big[1 \;-\; (-1) \Big] \;=\; \frac{2\pi}{3} \,|\, C \,|^{\,2} [2] \\
\Rightarrow \qquad &\frac{4\pi}{3} \,|\, C \,|^{\,2} \;=\; 1 \qquad \Rightarrow \qquad C \;=\; \sqrt{\frac{3}{4\pi}} \qquad \Rightarrow \qquad Y_{1,0} \;=\; \sqrt{\frac{3}{4\pi}} \cos\theta\,,
\end{aligned}$$

which is identical to $Y_{1,0}$ listed in table 12–1.

The third portion of this chapter returns to matrix operators, and continues the interpretation of a braket as a matrix element which was introduced in the discussion of the SHO. The culmination is an application of the general uncertainty relation to the component angular momentum operators which are related $\big[\, \mathcal{L}_i \,,\, \mathcal{L}_j \,\big] \;=\; i\hbar \mathcal{L}_k \qquad \Rightarrow \qquad \triangle \mathcal{L}_i \triangle \mathcal{L}_j \;\geq\; \frac{\hbar}{2} \Big| < \mathcal{L}_k > \Big|$.

12–42. Derive the $\mathcal{L}_z$ matrix operator for $l = 1$.

The component angular momentum operators in $\mathbb{C}^3$ have been given to be

$$\mathcal{L}_x \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar\,, \qquad \mathcal{L}_y \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar\,, \qquad \mathcal{L}_z \rightarrow \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\hbar$$

without proof. This and the next problem derive $\mathcal{L}_z$ and $\mathcal{L}_y$, and $\mathcal{L}_x$ is left as exercise 12–65.

The eigenvalues are properties of the operator. Knowing the eigenvalue/eigenvector equation linking an eigenvalue to a specific eigenstate, in this problem $\mathcal{L}_z\,|\,l\,,\,m> \;=\; m\hbar\,|\,l\,,\,m>$, enables the construction of the operator. This problem continues the interpretation of a braket of the form $<i\,|\,\mathcal{A}\,|\,j>$ as the element a_{ij} of the matrix form of the operator $\mathcal{A}$. In this case, $<1\,,\,m_i\,|\,\mathcal{L}_z\,|\,1\,,\,m_j>$ are the elements of $\mathcal{L}_z$ for $l = 1$.

$l = 1 \quad \Rightarrow \quad m \;=\; 1\,,\; 0\,,$ or $-1\,,$ and $\mathcal{L}_z$ can be represented

$$\mathcal{L}_z \;=\; \begin{pmatrix} <1\,,\,1\,|\,\mathcal{L}_z\,|\,1\,,\,1> & <1\,,\,1\,|\,\mathcal{L}_z\,|\,1\,,\,0> & <1\,,\,1\,|\,\mathcal{L}_z\,|\,1\,,-1> \\ <1\,,\,0\,|\,\mathcal{L}_z\,|\,1\,,\,1> & <1\,,\,0\,|\,\mathcal{L}_z\,|\,1\,,\,0> & <1\,,\,0\,|\,\mathcal{L}_z\,|\,1\,,-1> \\ <1\,,-1\,|\,\mathcal{L}_z\,|\,1\,,\,1> & <1\,,-1\,|\,\mathcal{L}_z\,|\,1\,,\,0> & <1\,,-1\,|\,\mathcal{L}_z\,|\,1\,,-1> \end{pmatrix}.$$

There are three eigenvalue/eigenvector equations in this matrix, namely

$$\begin{aligned} \mathcal{L}_z\,|\,1\,,\,1> \;&=\; 1\cdot\hbar\,|\,1\,,\,1> \;=\; \hbar\,|\,1\,,\,1>\,, \\ \mathcal{L}_z\,|\,1\,,\,0> \;&=\; 0\cdot\hbar\,|\,1\,,\,0> = 0\,, \\ \mathcal{L}_z\,|\,1\,,-1> \;&=\; -1\cdot\hbar\,|\,1\,,-1> \;=\; -\hbar\,|\,1\,,-1>\,. \end{aligned}$$

Using these in the above matrix,

$$\mathcal{L}_z \;=\; \begin{pmatrix} <1\,,\,1\,|\,\hbar\,|\,1\,,\,1> & <1\,,\,1\,|\,0 & <1\,,\,1\,|\,-\hbar\,|\,1\,,-1> \\ <1\,,\,0\,|\,\hbar\,|\,1\,,\,1> & <1\,,\,0\,|\,0 & <1\,,\,0\,|\,-\hbar\,|\,1\,,-1> \\ <1\,,-1\,|\,\hbar\,|\,1\,,\,1> & <1\,,-1\,|\,0 & <1\,,-1\,|\,-\hbar\,|\,1\,,-1> \end{pmatrix}$$

$$= \begin{pmatrix} \hbar\,<1\,,\,1\,|\,1\,,\,1> & 0 & -\hbar\,<1\,,\,1\,|\,1\,,-1> \\ \hbar\,<1\,,\,0\,|\,1\,,\,1> & 0 & -\hbar\,<1\,,\,0\,|\,1\,,-1> \\ \hbar\,<1\,,-1\,|\,1\,,\,1> & 0 & -\hbar\,<1\,,-1\,|\,1\,,-1> \end{pmatrix}.$$

Orthonormality dictates $<1\,,\,1\,|\,1\,,\,1> \;=\; <1\,,-1\,|\,1\,,-1> \;=\; 1\,,$ and all other inner products are zero. Thus

$$\mathcal{L}_z \;=\; \begin{pmatrix} \hbar\cdot 1 & 0 & -\hbar\cdot 0 \\ \hbar\cdot 0 & 0 & -\hbar\cdot 0 \\ \hbar\cdot 0 & 0 & -\hbar\cdot 1 \end{pmatrix} \;=\; \begin{pmatrix} \hbar & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\hbar \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\hbar\,.$$

Postscript: Since $l = 1$ does not change, the index for m alone will uniquely identify an eigenstate, and the notation can be simplified to $|\,1\,,\,1> \rightarrow |\,1>$, $|\,1\,,\,0> \rightarrow |\,0>$, and $|\,1\,,-1> \rightarrow |\,-1>$ for the next and other problems/exercises.

12–43. Derive the $\mathcal{L}_y$ matrix operator for $l = 1$.

It appears that we do not have an eigenvector/eigenvalue equation for $\mathcal{L}_y$, but remember that

$$\mathcal{L}_+ = \mathcal{L}_x + i\mathcal{L}_y \qquad \text{and} \qquad \mathcal{L}_- = \mathcal{L}_x - i\mathcal{L}_y \quad \Rightarrow \quad \mathcal{L}_+ - \mathcal{L}_- = 2i\mathcal{L}_y \quad \Rightarrow \quad \mathcal{L}_y = \frac{i}{2}(\mathcal{L}_- - \mathcal{L}_+)$$

and we can proceed as was done in the previous problem knowing

$$\mathcal{L}_\pm \,|\, l, m> \;=\; \sqrt{l(l+1) - m(m \pm 1)}\;\hbar \,|\, l, m \pm 1> \;.$$

Remembering that $l = 1$ and does not change in this problem,

$$\begin{aligned}
\mathcal{L}_- \,|\, 1, 1> \rightarrow \mathcal{L}_- \,|\, 1> &= \sqrt{1(1+1) - 1(1-1)}\;\hbar \,|\, 0> \;=\; \sqrt{2}\,\hbar \,|\, 0> \\
\mathcal{L}_- \,|\, 1, 0> \rightarrow \mathcal{L}_- \,|\, 0> &= \sqrt{1(1+1) - 0(0-1)}\;\hbar \,|\, -1> \;=\; \sqrt{2}\,\hbar \,|\, -1> \\
\mathcal{L}_- \,|\, 1, -1> \rightarrow \mathcal{L}_- \,|\, -1> &= 0 \quad \text{because it cannot be lowered.} \\
\mathcal{L}_+ \,|\, 1, 1> \rightarrow \mathcal{L}_+ \,|\, 1> &= 0 \quad \text{because it cannot be raised.} \\
\mathcal{L}_+ \,|\, 1, 0> \rightarrow \mathcal{L}_+ \,|\, 0> &= \sqrt{1(1+1) - 0(0+1)}\;\hbar \,|\, 1> \;=\; \sqrt{2}\,\hbar \,|\, 1> \\
\mathcal{L}_+ \,|\, 1, -1> \rightarrow \mathcal{L}_+ \,|\, -1> &= \sqrt{1(1+1) - (-1)(-1+1)}\;\hbar \,|\, 0> \;=\; \sqrt{2}\,\hbar \,|\, 0>
\end{aligned}$$

The matrix representation of $\mathcal{L}_y$ is

$$\mathcal{L}_y \;=\; \begin{pmatrix} <1\,|\,\mathcal{L}_y\,|\,1> & <1\,|\,\mathcal{L}_y\,|\,0> & <1\,|\,\mathcal{L}_y\,|\,-1> \\ <0\,|\,\mathcal{L}_y\,|\,1> & <0\,|\,\mathcal{L}_y\,|\,0> & <0\,|\,\mathcal{L}_y\,|\,-1> \\ <-1\,|\,\mathcal{L}_y\,|\,1> & <-1\,|\,\mathcal{L}_y\,|\,0> & <-1\,|\,\mathcal{L}_y\,|\,-1> \end{pmatrix}$$

$$= \frac{i}{2}\begin{pmatrix} <1\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,1> & <1\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,0> & <1\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,-1> \\ <0\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,1> & <0\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,0> & <0\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,-1> \\ <-1\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,1> & <-1\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,0> & <-1\,|\,\mathcal{L}_- - \mathcal{L}_+\,|\,-1> \end{pmatrix} =$$

$$\frac{i}{2}\begin{pmatrix} <1\,|\,\mathcal{L}_-\,|\,1> - <1\,|\,\mathcal{L}_+\,|\,1> & <1\,|\,\mathcal{L}_-\,|\,0> - <1\,|\,\mathcal{L}_+\,|\,0> & <1\,|\,\mathcal{L}_-\,|\,-1> - <1\,|\,\mathcal{L}_+\,|\,-1> \\ <0\,|\,\mathcal{L}_-\,|\,1> - <0\,|\,\mathcal{L}_+\,|\,1> & <0\,|\,\mathcal{L}_-\,|\,0> - <0\,|\,\mathcal{L}_+\,|\,0> & <0\,|\,\mathcal{L}_-\,|\,-1> - <0\,|\,\mathcal{L}_+\,|\,-1> \\ <-1|\mathcal{L}_-|1> - <-1|\mathcal{L}_+|1> & <-1|\mathcal{L}_-|0> - <-1|\mathcal{L}_+|0> & <-1|\mathcal{L}_-|-1> - <-1|\mathcal{L}_+|-1> \end{pmatrix}$$

$$= \frac{i}{2}\begin{pmatrix} <1\,|\,\sqrt{2}\,\hbar\,|\,0> - <1\,|\,0 & <1\,|\,\sqrt{2}\,\hbar\,|\,-1> - <1\,|\,\sqrt{2}\,\hbar\,|\,1> & <1\,|\,0 - <1\,|\,\sqrt{2}\,\hbar\,|\,0> \\ <0\,|\,\sqrt{2}\,\hbar\,|\,0> - <0\,|\,0 & <0\,|\,\sqrt{2}\,\hbar\,|\,-1> - <0\,|\,\sqrt{2}\,\hbar\,|\,1> & <0\,|\,0 - <0\,|\,\sqrt{2}\,\hbar\,|\,0> \\ <-1|\sqrt{2}\,\hbar\,|\,0> - <-1|0 & <-1|\sqrt{2}\,\hbar\,|\,-1> - <-1|\sqrt{2}\,\hbar\,|\,1> & <-1|0 - <-1|\sqrt{2}\,\hbar\,|\,0> \end{pmatrix}$$

$$= \frac{i\sqrt{2}\,\hbar}{2}\begin{pmatrix} <1\,|\,0> - 0 & <1\,|\,-1> - <1\,|\,1> & 0 - <1\,|\,0> \\ <0\,|\,0> - 0 & <0\,|\,-1> - <0\,|\,1> & 0 - <0\,|\,0> \\ <-1\,|\,0> - 0 & <-1\,|\,-1> - <-1\,|\,1> & 0 - <-1\,|\,0> \end{pmatrix}$$

$$= \frac{i\,\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 0-1 & 0 \\ 1 & 0-0 & -1 \\ 0 & 1-0 & 0 \end{pmatrix} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar\,.$$

12–44. Find the matrix form of the $\mathcal{L}_+$ operator for $l = 1$.

This problem demonstrates another method of obtaining a matrix representation of an operator.

$$\mathcal{L}_+ \;=\; \mathcal{L}_x + i\,\mathcal{L}_y \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\hbar \;+\; i\,\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\hbar$$

$$= \frac{\hbar}{\sqrt{2}}\left[\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}\right] \;=\; \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 2 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix} \;=\; \sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}\hbar$$

12–45. Apply the general uncertainty relation to the three component $l = 1$ operators.

From chapter 6, the general uncertainty relation is

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2 \;+\; \frac{1}{4}\,<\psi|\,\mathcal{C}\,|\,\psi>^2$$

for observables related by operators such that $\left[\mathcal{A}\,,\,\mathcal{B}\right] = i\mathcal{C}$. The product of uncertainties can only be minimized if $\frac{1}{4}\,<\psi|\,\left[\widehat{\mathcal{A}},\,\widehat{\mathcal{B}}\right]_+|\,\psi>^2 \;=\; 0\,,$ thus, consider only

$$\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\,<\psi|\,\mathcal{C}\,|\,\psi>^2$$

for $\left[\mathcal{L}_x\,,\,\mathcal{L}_y\right] \;=\; i\hbar\mathcal{L}_z$ and its cyclic permutations.

For $\left(\triangle\mathcal{A}\right)^2\left(\triangle\mathcal{B}\right)^2 \;\geq\; \frac{1}{4}\,<\psi|\,\mathcal{C}\,|\,\psi>^2,$ and $\left[\mathcal{L}_x\,,\,\mathcal{L}_y\right] \;=\; i\hbar\mathcal{L}_z\,,$ $\mathcal{A} \;\rightarrow\; \mathcal{L}_x\,,$ $\mathcal{B} \;\rightarrow\; \mathcal{L}_y\,,$ and $\mathcal{C} \;\rightarrow\; \hbar\mathcal{L}_z\,.$ When the component angular momentum operators are substituted, the minimal product general uncertainty relation reads

$$\left(\triangle\mathcal{L}_x\right)^2\left(\triangle\mathcal{L}_y\right)^2 \;\geq\; \frac{1}{4}\,<\psi|\,\hbar\mathcal{L}_z\,|\,\psi>^2$$

$$\Rightarrow \qquad \triangle\mathcal{L}_x\,\triangle\mathcal{L}_y \;\geq\; \frac{\hbar}{2}\left|\,<\mathcal{L}_z>\,\right|,$$

where the absolute value is appropriate because its square is positive definite. Remember that the expectation value $<\mathcal{L}_z>$ is understood to be dependent on a state vector. Similarly,

$$\left[\mathcal{L}_y\,,\,\mathcal{L}_z\right] \;=\; i\hbar\mathcal{L}_x \qquad \Rightarrow \qquad \triangle\mathcal{L}_y\,\triangle\mathcal{L}_z \;\geq\; \frac{\hbar}{2}\left|\,<\mathcal{L}_x>\,\right| \quad \text{and}$$

$$\left[\mathcal{L}_z\,,\,\mathcal{L}_x\right] \;=\; i\hbar\mathcal{L}_y \qquad \Rightarrow \qquad \triangle\mathcal{L}_z\,\triangle\mathcal{L}_x \;\geq\; \frac{\hbar}{2}\left|\,<\mathcal{L}_y>\,\right|.$$

These are frequently written as one relation, $\triangle\mathcal{L}_i\,\triangle\mathcal{L}_j \;\geq\; \frac{\hbar}{2}\left|\,<\mathcal{L}_k>\,\right|$ where subscripts are understood to be the cyclic permutations of $x\,,\;y\,,\;z\,.$

12–46. Find $<\mathcal{L}_x>$, $<\mathcal{L}_y>$, and $<\mathcal{L}_z>$ given $|\psi> = \frac{1}{\sqrt{14}}\begin{pmatrix}3\\1\\2i\end{pmatrix}$.

This is the first in a sequence of problems intended to provide numerical evidence of the minimal general uncertainty relations of the previous problem for the component angular momentum operators. The sequence also revisits material from the first six chapters demonstrating its utility in $\mathbb{C}^3$. The first step is to find expectation values using $<\mathcal{L}_i> = <\psi\,|\,\mathcal{L}_i\,|\,\psi>$, which is completed without eigenvectors or probabilities.

$$<\mathcal{L}_x> = \left(3,\ 1,\ -2i\right)\frac{1}{\sqrt{14}}\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\,\frac{1}{\sqrt{14}}\begin{pmatrix}3\\1\\2i\end{pmatrix}$$

$$= \frac{\hbar}{14\sqrt{2}}\left(3,\ 1,\ -2i\right)\begin{pmatrix}1\\3+2i\\1\end{pmatrix} = \frac{\hbar\sqrt{2}}{28}\left(3+3+2i-2i\right) = \frac{6\hbar\sqrt{2}}{28} = \frac{3\sqrt{2}}{14}\,\hbar$$

$$<\mathcal{L}_y> = \left(3,\ 1,\ -2i\right)\frac{1}{\sqrt{14}}\frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar\,\frac{1}{\sqrt{14}}\begin{pmatrix}3\\1\\2i\end{pmatrix}$$

$$= \frac{\hbar}{14\sqrt{2}}\left(3,\ 1,\ -2i\right)\begin{pmatrix}-i\\3i+2\\i\end{pmatrix} = \frac{\hbar\sqrt{2}}{28}\left(-3i+3i+2+2\right) = \frac{4\hbar\sqrt{2}}{28} = \frac{\sqrt{2}}{7}\,\hbar$$

$$<\mathcal{L}_z> = \left(3,\ 1,\ -2i\right)\frac{1}{\sqrt{14}}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar\,\frac{1}{\sqrt{14}}\begin{pmatrix}3\\1\\2i\end{pmatrix}$$

$$= \frac{\hbar}{14}\left(3,\ 1,\ -2i\right)\begin{pmatrix}3\\0\\-2i\end{pmatrix} = \frac{\hbar}{28}\left(9+0-4\right) = \frac{5}{14}\,\hbar$$

12–47. Find $<\mathcal{L}_x^2>$, $<\mathcal{L}_y^2>$, and $<\mathcal{L}_z^2>$ for $|\psi> = \frac{1}{\sqrt{14}}\begin{pmatrix}3\\1\\2i\end{pmatrix}$.

The next step is to calculate $<\mathcal{L}_i^2> = <\psi\,|\,\mathcal{L}_i\,\mathcal{L}_i\,|\,\psi>$.

$$<\mathcal{L}_x^2> = \left(3,\ 1,\ -2i\right)\frac{1}{\sqrt{14}}\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\,\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\,\frac{1}{\sqrt{14}}\begin{pmatrix}3\\1\\2i\end{pmatrix}$$

$$= \frac{\hbar^2}{28}\left(3,\ 1,\ -2i\right)\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}1\\3+2i\\1\end{pmatrix} = \frac{\hbar^2}{28}\left(3,\ 1,\ -2i\right)\begin{pmatrix}3+2i\\2\\3+2i\end{pmatrix}$$

$$= \frac{\hbar^2}{28}\left(9+6i+2-6i+4\right) = \frac{15}{28}\,\hbar^2$$

$$
\begin{aligned}
<\mathcal{L}_y^2> &= \left(3\,,\ 1\,,\ -2i\right)\frac{1}{\sqrt{14}}\,\frac{1}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}\hbar\,\frac{1}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}\hbar\,\frac{1}{\sqrt{14}}\begin{pmatrix}3\\ 1\\ 2i\end{pmatrix}\\
&= \frac{\hbar^2}{28}\left(3\,,\ 1\,,\ -2i\right)\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}\begin{pmatrix}-i\\ 3i+2\\ i\end{pmatrix} \;=\; \frac{\hbar^2}{28}\left(3\,,\ 1\,,\ -2i\right)\begin{pmatrix}3-2i\\ 2\\ -3+2i\end{pmatrix}\\
&= \frac{\hbar^2}{28}\left(9-6i+2+6i+4\right) \;=\; \frac{15}{28}\,\hbar^2
\end{aligned}
$$

$$
\begin{aligned}
<\mathcal{L}_z^2> &= \left(3\,,\ 1\,,\ -2i\right)\frac{1}{\sqrt{14}}\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}\hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}\hbar\,\frac{1}{\sqrt{14}}\begin{pmatrix}3\\ 1\\ 2i\end{pmatrix}\\
&= \frac{\hbar^2}{14}\left(3\,,\ 1\,,\ -2i\right)\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix}3\\ 0\\ -2i\end{pmatrix} \;=\; \frac{\hbar^2}{14}\left(3\,,\ 1\,,\ -2i\right)\begin{pmatrix}3\\ 0\\ 2i\end{pmatrix}\\
&= \frac{\hbar^2}{14}\left(9+0+4\right) \;=\; \frac{13}{14}\,\hbar^2
\end{aligned}
$$

Postscript: $\mathcal{L}^2 \;=\; \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; \mathcal{L}_z^2 \quad\Rightarrow\quad <\mathcal{L}^2> \;=\; <\mathcal{L}_x^2> \;+\; <\mathcal{L}_y^2> \;+\; <\mathcal{L}_z^2>$ which is $\frac{15}{28}\,\hbar^2 \;+\; \frac{15}{28}\,\hbar^2 \;+\; \frac{26}{28}\,\hbar^2 \;=\; \frac{56}{28}\,\hbar^2 \;=\; 2\hbar^2$ for this system, reinforcing problems 1–16 and 12–10.

12–48. Find $\triangle\mathcal{L}_x\,,\ \triangle\mathcal{L}_y\,,$ and $\triangle\mathcal{L}_z$ for this system.

Now compute $\triangle\mathcal{L}_i \;=\; \left[\,<\mathcal{L}_i^2> \;-\; <\mathcal{L}_i>^2\,\right]^{1/2}$.

$$\triangle\mathcal{L}_x \;=\; \left[\frac{15}{28}\,\hbar^2 \;-\; \left(\frac{3\sqrt{2}}{14}\,\hbar\right)^2\right]^{1/2} \;=\; \left[\frac{105}{196}\,\hbar^2 \;-\; \frac{18}{196}\,\hbar^2\right]^{1/2} \;=\; \left[\frac{87}{196}\,\hbar^2\right]^{1/2} \;=\; \frac{\sqrt{87}}{14}\,\hbar$$

$$\triangle\mathcal{L}_y \;=\; \left[\frac{15}{28}\,\hbar^2 \;-\; \left(\frac{\sqrt{2}}{7}\,\hbar\right)^2\right]^{1/2} \;=\; \left[\frac{105}{196}\,\hbar^2 \;-\; \frac{8}{196}\,\hbar^2\right]^{1/2} \;=\; \left[\frac{97}{196}\,\hbar^2\right]^{1/2} \;=\; \frac{\sqrt{97}}{14}\,\hbar$$

$$\triangle\mathcal{L}_z \;=\; \left[\frac{13}{14}\,\hbar^2 \;-\; \left(\frac{5}{14}\,\hbar\right)^2\right]^{1/2} \;=\; \left[\frac{182}{196}\,\hbar^2 \;-\; \frac{25}{196}\,\hbar^2\right]^{1/2} \;=\; \left[\frac{157}{196}\,\hbar^2\right]^{1/2} \;=\; \frac{\sqrt{157}}{14}\,\hbar$$

12–49. Show that $\quad \triangle \mathcal{L}_i \triangle \mathcal{L}_j \;\geq\; \dfrac{\hbar}{2} \left| < \mathcal{L}_k > \right| \quad$ for this system.

This is the primary reason to calculate the three uncertainties.

$$\triangle \mathcal{L}_x \triangle \mathcal{L}_y \;=\; \frac{\sqrt{87}}{14}\,\hbar\,\frac{\sqrt{97}}{14}\,\hbar \;=\; 0.4687\,\hbar^2 \quad \geq \quad \frac{\hbar}{2}\left| < \mathcal{L}_z > \right| \;=\; \frac{\hbar}{2}\,\frac{5}{14}\,\hbar \;=\; 0.1786\,\hbar^2$$

$$\triangle \mathcal{L}_y \triangle \mathcal{L}_z \;=\; \frac{\sqrt{97}}{14}\,\hbar\,\frac{\sqrt{157}}{14}\,\hbar \;=\; 0.6296\,\hbar^2 \quad \geq \quad \frac{\hbar}{2}\left| < \mathcal{L}_x > \right| \;=\; \frac{\hbar}{2}\,\frac{3\sqrt{2}}{14}\,\hbar \;=\; 0.1515\,\hbar^2$$

$$\triangle \mathcal{L}_z \triangle \mathcal{L}_x \;=\; \frac{\sqrt{157}}{14}\,\hbar\,\frac{\sqrt{87}}{14}\,\hbar \;=\; 0.5963\,\hbar^2 \quad \geq \quad \frac{\hbar}{2}\left| < \mathcal{L}_y > \right| \;=\; \frac{\hbar}{2}\,\frac{\sqrt{2}}{7}\,\hbar \;=\; 0.1010\,\hbar^2$$

Postscript: Notice that the minimal general uncertainty relation from problem 12–45 applied here to the component angular momentum operators is between the product of two uncertainties and a multiple of an expectation value, rather than involving three uncertainties.

Exercises

12–50. Show that (a) $\mathcal{L}_x$ does not commute with $\mathcal{L}_z$, and

(b) $\mathcal{L}_y$ does not commute with $\mathcal{L}_z$.

Component orbital angular momentum operators do not commute. See problem 12–2.

12–51. Show (a) $\left[\mathcal{X}, \mathcal{Y}\right] = 0$,

(b) $\left[\mathcal{P}_x, \mathcal{P}_y\right] = 0$, and

(c) $\left[\mathcal{X}, \mathcal{P}_x\right] = i\hbar$ in position space.

Let the indicated commutators operate on an arbitrary function, say $f(x, y, z)$, to obtain all three results. These three commutators are a representative sample supporting problem 12–4.

12–52. Show (a) $\left[\mathcal{X}, \mathcal{Y}\right] = 0$,

(b) $\left[\mathcal{P}_x, \mathcal{P}_y\right] = 0$, and

(c) $\left[\mathcal{X}, \mathcal{P}_x\right] = i\hbar$ in momentum space.

Similar to the last exercise, this time using the representations of component operators in momentum space. The arbitrary function should be $g(p_x, p_y, p_z)$ for momentum space representations.

12–53. Show that

$$\left[\mathcal{A} + \mathcal{B}, \mathcal{C}\right] = \left[\mathcal{A}, \mathcal{C}\right] + \left[\mathcal{B}, \mathcal{C}\right].$$

Follow the processes of problems 12–5, 12–6, and 12–7.

12–54. Prove that

$$\Big[\mathcal{A}, \left[\mathcal{B}, \mathcal{C}\right]\Big] + \Big[\mathcal{B}, \left[\mathcal{C}, \mathcal{A}\right]\Big] + \Big[\mathcal{C}, \left[\mathcal{A}, \mathcal{B}\right]\Big] = 0.$$

This relation is known as the Jacobi identity. Again, follow problems 12–5, 12–6, and 12–7.

12–55. (a) Given $|l,m> = |4,m>$, what measurements are possible for $\mathcal{L}^2$ and $\mathcal{L}_z$?

(b) For the eigenstate $|l,m> = |l,-3>$, what measurements are possible for $\mathcal{L}^2$ and $\mathcal{L}_z$?

Measurements must yield eigenvalues! See problems 12–23 and 12–24.

12–56. What are $\mathcal{L}_+$ and $\mathcal{L}_-$ operating on eigenstate $|3,-2>$?

Ladder operators become increasingly important. See problems 12–25 and 12–26.

12–57. Find $<\mathcal{L}_z>$ and $\triangle\mathcal{L}_z$ for the state vector

$$|\psi(t=0)> = A\big(|2,1> + 3|1,-1>\big)$$

used for problems 12–27 through 12–32.

These two details finish the sequence completely. You have eigenvalues and probabilities from problem 12–29. Calculations are procedurally similar to those of problems 12–30 and 12–31.

12–58. For the state vector of orbital angular momentum

$$|\psi(t=0)> = A\left(4|2,2> + |3,-2>\right),$$

(a) normalize the state vector.

(b) What are the possibilities for a measurement of $\mathcal{L}^2$?

(c) What are the probabilities for a measurement of $\mathcal{L}^2$?

(d) What are the possibilities for a measurement of $\mathcal{L}_z$?

(e) What are the probabilities for a measurement of $\mathcal{L}_z$?

(f) What is the expectation value of $\mathcal{L}^2$?

(g) What is the expectation value of $\mathcal{L}_z$?

(h) What is the uncertainty of $\mathcal{L}^2$?

(i) What is the uncertainty of $\mathcal{L}_z$?

(j) What is $\mathcal{L}_+|\psi(t=0)>$?

(k) What is $\mathcal{L}_-|\psi(t=0)>$?

(l) What is the time dependent state vector given that a Hamiltonian operator is not specified?

The sequence from problem 12–27 to 12–32 may be helpful. Part (l) intends that you write the state vector in terms of generic E_i, as was done in problem 12–32.

12–59. Consider the state vector of orbital angular momentum

$$|\,\psi(t=0)> \;=\; A\left(\,3\,|\,2,2> \;+\; 2\,|\,3,-2> \;+\; 5\,|\,0,0>\right).$$

(a) Normalize the state vector.

(b) What are the possibilities for a measurement of $\mathcal{L}^2$?

(c) What are the probabilities for a measurement of $\mathcal{L}^2$?

(d) What are the possibilities for a measurement of $\mathcal{L}_z$?

(e) What are the probabilities for a measurement of $\mathcal{L}_z$?

(f) What is the expectation value of $\mathcal{L}^2$?

(g) What is the expectation value of $\mathcal{L}_z$?

(h) What is the uncertainty of $\mathcal{L}^2$?

(i) What is the uncertainty of $\mathcal{L}_z$?

(j) What is $\mathcal{L}_+\,|\,\psi(t=0)>$?

(k) What is $\mathcal{L}_-\,|\,\psi(t=0)>$?

(l) What is the time dependent state vector given that a Hamiltonian operator is not specified?

Again, see the sequence from problems 12–27 to 12–32, and part (l) intends that you write the state vector in terms of generic E_i , as was done in problem 12–32 and exercise 12–58.

12–60. (a) Find $\mathcal{D}^2$ given $\quad \mathcal{D} \;=\; x\,\dfrac{\partial}{\partial y} \;+\; \dfrac{\partial}{\partial x}\,.$

(b) Find $\mathcal{K}^2$ given $\quad \mathcal{K} \;=\; x\,\dfrac{\partial}{\partial y} \;+\; y\,\dfrac{\partial}{\partial x}\,.$

(c) Find $\quad \mathcal{L}^2 \;=\; \mathcal{L}_x^2 \;+\; \mathcal{L}_y^2 \;+\; \mathcal{L}_z^2 \quad$ in spherical coordinates.

This exercise highlights the necessary use of the chain rule for differential operators, exposes some common notation, and is a practical conclusion to the position space representations in spherical coordinates for angular momentum operators.

Remember that an operator acts on a function, so for $f \;=\; f\,(x,\,y)\,,$

$$\mathcal{D}^2 \;=\; \left(x\,\frac{\partial}{\partial y} + \frac{\partial}{\partial x}\right)\left(x\,\frac{\partial}{\partial y} + \frac{\partial}{\partial x}\right) f \;=\; x\,\frac{\partial}{\partial y}\,x\,\frac{\partial f}{\partial y} \;+\; x\,\frac{\partial}{\partial y}\,\frac{\partial f}{\partial x} \;+\; \frac{\partial}{\partial x}\,x\,\frac{\partial f}{\partial y} \;+\; \frac{\partial}{\partial x}\,\frac{\partial f}{\partial x}$$

$$=\; x^2\,\frac{\partial^2 f}{\partial y^2} \;+\; x\,\frac{\partial^2 f}{\partial y \partial x} \;+\; \frac{\partial f}{\partial y} \;+\; x\,\frac{\partial^2 f}{\partial x \partial y} \;+\; \frac{\partial^2 f}{\partial x^2}$$

where the chain rule is required to evaluate $\quad \dfrac{\partial}{\partial x}\,x\,\dfrac{\partial f}{\partial y} \;=\; \dfrac{\partial f}{\partial y} \;+\; x\,\dfrac{\partial^2 f}{\partial x \partial y}\,.$ Assuming that the cross derivatives are interchangeable,

$$\mathcal{D}^2 \;=\; x^2\,\frac{\partial^2 f}{\partial y^2} \;+\; 2x\,\frac{\partial^2 f}{\partial x \partial y} \;+\; \frac{\partial f}{\partial y} \;+\; \frac{\partial^2 f}{\partial x^2}\,.$$

The function is normally only implied both in the reduction and the conclusion, so

$$\mathcal{D}^2 \;=\; x^2\,\frac{\partial^2}{\partial y^2} \;+\; 2x\,\frac{\partial^2}{\partial x \partial y} \;+\; \frac{\partial^2}{\partial x^2} \;+\; \frac{\partial}{\partial y}$$

is how this operator would normally be written. Part (b) will have six terms which become five under the assumption that the cross derivatives are interchangeable. The real operator of interest, $\mathcal{L}^2$, will have 15 terms initially that reduce to equation (20) on page 356 given that cross derivatives are interchangeable.

12–61. Find the spherical harmonic $Y_{4,2}$.

This exercise intends that you use the generating functions of problem 12–36. Start by finding the fourth Legendre polynomial $P_l(u) \;=\; \frac{(-1)^l}{2^l l!}\frac{d^l}{du^l}(1-u^2)^l$. Use this to find the second associated Legendre polynomial

$$P_{l,m}(u) \;=\; (-1)^m\sqrt{(1-u^2)^m}\,\frac{d^m}{du^m}P_l(u)\,,$$

from which $Y_{4,2}$ can be calculated using

$$Y_{l,m}(\theta,\phi) \;=\; (-1)^m\sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}P_{l,m}(\cos\theta)\,e^{im\phi}, \qquad m \;\geq\; 0\,.$$

You should find $\frac{3}{8}\sqrt{\frac{5}{2\pi}}\;\sin^2(\theta)\left(7\cos^2(\theta)-1\right)\,e^{2i\phi}$. These calculations have some value in assimilating the meanings and uses of these and other generating functions. The actual impact of this and the next exercise may be to convince you to see *Table of Spherical Harmonics* in Wikipedia or another source for higher $Y_{l,\,m}(\theta\,,\;\phi)$.

12–62. Find the spherical harmonic $Y_{5,-3}$.

See problem 12–36 and exercise 12–61 for guidance. The numerics for exercise 12–61 are somewhat involved and are more challenging for this exercise. It may be more valuable to find the answer online to become familiar with that resource rather than wading through the actual numerics. You must be careful with phase conventions when using online resources. The *Table of Spherical Harmonics* in Wikipedia has the same phase convention as adopted for this text. In fact, should you have the fortitude to suffer through the numerics, confirm your answer using this online resource.

12–63. Express the state vector of exercise 12–58 using spherical harmonics.

Use table 12–1. Interpret the eigenstates of angular momentum in Hilbert space into a position space representation. $\psi \;=\; \frac{1}{\sqrt{17}}\big(\,4\,|\,2\,,\;2> \;+\; |\,3\,,-2>\big)$ is the appropriate state vector.

12–64. Express the state vector of exercise 12–59 using spherical harmonics.

Similar to exercise 12–63 except slightly bigger, brighter, and shinier since the state vector is a linear combination of three eigenstates. Use $\psi = \frac{1}{\sqrt{38}}\big(3\,|\,2,\,2> + 2\,|\,3,-2> + 5\,|\,0,\,0>\big)$.

12–65. Derive the $\mathcal{L}_x$ matrix operator for $l = 1$.

Follow the processes of problems 12–42 and 12–43. The orthonormality of eigenstates is essential to the treatment of $<i\,|\,\mathcal{A}\,|\,j>$ as the element a_{ij} of the matrix form of the operator $\mathcal{A}$.

12–66. Find the matrix form of the $\mathcal{L}_-$ operator for $l = 1$.

A different method of obtaining a matrix form of an operator. See problem 12–44.

12–67. Verify that for

$$\mathcal{L}_x \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}\hbar\,, \qquad \mathcal{L}_y \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}\hbar\,, \qquad \mathcal{L}_z \rightarrow \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\hbar\,,$$

the eigenvectors for each eigenvalue are

$$\mathcal{L}_x: \quad |-\hbar> = \frac{1}{2}\begin{pmatrix}-1\\\sqrt{2}\\-1\end{pmatrix}, \qquad |\,0> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}, \qquad |\,\hbar> = \frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix},$$

$$\mathcal{L}_y: \quad |-\hbar> = \frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\,i\\-1\end{pmatrix}, \qquad |\,0> = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\1\end{pmatrix}, \qquad |\,\hbar> = \frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\,i\\-1\end{pmatrix},$$

$$\mathcal{L}_z: \quad |-\hbar> = \begin{pmatrix}0\\0\\1\end{pmatrix}, \qquad |\,0> = \begin{pmatrix}0\\1\\0\end{pmatrix}, \qquad |\,\hbar> = \begin{pmatrix}1\\0\\0\end{pmatrix}.$$

Intended is that you show $\mathcal{A}\,|\,v> = \alpha_i\,|\,v>$ for appropriate operators and vectors. The longer alternative is to solve the eigenvalue/eigenvector problem for all three operators. Realize that for the eigenvalue 0 you have significant latitude in choosing eigenvector components.

12–68. (a) Find the probabilities of obtaining $-\hbar\,,\ 0\,,$ or $\hbar$ from a measurement each of the component angular momentum operators given that the state vector is $|\,\psi> \;=\; \dfrac{1}{\sqrt{14}}\begin{pmatrix}3\\1\\2i\end{pmatrix}$.

(b) Find $<\mathcal{L}_x>\,,\ <\mathcal{L}_y>\,,$ and $<\mathcal{L}_z>$ using $<\mathcal{L}_j> \;=\; \sum P\,(\alpha_i)\,\alpha_i\,.$

The state vector is the same as used in problems 12–46 through 12–49. This is a confirmation of problem 12–46 as well as a reminder that a check for a calculation of $<\mathcal{L}_j>$ is available.

12–69. Show that $\quad \triangle\,\mathcal{L}_i\,\triangle\,\mathcal{L}_j \;\geq\; \dfrac{\hbar}{2}\,\Big|\,<\mathcal{L}_k>\,\Big|\quad$ for the state vector $\begin{pmatrix}2\\1\\2i\end{pmatrix}$.

This exercise is the general uncertainty relation applied to the three component $l = 1$ angular momentum operators. First, (a) normalize the state vector. Then (b) find $<\mathcal{L}_j>$. We get

$$<\mathcal{L}_x> \;=\; <\mathcal{L}_y> \;=\; \frac{2\sqrt{2}}{9}\,\hbar\,, \qquad \text{and} \qquad <\mathcal{L}_z> \;=\; 0\,.$$

(c) Then find

$$<\mathcal{L}_x^2> \;=\; <\mathcal{L}_y^2> \;=\; \frac{5}{9}\,\hbar^2\,, \qquad \text{and} \qquad <\mathcal{L}_z^2> \;=\; \frac{8}{9}\,\hbar^2\,,$$

and (d) obtain uncertainties using $\triangle\,\mathcal{L}_i \;=\; \left[\,<\mathcal{L}_i^2> \;-\; <\mathcal{L}_i>^2\,\right]^{1/2}$. Finally, (e) obtain the required products. Problems 12–46 through 12–49 should be good guides.

12–70. Find

$$<\mathcal{L}^2> \;=\; <\mathcal{L}_x^2> \;+\; <\mathcal{L}_y^2> \;+\; <\mathcal{L}_z^2>$$

using your numerical results from exercise 12–69.

Per the postscript to problem 12–47, you must get $2\hbar^2$.

Chapter 13

The Hydrogen Atom

All atoms are "boxes." The hydrogen atom with but one electron is a "particle in a box." The "box" is spherical. It has electrostatic walls. Electrostatic walls are "soft walls" rather than the "hard walls" examined earlier in our study of the infinite square well. The electron in a hydrogen atom is electrostatically bound to the nucleus composed of one proton. The electron can escape should it obtain enough energy from the process of absorbing a photon, but other than that, it is trapped in its spherical, electrostatic "box." Maybe a better description would be a "particle in a ball with indistinct, fuzzy walls." The electron in a hydrogen atom is a particle in a box with spherical, soft walls.

The hydrogen atom is one of the few realistic systems which can be solved analytically. The solution to the radial equation for a central potential is the only feature actually added in this chapter. This will not, however, be a short chapter because there is no easy solution to the radial equation for a central potential. One popular approach uses a power series solution. Our approach is to cast a portion of the radial equation into a form that can be recognized as the **associated Laguerre equation** which has a family of solutions known as **associated Laguerre polynomials** that are a major component to the solutions of the radial equation. The solutions to the radial equation will be combined with the spherical harmonics of the last chapter to obtain solutions in three dimensions for a central potential, which are the solutions to the hydrogen atom.

13–1. What is the Schrodinger equation in spherical coordinates?

The Schrodinger postulate and spherical symmetry dictate this step.

The time independent Schrodinger equation is

$$\mathcal{H}\,|\,E_i> \;=\; E_i\,|\,E_i>, \tag{1}$$

where E_i are eigenvalues and $|\,E_i>$ are energy eigenstates. We earlier developed a one dimensional position space representation of the time independent Schrodinger equation, using notation where $E_i \;\rightarrow\; E$, and $|\,E_i> \rightarrow\; \psi$. In three dimensions the Schrodinger equation generalizes to

$$\left(-\frac{\hbar^2}{2m}\nabla^2 \;+\; V\right)\psi \;=\; E\psi\,,$$

where ∇^2 is the Laplacian operator. Using the Laplacian in spherical coordinates, this is

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \;+\; \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) \;+\; \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi \;+\; V(r)\psi \;=\; E\psi\,. \tag{2}$$

Postscript: In spherical coordinates, $\psi \;=\; \psi\,(r,\theta,\phi)$, and we shall seek a variables separable solution where $\psi(r,\theta,\phi) \;=\; R\,(r)\,Y(\theta,\phi)$. We will find solutions where $Y(\theta,\phi)$ are the spherical harmonic functions and $R(r)$ is expressible in terms of **associated Laguerre functions**.

13–2. Show that the Laplacian can be expressed

$$\nabla^2 \;=\; \frac{\partial^2}{\partial r^2} \;+\; \frac{2}{r}\frac{\partial}{\partial r} \;+\; \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} \;+\; \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} \;+\; \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right). \tag{3}$$

in spherical coordinates.

It is imperative to find a complete set of commuting observables. The previous chapter on orbital angular momentum and the postscript to problem 13–1 suggest $\mathcal{L}^2$ and $\mathcal{L}_z$ will suffice for the angular portion. Our intent is to show that the Hamiltonian commutes with both of these operators, so that $\mathcal{H}$, $\mathcal{L}^2$ and $\mathcal{L}_z$ form a complete set of commuting observables for the hydrogen atom. This problem is an intermediate step in that process that makes calculation toward this end both more convenient and more accessible.

Starting with the Laplacian included in equation (2),

$$\begin{aligned}
\nabla^2 \;&=\; \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \;+\; \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) \;+\; \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\
&=\; \frac{1}{r^2}\left(2r\frac{\partial}{\partial r} \;+\; r^2\frac{\partial^2}{\partial r^2}\right) \;+\; \frac{1}{r^2\sin\theta}\left(\cos\theta\frac{\partial}{\partial\theta} \;+\; \sin\theta\frac{\partial^2}{\partial\theta^2}\right) \;+\; \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\
&=\; \frac{\partial^2}{\partial r^2} \;+\; \frac{2}{r}\frac{\partial}{\partial r} \;+\; \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} \;+\; \frac{1}{r^2\tan\theta}\frac{\partial}{\partial\theta} \;+\; \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \\
&=\; \frac{\partial^2}{\partial r^2} \;+\; \frac{2}{r}\frac{\partial}{\partial r} \;+\; \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} \;+\; \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} \;+\; \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right),
\end{aligned}$$

which is the form of equation (3).

13–3. Express the Schrodinger equation in terms of $\mathcal{L}^2$.

This is another step in finding a complete set of commuting observables. The position space representation of $\mathcal{L}^2$ in spherical coordinates is given as equation (20) on page 356.

The terms in parenthesis are $-\mathcal{L}^2/\hbar^2$, so the Laplacian can be written

$$\nabla^2 \;=\; \frac{\partial^2}{\partial r^2} \;+\; \frac{2}{r}\frac{\partial}{\partial r} \;-\; \frac{\mathcal{L}^2}{r^2\hbar^2},$$

when spherical symmetry is intrinsic. The Schrodinger equation becomes

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} \;+\; \frac{2}{r}\frac{\partial}{\partial r} \;-\; \frac{\mathcal{L}^2}{r^2\hbar^2}\right) \;+\; V(r)\right]\psi \;=\; E\psi. \tag{4}$$

13–4. Show $\left[\mathcal{H},\, \mathcal{L}^2\right] \,=\, 0\,.$

This is a necessary step to establish a complete set of commuting observables. Though not yet explicitly introduced, the Coulomb potential is

$$V\,(r) \;=\; -\frac{Z\,e^2}{r} \quad \text{in general} \qquad \Rightarrow \qquad V\,(r) \;=\; -\frac{e^2}{r}$$

for the hydrogen atom. Notice the potential has no angular dependence, and is a function solely of the radial component.

$$\left[\mathcal{H},\, \mathcal{L}^2\right] \;=\; \mathcal{H}\,\mathcal{L}^2 \;-\; \mathcal{L}^2\,\mathcal{H}$$

$$= \;\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} \,+\, \frac{2}{r}\frac{\partial}{\partial r} \,-\, \frac{\mathcal{L}^2}{r^2\hbar^2}\right) \,+\, V(r)\right]\mathcal{L}^2 \;-\; \mathcal{L}^2\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} \,+\, \frac{2}{r}\frac{\partial}{\partial r} \,-\, \frac{\mathcal{L}^2}{r^2\hbar^2}\right) \,+\, V(r)\right]$$

$$= \;-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\mathcal{L}^2 \;-\; \frac{\hbar^2}{2m}\frac{2}{r}\frac{\partial}{\partial r}\mathcal{L}^2 \;+\; \frac{\hbar^2}{2m}\frac{\mathcal{L}^4}{r^2\hbar^2} \;+\; V(r)\,\mathcal{L}^2$$

$$+\; \frac{\hbar^2}{2m}\mathcal{L}^2\frac{\partial^2}{\partial r^2} \;+\; \frac{\hbar^2}{2m}\mathcal{L}^2\frac{2}{r}\frac{\partial}{\partial r} \;-\; \frac{\hbar^2}{2m}\frac{\mathcal{L}^4}{r^2\hbar^2} \;-\; \mathcal{L}^2\,V(r)$$

$$= \;-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\mathcal{L}^2 \;-\; \frac{\hbar^2}{2m}\frac{2}{r}\frac{\partial}{\partial r}\mathcal{L}^2 \;+\; V(r)\,\mathcal{L}^2 \;+\; \frac{\hbar^2}{2m}\mathcal{L}^2\frac{\partial^2}{\partial r^2} \;+\; \frac{\hbar^2}{2m}\mathcal{L}^2\frac{2}{r}\frac{\partial}{\partial r} \;-\; \mathcal{L}^2\,V(r)$$

where the third and seventh terms in $\mathcal{L}^4$ sum to zero. The spherical coordinate representation of $\mathcal{L}^2$ is

$$\mathcal{L}^2 \;=\; -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} \,+\, \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} \,+\, \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

and has angular dependence only. The partial derivatives with respect to the radial variable do not affect terms without radial dependence. Partial derivatives with respect to angular variables do not affect the potential which is a function only of the radial variable. Therefore, the order of the operator products is interchangeable, and

$$\left[\mathcal{H},\, \mathcal{L}^2\right] \;=\; -\,\frac{\hbar^2}{2m}\mathcal{L}^2\frac{\partial^2}{\partial r^2} \;-\; \frac{\hbar^2}{2m}\mathcal{L}^2\frac{2}{r}\frac{\partial}{\partial r} \;+\; \mathcal{L}^2\,V(r)$$

$$+\,\frac{\hbar^2}{2m}\mathcal{L}^2\frac{\partial^2}{\partial r^2} \;+\; \frac{\hbar^2}{2m}\mathcal{L}^2\frac{2}{r}\frac{\partial}{\partial r} \;-\; \mathcal{L}^2\,V(r) \;=\; 0\,.$$

Postscript: Instead of the verbal argument, we could substitute the angular representation of $\mathcal{L}^2$, form the 18 resultant terms, explicitly interchange nine of them, and get the same result.

13–5. Show $\left[\mathcal{H},\, \mathcal{L}_z\right] \,=\, 0\,.$

This is the last step in obtaining a complete set of commuting observables for the hydrogen atom.

$$\left[\mathcal{H},\, \mathcal{L}_z\right] \,=\, \mathcal{H}\,\mathcal{L}_z \,-\, \mathcal{L}_z\,\mathcal{H}$$

$$= \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\mathcal{L}^2}{r^2\hbar^2}\right) + V\,(r)\right]\mathcal{L}_z \,-\, \mathcal{L}_z\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{\mathcal{L}^2}{r^2\hbar^2}\right) + V\,(r)\right]$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\mathcal{L}_z \,-\, \frac{\hbar^2}{2m}\frac{2}{r}\frac{\partial}{\partial r}\mathcal{L}_z \,+\, \frac{\hbar^2}{2m}\frac{\mathcal{L}^2\,\mathcal{L}_z}{r^2\hbar^2} \,+\, V\,(r)\,\mathcal{L}_z$$

$$+\, \frac{\hbar^2}{2m}\mathcal{L}_z\frac{\partial^2}{\partial r^2} \,+\, \frac{\hbar^2}{2m}\mathcal{L}_z\frac{2}{r}\frac{\partial}{\partial r} \,-\, \frac{\hbar^2}{2m}\frac{\mathcal{L}_z\,\mathcal{L}^2}{r^2\hbar^2} \,-\, \mathcal{L}_z\,V\,(r)$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\mathcal{L}_z \,-\, \frac{\hbar^2}{2m}\frac{2}{r}\frac{\partial}{\partial r}\mathcal{L}_z \,+\, V\,(r)\,\mathcal{L}_z \,+\, \frac{\hbar^2}{2m}\mathcal{L}_z\frac{\partial^2}{\partial r^2} \,+\, \frac{\hbar^2}{2m}\mathcal{L}_z\frac{2}{r}\frac{\partial}{\partial r} \,-\, \mathcal{L}_z\,V\,(r)$$

where the third and seventh terms in $\mathcal{L}^2\,\mathcal{L}_z$ sum to zero, since we already know that those two operators commute. The spherical coordinate representation of $\mathcal{L}_z$ is

$$\mathcal{L}_z \,=\, -i\hbar\frac{\partial}{\partial\phi}$$

and has angular dependence only. Again there are no partial derivatives which affect any term of the other operator, or the potential $V\,(r)$, in any of the operator products. Therefore, the order of the operator products is interchangeable, and

$$\left[\mathcal{H},\, \mathcal{L}_z\right] \,=\, -\,\frac{\hbar^2}{2m}\mathcal{L}_z\frac{\partial^2}{\partial r^2} \,-\, \frac{\hbar^2}{2m}\mathcal{L}_z\frac{2}{r}\frac{\partial}{\partial r} \,+\, \mathcal{L}_z\,V\,(r)$$

$$+\, \frac{\hbar^2}{2m}\mathcal{L}_z\frac{\partial^2}{\partial r^2} \,+\, \frac{\hbar^2}{2m}\mathcal{L}_z\frac{2}{r}\frac{\partial}{\partial r} \,-\, \mathcal{L}_z\,V\,(r) \,=\, 0\,.$$

13–6. Merge the results of the first five problems with those from chapter 12.

We have simply complicated the system of orbital angular momentum by adding a radial component. Without the radial variable, we have a complete set of commuting observables for the angular momentum operators in $\mathcal{L}^2$ and $\mathcal{L}_z$. Including the radial variable, we need a minimum of one more operator, if that operator commutes with both $\mathcal{L}^2$ and $\mathcal{L}_z$. The total energy operator, the Hamiltonian, satisfies the requirements, since

$$\left[\mathcal{H},\, \mathcal{L}^2\right] \,=\, 0\,, \qquad \text{and} \qquad \left[\mathcal{H},\, \mathcal{L}_z\right] \,=\, 0\,,$$

so the Hamiltonian is a suitable choice. A complete set of commuting observables is $\mathcal{H}$, $\mathcal{L}^2$, and $\mathcal{L}_z$, which is the conventional choice for the hydrogen atom. We have all the eigenvalue/eigenvector equations, because the time independent Schrodinger equation is eigenvalue/eigenvector equation (1) for the Hamiltonian operator, thus the eigenvalue/eigenvector equations are

$$\begin{aligned}
\mathcal{H}\,|\,\psi> &= E_n\,|\,\psi>, \\
\mathcal{L}^2\,|\,\psi> &= l(l+1)\hbar^2\,|\,\psi>, \\
\mathcal{L}_z\,|\,\psi> &= m\hbar\,|\,\psi>,
\end{aligned}$$

where we subscripted the energy eigenvalue with an n because that is the symbol conventionally used for the energy quantum number (per the infinite square well and the SHO). Then the solution to the problem is the eigenstate which satisfies all three, denoted $|\,n,l,m>$ in abstract Hilbert space. The representation in position space in spherical coordinates is

$$<r,\theta,\phi\,|\,n,l,m> \;\rightarrow\; \psi_{nlm}(r,\theta,\phi)\,.$$

13–7. Separate the radial and angular dependence of equation (2)

In this and the following three problems, we illustrate how the angular momentum and magnetic moment quantum numbers enter the symbology from a calculus based argument. Equation (2) is a representation in position space, so is no longer in abstract Hilbert space. One of the consequences of the process of representation is the arguments of linear algebra are obscured. They are still there, simply obscured because the special functions we use are orthogonal, so can be made orthonormal; and complete, meaning the space is spanned. The primary reason to proceed in terms of a position space representation is to obtain a position space description.

As noted, we assume a variables separable solution to equation (2) of the form

$$\psi\,(r,\theta,\phi) \;=\; R\,(r)\;Y(\theta,\phi)\,. \tag{5}$$

An often asked question is "How do you know you can assume that?" You do not know. You assume it, and if it works, you have found a solution. If it does not work, you need to attempt other methods or techniques. Here, it will work.

Using equation (5), equation (2) can be written

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R\,(r)\;Y\,(\theta,\phi) \;+\; \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)R\,(r)\;Y\,(\theta,\phi)$$

$$+\;\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\;R\,(r)\,Y\,(\theta,\phi) \;-\; \frac{2m}{\hbar^2}\Big[V(r)-E\Big]R\,(r)\,Y\,(\theta,\phi) \;=\; 0$$

$$\Rightarrow\quad Y\,(\theta,\phi)\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R\,(r) \;+\; R\,(r)\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y\,(\theta,\phi)$$

$$+\;R\,(r)\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\;Y\,(\theta,\phi) \;-\; \frac{2m}{\hbar^2}\Big[V(r)-E\Big]R\,(r)\;Y\,(\theta,\phi) \;=\; 0\,.$$

Dividing the equation by $R\,(r)\;Y\,(\theta,\phi)$, multiplying by r^2, and rearranging terms, this becomes

$$\left\{\frac{1}{R(r)}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R(r) \;-\; \frac{2mr^2}{\hbar^2}\Big[V(r)-E\Big]\right\}$$

$$+\left[\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) \;+\; \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,Y(\theta,\phi)\right] \;=\; 0\,.$$

The two terms in the curly braces depend only on r, and the two terms in the square brackets depend only upon angles. With the exception of a trivial solution, the only way the sum of the groups can be zero is if each group is equal to the same constant. The constant chosen is known as the **separation constant**. Normally, an arbitrary separation constant, like K, is selected and then you solve for K later. In this example, we are instead going to stand on the shoulders of some of the physicists and mathematicians of the previous 300 years, and make the enlightened choice of $l(l+1)$ as the separation constant. It should become clear l is the angular momentum quantum number introduced in the last chapter. Then

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) \;-\; \frac{2mr^2}{\hbar^2}\Big[V(r)-E\Big] \;=\; l(l+1) \tag{6}$$

which we call the **radial equation**, and

$$\frac{1}{Y(\theta,\phi)\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)Y(\theta,\phi) \;+\; \frac{1}{Y(\theta,\phi)\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,Y(\theta,\phi) \;=\; -l(l+1)\,, \tag{7}$$

which we call the **angular equation**. Notice the signs on the right side of equations (6) and (7) are opposite so they do, in fact, sum to zero.

13–8. Separate the angular equation into azimuthal and polar angle equations.

The solutions to equation (7), the $Y(\theta,\phi)$, are the spherical harmonic functions, and the l used in the separation constant is the same used as the index l in the spherical harmonics $Y_{l,m}(\theta,\phi)$. In fact, it is the angular momentum quantum number. But where is the index m? How is the magnetic moment quantum number introduced? To answer these questions, remember the spherical harmonics are also separable, *i.e.*, $Y_{l,m}(\theta,\phi) = f_{l,m}(\theta)\,g_m(\phi)$. We will use such a solution in the angular equation, without the indices until we see where they originate.

Using the solution $Y(\theta,\phi) = f(\theta)\,g(\phi)$ in equation (7),

$$\frac{1}{f(\theta)\,g(\phi)\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta)\,g(\phi) \;+\; \frac{1}{f(\theta)\,g(\phi)\,\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,f(\theta)\,g(\phi) \;=\; -l(l+1)$$

$$\Rightarrow\quad \frac{1}{f(\theta)\,\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta) \;+\; \frac{1}{g(\phi)\,\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\,g(\phi) \;=\; -l(l+1)\,.$$

Multiplying the equation by $\sin^2\theta$ and rearranging,

$$\frac{\sin\theta}{f(\theta)}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)f(\theta) \;+\; l(l+1)\,\sin^2\theta \;+\; \frac{1}{g(\phi)}\frac{\partial^2}{\partial\phi^2}\,g(\phi) \;=\; 0\,.$$

The first two terms depend only on θ, and the last term depends only on ϕ. Again, the only non–trivial solution such that the sum is zero is if the groups of terms each dependent on a single variable is equal to the same constant. Again using an enlightened choice, we pick m^2 as the separation constant, so

$$\frac{\sin\theta}{f\,(\theta)}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)f\,(\theta)\;+\;l(l+1)\,\sin^2\theta\;=\;m^2\,, \tag{8}$$

$$\frac{1}{g\,(\phi)}\frac{d^2}{d\phi^2}\;g\,(\phi)\;=\;-m^2\,, \tag{9}$$

and that is how the magnetic moment quantum number is introduced. Again, (8) and (9) need to sum to zero so the separation constant has opposite signs on the right side in the two equations.

13–9. Solve the azimuthal angle equation.

The solution to the azimuthal angle equation, equation (9), is

$$g\,(\phi)\;=\;e^{im\phi}\qquad\Rightarrow\qquad g_m(\phi)\;=\;e^{im\phi}\,, \tag{10}$$

where the subscript m is added to $g(\phi)$ because it is now clear there are as many solutions as there are allowed values of m.

Solving differential equations is an art. Likely one of the easier methods used is to "guess" the answer, then show it is a solution. The quality of the "guess" is likely proportional to the experience of the person doing the guessing. A person with experience may recognize the form of an equation that makes them try a solution of a particular form. The discussion of orbital angular momentum in the last chapter may help justify our current "guess."

To show $g_m(\phi)\;=\;e^{im\phi}$ is a solution to equation (9),

$$\frac{d^2}{d\phi^2}\,g_m(\phi)\;=\;\frac{d^2}{d\phi^2}\,e^{im\phi}\;=\;\frac{d}{d\phi}\,(im)\,e^{im\phi}\;=\;(im)^2\,e^{im\phi}\;=\;-m^2\,g_m(\phi)\,.$$

Using this in equation (9),

$$\frac{1}{g_m(\phi)}\frac{d^2}{d\phi^2}\,g_m(\phi)\;=\;-m^2\qquad\Rightarrow\qquad\frac{1}{g_m(\phi)}\Big(-m^2g_m(\phi)\Big)\;=\;-m^2\qquad\Rightarrow\qquad-m^2\;=\;-m^2\,,$$

therefore $g_m(\phi)\;=\;e^{im\phi}$ is a solution to equation (9).

13–10. Solve the polar angle equation.

This problem is a little more substantial than the last. Equation (8) can be written

$$\sin\theta\,\frac{d}{d\theta}\left(\sin\theta\,\frac{d}{d\theta}\right)f(\theta)\;+\;l(l+1)\,\sin^2\theta\,f(\theta)\;-\;m^2\,f(\theta)\;=\;0\,.$$

We can evaluate the derivative in the first term. We are then going to change variables to $x = \cos\theta$ for the purpose of obtaining an elementary form which will reduce to the **associated Legendre equation** introduced in the last chapter. The solutions to the associated Legendre equation are the **associated Legendre polynomials**, which are well known and are, in fact, solutions to our polar angle equation remembering $x = \cos\theta$ in our development.

Evaluating the first term,

$$\begin{aligned}\sin\theta\,\frac{d}{d\theta}\left(\sin\theta\,\frac{d}{d\theta}\right)f(\theta)\;&=\;\sin\theta\,\frac{d}{d\theta}\left(\sin\theta\,\frac{df(\theta)}{d\theta}\right)\\&=\;\sin\theta\,\left(\cos\theta\,\frac{df(\theta)}{d\theta}\;+\;\sin\theta\,\frac{d^2f(\theta)}{d\theta^2}\right)\\&=\;\sin^2\theta\,\frac{d^2f(\theta)}{d\theta^2}\;+\;\sin\theta\,\cos\theta\,\frac{df(\theta)}{d\theta}\,.\end{aligned}$$

Using this, equation (8) becomes

$$\sin^2\theta\,\frac{d^2f(\theta)}{d\theta^2}\;+\;\sin\theta\,\cos\theta\,\frac{df(\theta)}{d\theta}\;+\;l(l+1)\,\sin^2\theta\,f(\theta)\;-\;m^2\,f(\theta)\;=\;0\,.\qquad(11)$$

Changing variables to $x = \cos\theta$, we need the derivatives with respect to x instead of θ, so

$$\frac{df(\theta)}{d\theta}\;=\;\frac{df(x)}{dx}\frac{dx}{d\theta}\;=\;\frac{df(x)}{dx}\big(-\sin\theta\big)\;=\;-\sin\theta\,\frac{df(x)}{dx}\,,$$

is the first derivative, and the second derivative is

$$\begin{aligned}\frac{d^2f(\theta)}{d\theta^2}\;&=\;\frac{d}{d\theta}\left(-\sin\theta\,\frac{df(x)}{dx}\right)\;=\;-\cos\theta\,\frac{df(x)}{dx}\;-\;\sin\theta\,\frac{d}{d\theta}\,\frac{df(x)}{dx}\\&=\;-\cos\theta\,\frac{df(x)}{dx}\;-\;\sin\theta\,\frac{d}{dx}\,\frac{dx}{d\theta}\,\frac{df(x)}{dx}\\&=\;-\cos\theta\,\frac{df(x)}{dx}\;-\;\sin\theta\,\frac{d}{dx}\big(-\sin\theta\big)\,\frac{df(x)}{dx}\\&=\;-\cos\theta\,\frac{df(x)}{dx}\;+\;\sin^2\theta\,\frac{d^2f(x)}{dx^2}\,.\end{aligned}$$

Substituting just the derivatives in equation (11),

$$\begin{aligned}\sin^2\theta\left(\sin^2\theta\,\frac{d^2f(x)}{dx^2}\;-\;\cos\theta\,\frac{df(x)}{dx}\right)\;+\;\sin\theta\cos\theta\left(-\sin\theta\,\frac{df(x)}{dx}\right)&\\+\;l(l+1)\sin^2\theta f(x)\;-\;m^2\,f(x)\;=\;0\,,&\end{aligned}$$

which gives us an equation in both θ and x, which is not formally appropriate, however, it becomes difficult to keep track of the terms if all the substitutions and reductions are done at once so this intermediate step may be illustrative. Dividing by $\sin^2\theta$, we get

$$\sin^2\theta\,\frac{d^2f(x)}{dx^2} \;-\; \cos\theta\,\frac{df(x)}{dx} \;-\; \cos\theta\,\frac{df(x)}{dx} \;+\; l(l+1)\,f(x) \;-\; \frac{m^2}{\sin^2\theta}f(x) \;=\; 0\,.$$

The change of variables is complete upon summing the two first derivatives, using $\cos\theta = x$, and $\sin^2\theta = 1 - \cos^2\theta = 1 - x^2$, which is

$$\left(1-x^2\right)\frac{d^2f(x)}{dx^2} \;-\; 2x\,\frac{df(x)}{dx} \;+\; l(l+1)\,f(x) \;-\; \frac{m^2}{1-x^2}f(x) \;=\; 0\,.$$

This is the **associated Legendre equation**. It reduces to **Legendre equation** when $m = 0$. The function has a single argument so there is no confusion if the derivatives are indicated with primes, and the associated Legendre equation is often written

$$\left(1-x^2\right)f''(x) \;-\; 2x\,f'(x) \;+\; l(l+1)\,f(x) \;-\; \frac{m^2}{1-x^2}f(x) \;=\; 0\,,$$

and becomes the Legendre equation,

$$\left(1-x^2\right)f''(x) \;-\; 2x\,f'(x) \;+\; l(l+1)\,f(x) \;=\; 0\,,$$

when $m = 0$. The solutions to the associated Legendre equation are the associated Legendre polynomials discussed briefly in the last chapter. To review that in the current context, associated Legendre polynomials can be generated from Legendre polynomials using

$$P_{l,m}(x) \;=\; (-1)^m\sqrt{(1-x^2)^m}\,\frac{d^m}{dx^m}\;P_l(x)\,,$$

where the $P_l(x)$ are Legendre polynomials. Legendre polynomials can be generated using

$$P_l(x) \;=\; \frac{(-1)^l}{2^l l!}\,\frac{d^l}{dx^l}\,(1-x^2)^l\,.$$

The use of these generating functions was illustrated in the last chapter as intermediate results in calculating spherical harmonic functions.

The first few Legendre polynomials are listed in table 13–1. Our interest is to generate associated Legendre functions. Some associated Legendre polynomials are seen in table 13–2.

$P_0(x)$	$= 1$	$P_3(x)$	$= \frac{1}{2}\left(5x^3 - 3x\right)$
$P_1(x)$	$= x$	$P_4(x)$	$= \frac{1}{8}\left(35x^4 - 30x^2 + 3\right)$
$P_2(x)$	$= \frac{1}{2}\left(3x^2 - 1\right)$	$P_5(x)$	$= \frac{1}{8}\left(63x^5 - 70x^3 + 15x\right)$

Table 13 – 1. The First Six Legendre Polynomials.

$P_{0,0}(x)$	$= 1$	$P_{2,0}(x)$	$= \frac{1}{2}\big(3x^2 - 1\big)$
$P_{1,1}(x)$	$= -\sqrt{1 - x^2}$	$P_{3,3}(x)$	$= -15\big(\sqrt{1 - x^2}\big)^3$
$P_{1,0}(x)$	$= x$	$P_{3,2}(x)$	$= 15x\,\big(1 - x^2\big)$
$P_{2,2}(x)$	$= 3\big(1 - x^2\big)$	$P_{3,1}(x)$	$= -\frac{3}{2}\big(5x^2 - 1\big)\sqrt{1 - x^2}$
$P_{2,1}(x)$	$= -3x\,\sqrt{1 - x^2}$	$P_{3,0}(x)$	$= \frac{1}{2}\big(5x^3 - 3x\big)$

Table 13 – 2. The First Few Associated Legendre Polynomials.

Postscript: Notice $P_l = P_{l,0}$. The solutions to the Legendre equation and the associated Legendre equation must be the same when $m = 0$. Also, many authors will use a positive sign for all associated Legendre polynomials. This is a different choice of phase. We choose to include a factor of $(-1)^m$ with the associated Legendre polynomials, for the purpose that the sign of all spherical harmonics will be positive as a result.

The change of variables $x = \cos\theta$ was done to put the differential equation in a more elementary form. A dominant use of associated Legendre polynomials is in applications where the argument is $\cos\theta$. One example is the generating function for spherical harmonic functions,

$$Y_{l,m}(\theta,\phi) \;=\; (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}\; P_{l,m}(\cos\theta)\; e^{im\phi}\,, \qquad m \,\geq\, 0\,, \tag{12}$$

$$\text{and} \qquad Y_{l,-m}(\theta,\phi) \;=\; Y^*_{l,m}(\theta,\phi), \qquad m \,<\, 0\,,$$

where the $P_{l,m}(\cos\theta)$ are associated Legendre polynomials. Calculate a spherical harmonic with $m < 0$ by obtaining the spherical harmonic with $m = |\,m\,|$ and forming the adjoint.

To summarize, the angular equation is separated into an azimuthal and a polar portion. The solutions to the azimuthal angle equation are exponentials including the magnetic moment quantum number in the argument. The solutions to the polar angle equation are the associated Legendre polynomials including both orbital angular momentum and magnetic moment quantum number. Both quantum numbers are introduced into the respective differential equations as separation constants. The solutions to the original angular equation (7) are proportional to the products $P_{l,m}(\cos\theta)\,e^{im\phi}$. These products $P_{l,m}(\cos\theta)\,e^{im\phi} \,\propto\, Y_{l,m}(\theta,\phi)$ are the spherical harmonic functions; the alternating sign and radical serve only to make the orthogonal set orthonormal.

13–11. What are associated Laguerre polynomials and Laguerre functions?

There is no easy way to solve the radial equation. A power series solution is often used. (See Griffiths[1], or Cohen–Tannoudji[2]). Our approach will be to relate the radial equation to the associated Laguerre equation, for which the associated Laguerre polynomials are solutions.

[1] Griffiths, *Introduction to Quantum Mechanics* (Prentice Hall, Englewood Cliffs, New Jersey, 1995), pp. 134–141.

[2] Cohen–Tannoudji, Diu, and Laloe, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), pp. 794–797.

Laguerre polynomials are solutions to the Laguerre equation

$$x\,L_j^{''}(x) \;+\; \big(1-x\big)\,L_j^{'}(x) \;+\; j\;L_j(x) \;=\; 0\,.$$

The first few Laguerre polynomials are listed in table 13–3.

$$\begin{aligned}
L_0(x) &= 1\\
L_1(x) &= -x+1\\
L_2(x) &= x^2-4x+2\\
L_3(x) &= -x^3+9x^2-18x+6\\
L_4(x) &= x^4-16x^3+72x^2-96x+24\\
L_5(x) &= -x^5+25x^4-200x^3+600x^2-600x+120\\
L_6(x) &= x^6-36x^5+450x^4-2400x^3+5400x^2-4320x+720
\end{aligned}$$

Table 13 – 3. The First Seven Laguerre Polynomials.

Laguerre polynomials of any order can be calculated using the generating function

$$L_j(x) \;=\; e^x\,\frac{d^j}{dx^j}\;e^{-x}\,x^j\,.$$

The Laguerre polynomials do not form an orthogonal set. The related set of **Laguerre functions**,

$$\phi_j(x) \;=\; e^{-x/2}\;L_j(x) \tag{13}$$

is orthogonal on the interval $0 \le x < \infty$. Laguerre functions are not themselves solutions to the Laguerre equation.

Just as the Legendre equation becomes the associated Legendre equation by adding an appropriate term containing a second index, the associated Laguerre equation is

$$x\,L_j^{k\,''}(x) \;+\; \big(1-x+k\big)\,L_j^{k\,'}(x) \;+\; j\;L_j^k(x) \;=\; 0, \tag{14}$$

which reduces to the Laguerre equation when $k=0$. Some associated Laguerre polynomials are listed in table 13–4.

$$\begin{aligned}
L_0^0(x) &= L_0(x) & L_0^2(x) &= 2\\
L_1^0(x) &= L_1(x) & L_3^0(x) &= L_3(x)\\
L_1^1(x) &= -2x+4 & L_3^1(x) &= -4x^3+48x^2-144x+96\\
L_0^1(x) &= 1 & L_2^3(x) &= 60x^2-600x+1200\\
L_2^0(x) &= L_2(x) & L_3^3(x) &= -120x^3+2160x^2-10800x+14400\\
L_2^1(x) &= 3x^2-18x+18 & L_3^2(x) &= -20x^3+300x^2-1200x+1200\\
L_2^2(x) &= 12x^2-96x+144 & L_1^3(x) &= -24x+96\\
L_1^2(x) &= -6x+18 & L_0^3(x) &= 6
\end{aligned}$$

Table 13 – 4. The first few Associated Laguerre Polynomials.

Postscript: Notice $L_j^0 = L_j$. Either index may assume any non-negative integral value. We will be interested only in $L_j^k(x)$ where $k < j$ for hydrogen atom wave functions.

The $L_j^k(x)$ can be calculated from Laguerre polynomials using the generating function

$$L_j^k(x) \;=\; \big(-1\big)^k \frac{d^k}{dx^k}\; L_{j+k}(x)\,.$$

13–12. Calculate $L_3^1(x)$ starting with the generating function for $L_j(x) = e^x \dfrac{d^j}{dx^j}\; e^{-x}\, x^j$.

Given the intent to relate the radial equation to the associated Laguerre equation, this problem is a straight forward numerical calculation consistent with our approach.

We first need to calculate $L_4(x)$, because

$$L_j^k(x) \;=\; \big(-1\big)^k \frac{d^k}{dx^k}\, L_{j+k}(x) \qquad \Rightarrow \qquad L_3^1(x) \;=\; \big(-1\big)^1 \frac{d^1}{dx^1}\; L_{3+1}(x) \;=\; -\frac{d}{dx}\, L_4(x)\,.$$

Similarly, if you want to calculate L_3^2, you need to start with L_5, and to calculate L_4^3, you need to start with L_7. So using the generating function,

$$\begin{aligned}
L_4(x) \;&=\; e^x \frac{d^4}{dx^4}\, e^{-x} x^4 \\
&=\; e^x \frac{d^3}{dx^3}\Big(-e^{-x}x^4 + e^{-x}\,4x^3\Big) \\
&=\; e^x \frac{d^2}{dx^2}\Big(e^{-x}x^4 - e^{-x}\,4x^3 - e^{-x}\,4x^3 + e^{-x}\,12x^2\Big) \\
&\qquad\qquad =\; e^x \frac{d^2}{dx^2}\Big(e^{-x}x^4 - e^{-x}\,8x^3 + e^{-x}\,12x^2\Big) \\
&=\; e^x \frac{d}{dx}\Big(-e^{-x}x^4 + e^{-x}\,4x^3 + e^{-x}\,8x^3 - e^{-x}\,24x^2 - e^{-x}\,12x^2 + e^{-x}\,24x\Big) \\
&\qquad\qquad =\; e^x \frac{d}{dx}\Big(-e^{-x}x^4 + e^{-x}\,12x^3 - e^{-x}\,36x^2 + e^{-x}\,24x\Big) \\
&=\; e^x\Big(e^{-x}x^4 - e^{-x}\,4x^3 - e^{-x}\,12x^3 + e^{-x}\,36x^2 + e^{-x}\,36x^2 - e^{-x}\,72x - e^{-x}\,24x + e^{-x}\,24\Big) \\
&=\; e^x e^{-x}\Big(x^4 - 16x^3 + 72x^2 - 96x + 24\Big) \\
&=\; x^4 - 16x^3 + 72x^2 - 96x + 24\,,
\end{aligned}$$

per table 13–3. Then to get $L_3^1(x)$,

$$\begin{aligned}
L_3^1 \;&=\; -\frac{d}{dx}\, L_4(x) \\
&=\; -\frac{d}{dx}\big(x^4 - 16x^3 + 72x^2 - 96x + 24\big) \\
&=\; -\big(4x^3 - 48x^2 + 144x - 96\big) \\
&=\; -4x^3 + 48x^2 - 144x + 96\,,
\end{aligned}$$

per table 13–4.

Postscript: Associated Laguerre polynomials are not orthogonal. **Associated Laguerre functions**

$$\Phi_j^k(x) \;=\; e^{-x/2}x^{k/2}L_j^k(x)$$

are orthogonal on the interval $0 \le x < \infty$, so can be made an orthonormal set. Again, the $\Phi_j^k(x)$ are not themselves solutions to the associated Laguerre equation.

We are specifically interested in a slightly different associated Laguerre function than the usual first choice indicated above, *i.e.*, we are interested in

$$y_j^k(x) \;=\; e^{-x/2}x^{(k+1)/2}\; L_j^k(x). \tag{15}$$

These are also not solutions to the associated Laguerre equation, but they are solutions to

$$y_j^{k''}(x) \;+\; \left(-\frac{1}{4} \;+\; \frac{2j+k+1}{2x} \;-\; \frac{k^2-1}{4x^2}\right) y_j^k(x) \;=\; 0\,. \tag{16}$$

Equation (16) is a form of the radial equation with solutions given by equation (15), so the radial functions $R(r)$ we seek are $R_{n,l}(r) = A\,y_n^l(r)$, where A is a normalization constant.

13–13. Show equation (15) satisfies equation (16).

This is a critical connection. The result is a direct link to the solution of the radial equation. We are going to simplify the notation to minimize clutter, and will explain as we progress.

To obtain the second derivative, we need the first derivative, and use the notation

$$y \;=\; e^{-x/2}\,x^{(k+1)/2}\,v\,,$$

for equation (15) where $v = L_j^k(x)$, because the indices do not change and only serve to add clutter, and we can remember the independent variable is x. The first derivative is

$$\begin{aligned} y' \;&=\; -\frac{1}{2}\,e^{-x/2}\,x^{(k+1)/2}\,v \;+\; e^{-x/2}\left(\frac{k+1}{2}\right)x^{(k-1)/2}\,v \;+\; e^{-x/2}\,x^{(k+1)/2}\,v' \\ &=\; \left[-\frac{1}{2}\,v \;+\; \left(\frac{k+1}{2x}\right)v \;+\; v'\right]e^{-x/2}x^{(k+1)/2} \\ &\Rightarrow\quad \left(e^{x/2}\,x^{-(k+1)/2}\right)y' \;=\; -\frac{1}{2}\,v \;+\; \frac{k+1}{2x}\,v \;+\; v'\,. \end{aligned}$$

Notice we adjusted the second term on the right to do the factoring. Using the same adjustment technique, we will factor these terms out of the second derivative as we go. These are also factors common to equation (15). Since the right side of equation (16) is zero, after we substitute the second derivative and the function into (16), we will simplify the equation by dividing by common factors, therefore, none of the common factors will enter into the final solution. The exponentials and powers still need to be considered in differentiation, but their inverses will appear on the left and only the terms which have impact will appear on the right (see appendix D).

$$\begin{aligned} \left(e^{x/2}x^{-(k+1)/2}\right)y'' \;=\; &\frac{1}{4}v \;-\; \frac{1}{2}\frac{k+1}{2x}\,v \;-\; \frac{1}{2}v' \;-\; \frac{1}{2}\frac{k+1}{2x}\,v \\ &+\; \frac{k+1}{2x}\,\frac{k-1}{2x}\,v \;+\; \frac{k+1}{2x}\,v' \;-\; \frac{1}{2}\,v' \;+\; \frac{k+1}{2x}\,v' \;+\; v''\,. \end{aligned}$$

Substituting the second derivative and the function into equation (16),

$$y'' \;+\; \left(-\frac{1}{4} \;+\; \frac{2j+k+1}{2x} \;-\; \frac{k^2-1}{4x^2}\right) y \;=\; 0\,,$$

and dividing by the common factor of $e^{-x/2}x^{(k+1)/2}$, the remaining terms are

$$\left(\frac{1}{4}\,v \;-\; \frac{1}{2}\frac{k+1}{2x}\,v \;-\; \frac{1}{2}\,v' \;-\; \frac{1}{2}\frac{k+1}{2x}\,v \;+\; \frac{k+1}{2x}\,\frac{k-1}{2x}\,v \;+\; \frac{k+1}{2x}\,v' \;-\; \frac{1}{2}\,v' \;+\; \frac{k+1}{2x}\,v' \;+\; v''\right)$$

$$+\; \left(-\frac{1}{4} \;+\; \frac{2j+k+1}{2x} \;-\; \frac{k^2-1}{4x^2}\right) v \;=\; 0$$

$$\Rightarrow \quad v'' \;+\; \cancel{\frac{1}{4}}\,v \;-\; \frac{1}{2}\frac{k+1}{2x}\,v \;-\; \frac{1}{2}\,v' \;-\; \frac{1}{2}\,\frac{k+1}{2x}\,v \;+\; \cancel{\frac{k^2-1}{4x^2}}\,v \;+\; \frac{k+1}{2x}\,v' \;-\; \frac{1}{2}\,v' \;+\; \frac{k+1}{2x}\,v'$$

$$-\; \cancel{\frac{1}{4}}\,v \;+\; \frac{2j+k+1}{2x}\,v \;-\; \cancel{\frac{k^2-1}{4x^2}}\,v \;=\; 0$$

$$\Rightarrow \quad v'' \;-\; \cancel{\frac{k-1}{4x}}\,v \;-\; \frac{1}{2}\,v' \;-\; \cancel{\frac{k-1}{4x}}\,v \;+\; \frac{k+1}{x}\,v' \;-\; \frac{1}{2}\,v' \;+\; \frac{j}{x}\,v \;+\; \cancel{\frac{k-1}{2x}}\,v \;=\; 0$$

$$\Rightarrow \quad v'' \;-\; v' \;+\; \frac{k+1}{x}\,v' \;+\; \frac{j}{x}\,v \;=\; 0$$

$$\Rightarrow \quad x\,v'' \;-\; x\,v' \;+\; (k+1)\,v' \;+\; j\,v \;=\; 0$$

$$\Rightarrow \quad x\,v'' \;+\; (1-x+k)\,v' \;+\; j\,v \;=\; 0 \qquad (17)$$

which is the associated Laguerre equation. Since $v \;=\; L_j^k(x)$, equation (17) is

$$x\,L_j^{k''}(x) \;+\; \big(1-x+k\big)\,L_j^{k'}(x) \;+\; j\;L_j^k(x) \;=\; 0\,, \qquad \text{and}$$

$$y \;=\; e^{-x/2}\,x^{(k+1)/2}\,v$$

$$=\; e^{-x/2}\,x^{(k+1)/2}\,L_j^k(\,x\,) \qquad \text{are solutions to equation (16).}$$

Postscript: Equation (2) describes a single particle in a central potential. The hydrogen atom is not actually a central potential, rather it is a two body problem. Were we able to anchor the nucleus to a stationary location, equation (2) would be an accurate description. This is not possible, but we can reach a similar end by picturing the center of mass being anchored to a fixed location. If we use the **reduced mass** in place of the electron mass,

$$\mu \;=\; \frac{m_p\,m_e}{m_p+m_e}\,,$$

the radial coordinate r accurately describes the distance between the center of mass and the electron. The effect in equation (2) is largely cosmetic; where there was an m representing m_e, it is replaced by μ. Because the proton is about 1836 times more massive than the electron, the reduced mass is nearly identically the electron mass. Many authors simply retain the electron mass. The details of reducing a two particle problem to a one particle problem are covered in numerous texts, including Cohen–Tannoudji[3], Levine[4], and many classical mechanics texts.

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[3] Cohen–Tannoudji, Diu, and Laloe, *Quantum Mechanics* (John Wiley & Sons, New York, 1977), pp. 784–788.

[4] Levine, *Quantum Chemistry* (Allyn and Bacon, Inc., Boston, 1983), pp. 101–106.

13–14. Solve the radial equation.

The plan is to explicitly use the Coulomb potential in equation (6), then rearrange the radial equation into a form comparable to equation (16) for which we have the solutions, which are the family constructed using associated Laguerre polynomials denoted in equation (15). We will make three substitutions to obtain this end. There is a significant amount of algebra in this problem.

An advantage to proceeding in this manner is that we will be able to glean additional information by comparing different equations term by term. The energy levels of the hydrogen atom and the meaning of the indices of the associated Laguerre polynomials, which will be quantum numbers for the hydrogen atom, will come from the comparison of individual terms.

The radial equation (6) using the reduced mass and the Coulomb potential, is

$$\begin{aligned}
&\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) \;-\; \frac{2\mu r^2}{\hbar^2}\Big[-\frac{e^2}{r}-E\Big] \;-\; l(l+1) \;=\; 0 \\
\Rightarrow\qquad &\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) \;-\; \frac{2\mu r^2}{\hbar^2}\Big[-\frac{e^2}{r}-E\Big]R(r) \;-\; l(l+1)\,R(r) \;=\; 0 \\
\Rightarrow\qquad &\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) \;+\; \left[\frac{2\mu r^2}{\hbar^2}\frac{e^2}{r}+\frac{2\mu r^2}{\hbar^2}E-l(l+1)\right]R(r) \;=\; 0\,. \qquad (18)
\end{aligned}$$

We will make three substitutions to get equation (18) into the form of equation (16). The first is

$$y(r) \;=\; r\,R(r) \qquad\Rightarrow\qquad R(r) \;=\; \frac{y(r)}{r}\,. \qquad (19)$$

Making this substitution in the first term and evaluating the derivatives

$$\begin{aligned}
\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r) \;&=\; \frac{d}{dr}\left(r^2\frac{d}{dr}\right)\left(r^{-1}\right)y(r) \\
&=\; \frac{d}{dr}\,r^2\left[\left(-r^{-2}\right)y(r) \;+\; \left(r^{-1}\right)\frac{dy(r)}{dr}\right] \\
&=\; \frac{d}{dr}\left[-y(r) \;+\; r\,\frac{dy(r)}{dr}\right] \\
&=\; -\frac{dy(r)}{dr} \;+\; \frac{dy(r)}{dr} \;+\; r\,\frac{d^2y(r)}{dr^2} \\
&=\; r\,\frac{d^2y(r)}{dr^2}\,.
\end{aligned}$$

The substitution serves to consolidate the first derivatives. Equation (18) becomes

$$\begin{aligned}
&r\,\frac{d^2y(r)}{dr^2} \;+\; \left[\frac{2\mu re^2}{\hbar^2} \;+\; \frac{2\mu r^2}{\hbar^2}E \;-\; l(l+1)\right]\frac{y(r)}{r} \;=\; 0 \\
\Rightarrow\qquad &\frac{d^2y(r)}{dr^2} \;+\; \left[\frac{2\mu e^2}{r\,\hbar^2} \;+\; \frac{2\mu E}{\hbar^2} \;-\; \frac{l(l+1)}{r^2}\right]y(r) \;=\; 0\,.
\end{aligned}$$

The second substitution is essentially to simplify the notation, and is

$$\left(\frac{\epsilon}{2}\right)^2 \;=\; -\,\frac{2\mu E}{\hbar^2} \tag{20}$$

where the negative sign on the right indicates we are looking for bound states such that $E < 0$. Including the negative sign here lets us have an ϵ which is real. The radial equation becomes

$$\frac{d^2\,y\,(r)}{dr^2} \;+\; \left[\,\frac{2\mu e^2}{r\,\hbar^2} \;-\; \frac{\epsilon^2}{4} \;-\; \frac{l\,(l+1)}{r^2}\right] y\,(r) \;=\; 0\,.$$

The third substitution is a change of variables,

$$x \;=\; r\epsilon \qquad \Rightarrow \qquad r \;=\; \frac{x}{\epsilon}\,, \tag{21}$$

$$\Rightarrow \quad dr \;=\; \frac{dx}{\epsilon} \quad \Rightarrow \quad \frac{d^2\,y\,(r)}{dr^2} \;=\; \frac{d}{dr}\frac{d\,y\,(r)}{dr} \;=\; \epsilon\frac{d}{dx}\,\epsilon\frac{d\,y(x)}{dx} \;=\; \epsilon^2\frac{d^2\,y\,(x)}{dx^2}\,,$$

so our radial equation becomes

$$\epsilon^2\frac{d^2\,y\,(x)}{dx^2} \;+\; \left[\,\frac{2\mu e^2\epsilon}{x\,\hbar^2} \;-\; \frac{\epsilon^2}{4} \;-\; \epsilon^2\frac{l\,(l+1)}{x^2}\right] y\,(x) \;=\; 0$$

$$\Rightarrow \qquad \frac{d^2\,y\,(x)}{dx^2} \;+\; \left[-\frac{1}{4} \;+\; \frac{2\mu e^2}{\hbar^2\epsilon x} \;-\; \frac{l\,(l+1)}{x^2}\right] y\,(x) \;=\; 0\,, \tag{22}$$

and equation (22) is equation (16) where

$$l\,(l+1) \;=\; \frac{k^2-1}{4}, \tag{23}$$

and

$$\frac{2\mu e^2}{\hbar^2\epsilon} \;=\; \frac{2j+k+1}{2}\,, \tag{24}$$

As demonstrated earlier, the solutions are equation (15),

$$y_j^k(x) \;=\; e^{-x/2}\,x^{(k+1)/2}\,L_j^k(x)\,.$$

Postscript: Evaluation of these results is completed in problem 13–16.

13–15. Show $a_0 = 0.529\,\text{Å}$, using both the electron mass and the reduced mass.

We are going to take what appears to be a slight diversion to evaluate the particular set of factors in equation (24), $\hbar^2/\mu e^2$, which recurs repeatedly. Going back to the old quantum theory, this is called the Bohr radius, that is

$$a_0 \;=\; \frac{\hbar^2}{\mu e^2} \;=\; 0.529\,\text{Å}\,. \tag{25}$$

This example is intended to illustrate three things. First, $a_0 = 0.529\,\text{Å}$, second is to work out the CGS units for e^2, and then to show the electron mass is a good approximation to the reduced mass in hydrogen. The Bohr radius is a natural length for the hydrogen atom.

The electrostatic force in MKS and CGS systems is defined

$$\frac{1}{4\pi\epsilon_0}\frac{e^2_{\text{MKS}}}{r^2} \;=\; F \;=\; \frac{e^2_{\text{CGS}}}{r^2}$$

$$\begin{aligned}
\Rightarrow \quad e^2_{\text{CGS}} \;&=\; \frac{e^2_{\text{MKS}}}{4\pi\epsilon_0} \;=\; \left(1.602\times10^{-19}\,C\right)^2\left(8.988\times10^{9}\,N\cdot m^2/C^2\right)\\
&=\; 2.307\times10^{-28}\,N\cdot m^2 \;=\; 2.307\times10^{-19}\,dyne\cdot cm^2\\
&=\; 2.307\times10^{-19}\,erg\cdot cm \;=\; 14.42\;eV\cdot\text{Å}\,.
\end{aligned}$$

So

$$a_0 \;=\; \frac{\hbar^2}{m_e e^2} \;=\; \frac{1}{4\pi^2}\frac{(hc)^2}{m_e c^2 e^2} \;=\; \frac{1}{4\pi^2}\frac{(1.240\times10^4\,eV\cdot\text{Å})^2}{(0.5110\times10^6\,eV)(14.42\,eV\cdot\text{Å})} \;=\; 0.5286\,\text{Å}\,.$$

The reduced mass is

$$\mu \;=\; \frac{m_p\,m_e}{m_p+m_e} \;=\; \frac{1.673\times10^{-24}}{1.673\times10^{-24}+9.110\times10^{-28}}m_e \;=\; 0.9995\,m_e\,,$$

$$\Rightarrow \quad \frac{\hbar^2}{\mu e^2} \;=\; \frac{\hbar^2}{0.9995 m_e e^2} \;=\; \frac{0.5286\,\text{Å}}{0.9995} \;=\; 0.5288\,\text{Å}\,.$$

Postscript: There is 0.03% difference between the electron mass and reduced mass values. Many authors simply use the electron mass and it yields a good approximation. The CGS value of e^2 can be mysterious for those who have worked primarily in MKS units. By the way, the square root $e = 3.797\,(eV\cdot\text{Å})^{1/2}$ can be a convenient way to express the charge on the electron in CGS units.

13–16. Find the eigenenergies of hydrogen from the solution of the radial equation.

Eigenenergies of hydrogen follow directly from equation (24). This problem also shows how the principal quantum number for the hydrogen atom emerges from the mathematics.

Starting with equation (23)

$$\frac{k^2-1}{4} \;=\; l(l+1)$$

$$\begin{aligned} \Rightarrow \quad k^2 &= 4l(l+1) + 1 \\ &= 4l^2 + 4l + 1 \\ &= \left(2l+1\right)^2 \\ \Rightarrow \quad k &= 2l + 1\,. \end{aligned}$$

Equation (24) gives us the eigenenergies of the hydrogen atom, but requires some development. Since $k = 2l + 1$,

$$\frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = j + l + 1\,.$$

From the discussion on associated Laguerre polynomials, the indices j and k are non–negative integers. The sum $j + l + 1$ can, therefore, assume any integer values of 1 or greater. We are going to rename it n, or

$$n = j + l + 1\,. \tag{26}$$

The new integer index n is known as the **principal quantum number**. Equation (24) is

$$\frac{2\mu e^2}{\hbar^2 \epsilon} = \frac{2j+k+1}{2}$$

$$\Rightarrow \quad j + l + 1 = n = \frac{2\mu e^2}{\hbar^2 \epsilon}$$

$$\Rightarrow \quad \epsilon = \frac{2\mu e^2}{\hbar^2 n}$$

$$\Rightarrow \quad \epsilon^2 = \frac{4\mu^2 e^4}{\hbar^4 n^2}\,.$$

Substituting equation (20) to eliminate ϵ and insert energy explicitly,

$$-4\,\frac{2\mu E}{\hbar^2} = \frac{4\mu^2 e^4}{\hbar^4 n^2}$$

$$\Rightarrow \quad E = -\frac{\mu^2 e^4 \hbar^2}{2\mu\hbar^4 n^2} = -\left(\frac{\mu e^2}{\hbar^2}\right)^2 \frac{\hbar^2}{2\mu n^2}$$

$$\Rightarrow \quad E_n = -\frac{\hbar^2}{2\mu a_0^2\, n^2}\,.$$

Inserting numerical values,

$$\begin{aligned} E_n &= -\frac{\hbar^2}{2\mu a_0^2 n^2} = -\frac{1}{4\pi^2}\frac{(hc)^2}{2(\mu c^2)a_0^2 n^2} \\ &= -\frac{1}{4\pi^2}\frac{(1.24\times 10^4\, eV\cdot \text{Å})^2}{2(0.511\times 10^6\, eV)(0.529\,\text{Å})^2 n^2} = -\frac{13.6\, eV}{n^2}\,, \end{aligned}$$

so summarizing,

$$E_n = -\frac{\hbar^2}{2\mu a_0^2 n^2} = -\frac{13.6\, eV}{n^2} \tag{27}$$

are the eigenenergies of hydrogen.

Postscript: The quantity $13.6\,eV$ is called the **Rydberg**, and is usually denoted R or Ry.

Notice that $n = j + l + 1$ where j and l are non-negative integers, thus $l_{\max} = n - 1$.

Remember that the observables postulate indicates that these are the only energies of hydrogen that can possibly be observed. Indeed, the numerical expression

$$E_n \;=\; -\,\frac{13.6\,eV}{n^2}$$

was developed from the spectra of visible light long before any explanation existed.

13–17. Create the radial wave functions from the solution of the radial equation.

The state vector postulate indicates that eventually we are seeking an $|\,n,l,m>$ which represents the possible states of hydrogen. In abstract Hilbert space, this is

$$<r,\theta,\phi\,|\,n,l,m> \;\rightarrow\; R_{n,l}(r)\,Y_{l,m}(\theta,\phi)$$

for our development in position space. This is conventionally denoted

$$\psi_{nlm}(r,\theta,\phi) \;=\; R_{n,l}(r)\,Y_{l,m}(\theta,\phi)$$

in position space. The next step is to develop the possible radial wave functions. Once those are obtained, our wave function is a simple product of the $R_{n,l}(r)$ and the spherical harmonics.

To obtain the $R_{n,l}(r)$, start with

$$y_j^k(x) \;=\; e^{-x/2}\,x^{(k+1)/2}\,L_j^k(x)$$

which are the family of solutions to the radial equation. Since $x = \epsilon r$, we need to convert back to r, to be consistent with the spherical coordinate system. Then $y(r) = r\,R(r)$, and the solutions can be expressed as radial functions $R(r)$. The final step for this problem will be to express the indices in the family of solutions in terms of the principal and angular momentum quantum numbers remembering $k = 2l + 1$ and $n = j + l + 1$.

The family of solutions of the radial equation is given by equation (15)

$$y_j^k(x) \;=\; e^{-x/2}\,x^{(k+1)/2}\,L_j^k(x)\,.$$

The independent variable is still $x = \epsilon r$. We need an independent variable r, or at least in terms of r, to be consistent with the spherical coordinate system. Using equations (20) and (27), we can solve for ϵ in terms of the Bohr radius and the principal quantum number,

$$\left(\frac{\epsilon}{2}\right)^2 \;=\; -\frac{2\mu E}{\hbar^2} \;=\; -\frac{2\mu}{\hbar^2}\left(-\frac{\hbar^2}{2\mu a_0^2 n^2}\right) \;=\; \frac{1}{a_0^2 n^2}$$

$$\Rightarrow \quad \epsilon^2 \;=\; \frac{4}{a_0^2 n^2} \quad \Rightarrow \quad \epsilon \;=\; \frac{2}{a_0 n}\,, \qquad \text{and}$$

$$x \;=\; \epsilon r \qquad \Rightarrow \qquad x \;=\; \frac{2r}{na_0}\,,$$

and this is in terms of the desired independent variable. Upon substituting

$$y_j^k\left(\frac{2r}{na_0}\right) \;=\; e^{-r/na_0}\left(\frac{2r}{na_0}\right)^{(k+1)/2} L_j^k\left(\frac{2r}{na_0}\right).$$

Remember $y\,(r) \;=\; r\,R\,(r)$, so

$$r\,R_{n,l}(r) \;=\; e^{-r/na_0}\left(\frac{2r}{na_0}\right)^{(k+1)/2} L_j^k\left(\frac{2r}{na_0}\right)$$

$$\Rightarrow \qquad R_{n,l}(r) \;=\; \left(\frac{2}{na_0}\right) e^{-r/na_0}\left(\frac{2r}{na_0}\right)^{(k-1)/2} L_j^k\left(\frac{2r}{na_0}\right)$$

after dividing both sides by r. Expressing the indices in terms of the quantum numbers n and l,

$$k \;=\; 2l+1 \qquad \Rightarrow \qquad \frac{k-1}{2} \;=\; l \qquad \text{and} \qquad j+l+1 \;=\; n \qquad \Rightarrow \qquad j \;=\; n-l-1\,, \qquad \text{thus}$$

$$R_{n,l}(r) \;=\; A\,e^{-r/na_0}\left(\frac{2r}{na_0}\right)^{l} L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)$$

in terms of the quantum numbers. We have added a normalization constant A which has absorbed the factor $2/na_0$ from the power term when we divided through by the factor of r. This still needs to be normalized. We want the radial functions to be individually normalized so the products of the radial wave functions and spherical harmonics, the hydrogen wave functions, are normalized. The normalized radial wave functions are

$$R_{n,l}(r) \;=\; \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n\big[\,(n+l)!\,\big]^3}}\; e^{-r/na_0}\left(\frac{2r}{na_0}\right)^{l} L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right). \tag{28}$$

The first few normalized radial wave functions are listed in table 13–5.

$$\begin{aligned}
R_{1,0}(r) &= 2a_0^{-3/2}e^{-r/a_0} \\
R_{2,0}(r) &= \frac{1}{\sqrt{2}}a_0^{-3/2}\left(1 - \frac{r}{2a_0}\right)e^{-r/2a_0} \\
R_{2,1}(r) &= \frac{1}{\sqrt{24}}a_0^{-3/2}\frac{r}{a_0}\,e^{-r/2a_0} \\
R_{3,0}(r) &= \frac{2}{\sqrt{27}}a_0^{-3/2}\left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2}\right)e^{-r/3a_0} \\
R_{3,1}(r) &= \frac{8}{27\sqrt{6}}a_0^{-3/2}\left(1 - \frac{r}{6a_0}\right)\frac{r}{a_0}e^{-r/3a_0} \\
R_{3,2}(r) &= \frac{4}{81\sqrt{30}}a_0^{-3/2}\frac{r^2}{a_0^2}\,e^{-r/3a_0}
\end{aligned}$$

Table $13-5$. The First Six Radial Wave Functions for Hydrogen.

13–18. Show equation (28) is properly normalized.

The probability postulate is of diminished usefulness without normalized wave functions. The complicated radical in equation (28) is simply a normalization constant. This calculation is retained in the body of the text to illustrate a general normalization processes in position space. Should you have a particular interest in mathematical physics and special functions, the details of this problem may be interesting. Otherwise, briefly scan the arguments and proceed to the next problem.

We want to normalize

$$R_{n,l}(r) \;=\; A\, e^{-r/na_0} \left(\frac{2r}{na_0}\right)^l L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right) .$$

The normalization condition for a function of the radial variable in spherical coordinates is

$$<\psi\,(r)\,|\,\psi\,(r)> \;=\; 1 \;=\int_0^\infty \Big(R_{n,l}(r)\Big)^* R_{n,l}(r)\, r^2\, dr$$

where the factor of r^2 is the radial portion of the volume element in spherical coordinates. Using the radial wave functions, this is

$$\begin{aligned} 1 \;&=\; \int_0^\infty \left(A\, e^{-r/na_0} \left(\frac{2r}{na_0}\right)^l L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right)\right)^* A\, e^{-r/na_0} \left(\frac{2r}{na_0}\right)^l L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right) r^2\, dr \\ &=\; \int_0^\infty A^* A\; e^{-2r/na_0} \left(\frac{2r}{na_0}\right)^{2l} \left(r^2\right)\; L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right) L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right)\, dr \\ &=\; |\,A\,|^2 \left(\frac{na_0}{2}\right)^3 \int_0^\infty e^{-2r/na_0} \left(\frac{2r}{na_0}\right)^{2l+2} L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right) L^{2l+1}_{n-l-1}\left(\frac{2r}{na_0}\right)\, d\left(\frac{2r}{na_0}\right) , \end{aligned} \tag{29}$$

where the cubic factor preceding the integral comes from the fact we have grouped the factor of r^2 with the other powers of r, and also have expressed the differential in terms of the argument of the associated Laguerre polynomial. We are going to borrow two relations from Morse and Feshbach[5], the first of which is

$$\int_0^\infty z^a\, e^{-z}\, L^a_b(z)\, L^a_c(z)\, dz \;=\; \delta_{b,c}\, \frac{[\,\Gamma(a+b+1)\,]^3}{\Gamma(b+1)} . \tag{30}$$

There are some things to notice about equation (30). The Kronecker delta $\delta_{b,c}$ reflects the orthogonality of the associated Laguerre polynomials. The integral is zero unless the lower indices of the two associated Laguerre polynomials are identical. Also, we expect all indices to be integers, so expect the gamma functions to become factorials. Comparing (29) and (30), the argument of the associated Laguerre polynomial, the base of the power term, and the differential are all the same in both equations. The upper index of the associated Laguerre polynomials and the power term

[5] Morse and Feshbach, *Methods of Theoretical Physics* (McGraw–Hill, New York, 1953), pp. 784–785

are the same in (30), but differ in (29). We can adjust (29) using a recursion relation from Morse and Feshbach,

$$z\,L_b^a(z) \;=\; \big(a+2b+1\big)\,L_b^a(z) \;-\; \frac{b+1}{a+b+1}\,L_{b+1}^a(z) \;-\; \big(a+b\big)^2\,L_{b-1}^a(z)\,.$$

If we take one factor of the power term and group it with the first associated Laguerre polynomial,

$$1 \;=\; \big|\,A\,\big|^2\left(\frac{na_0}{2}\right)^3\int_0^\infty e^{-2r/na_0}\left(\frac{2r}{na_0}\right)^{2l+1}\left\{\left(\frac{2r}{na_0}\right)L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)\right\}L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)\,d\left(\frac{2r}{na_0}\right)\,,$$

which makes the exponent of the power term match the upper index of the associated Laguerre polynomial, we can evaluate the term in braces using the recursion relation. For $a \,=\, 2l+1$ and $b \,=\, c \,=\, n-l-1\,,$ this is

$$\begin{aligned}\left(\frac{2r}{na_0}\right)L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right) \;&=\; \big(2l+1+2n-2l-2+1\big)L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)\\ &\quad-\,\frac{n-l-1+1}{2l+1+n-l-1+1}L_{n-l}^{2l+1}\left(\frac{2r}{na_0}\right) \;-\; \big(2l+1+n-l-1\big)^2L_{n-l-2}^{2l+1}\left(\frac{2r}{na_0}\right)\\ &=\; 2n\,L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right) \;-\; \frac{n-l}{n+l+1}L_{n-l}^{2l+1}\left(\frac{2r}{na_0}\right) \;-\; \big(n+l\big)^2L_{n-l-2}^{2l+1}\left(\frac{2r}{na_0}\right).\end{aligned}$$

We are going to ignore all but the first term. We could substitute all three terms into the integral, distribute other factors, break the integral into three integrals, and evaluate each one using equation (30). But the Kronecker delta tells us integrals with unequal lower associated Laguerre polynomial indices will be zero. The only non–vanishing integral will come from the first term, so

$$\begin{aligned}1 \;&=\; \big|\,A\,\big|^2\left(\frac{na_0}{2}\right)^3\int_0^\infty e^{-2r/na_0}\left(\frac{2r}{na_0}\right)^{2l+1}\left\{2n\,L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)\right\}L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)\,d\left(\frac{2r}{na_0}\right)\,,\\ &=\; \big|\,A\,\big|^2\,2n\left(\frac{na_0}{2}\right)^3\int_0^\infty e^{-2r/na_0}\left(\frac{2r}{na_0}\right)^{2l+1}L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)\,d\left(\frac{2r}{na_0}\right)\,,\end{aligned}$$

and we are ready to evaluate this integral using equation (30) where

$$z \;=\; \left(\frac{2r}{na_0}\right), \qquad a \;=\; 2l+1\,, \qquad b \;=\; c \;=\; n-l-1\,,$$

and for integers $\Gamma(j) \,=\, (j-1)\,!\,.$ Then

$$\begin{aligned}1 \;&=\; \big|\,A\,\big|^2\,2n\left(\frac{na_0}{2}\right)^3\frac{\big[\,\Gamma\,(2l+1+n-l-1+1)\,\big]^3}{\Gamma(n-l-1+1)}\\ &=\; \big|\,A\,\big|^2\,2n\left(\frac{na_0}{2}\right)^3\frac{\big[\,\Gamma\,(n+l+1)\,\big]^3}{\Gamma(n-l)}\\ &=\; \big|\,A\,\big|^2\,2n\left(\frac{na_0}{2}\right)^3\frac{\big[\,(n+l)!\,\big]^3}{(n-l-1)!}\end{aligned}$$

$$\Rightarrow \quad A = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n\big[\,(n+l)!\,\big]^3}}$$

$$\Rightarrow \quad R_{n,l}(r) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n\big[\,(n+l)!\,\big]^3}}\, e^{-r/na_0} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right).$$

13–19. Calculate $R_{3,1}(r)$ from equation (28).

Once the indices are established in terms of the quantum numbers n and l, most of the calculation is arithmetic. The associated Laguerre polynomial is a look–it–up factor using table 13–4.

For $n = 3$, $l = 1$,

$$\begin{aligned} R_{3,1}(r) &= \sqrt{\left(\frac{2}{3a_0}\right)^3 \frac{(3-1-1)!}{2(3)\big[\,(3+1)!\,\big]^3}}\, e^{-r/3a_0} \left(\frac{2r}{3a_0}\right)^1 L_{3-1-1}^{2(1)+1}\left(\frac{2r}{3a_0}\right) \\ &= \frac{2}{3}\sqrt{\left(\frac{2^3}{3^3 a_0^3}\right) \frac{1}{2\cdot 3\big[\,(4\cdot 3\cdot 2)\,\big]^3}}\, e^{-r/3a_0} \left(\frac{r}{a_0}\right) L_1^3\left(\frac{2r}{3a_0}\right) \\ &= \frac{2}{3}\sqrt{\frac{2^2}{3^4\big[\,2^6\cdot 3^3\cdot 2^3\,\big]}}\, a_0^{-3/2} e^{-r/3a_0} \left(\frac{r}{a_0}\right)\left(-24\left(\frac{2r}{3a_0}\right)+96\right) \\ &= 96\cdot\frac{2}{3}\sqrt{\frac{2^2}{2^9\cdot 3^7}}\, a_0^{-3/2}\left(-\left(\frac{r}{6a_0}\right)+1\right)\frac{r}{a_0}\, e^{-r/3a_0}, \end{aligned}$$

and because $96 = 2^5\cdot 3$,

$$\begin{aligned} R_{3,1}(r) &= \frac{2^6}{2^3\cdot 3^3}\sqrt{\frac{1}{2\cdot 3}}\, a_0^{-3/2}\left(1-\frac{r}{6a_0}\right)\frac{r}{a_0}\, e^{-r/3a_0} \\ &= \frac{8}{27\sqrt{6}}\, a_0^{-3/2}\left(1-\frac{r}{6a_0}\right)\frac{r}{a_0}\, e^{-r/3a_0}, \end{aligned}$$

in agreement with table 13–5.

13–20. Sketch the first six radial wave functions.

The radial wave functions listed in table 13–5 are sketched in figure 13–1.

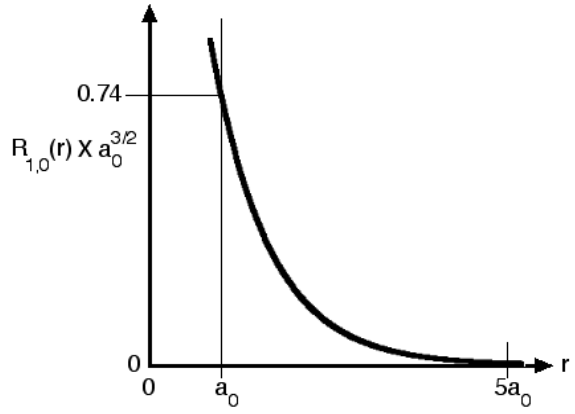

Figure 13-1a. Radial wave function for n = 1, l = 0.

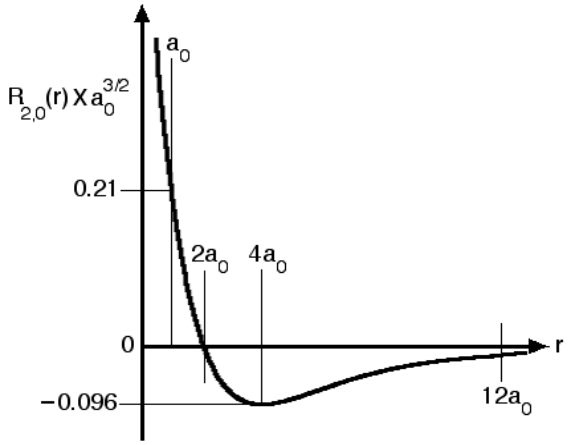

Figure 13-1b. Radial wave function for n = 2, l = 0.

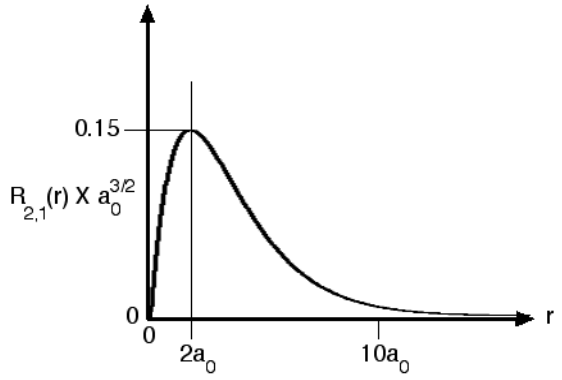

Figure 13-1c. Radial wave function for n = 2, l = 1.

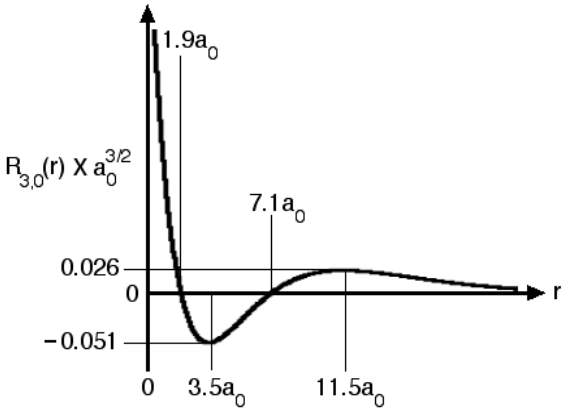

Figure 13-1d. Radial wave function for n = 3, l = 0.

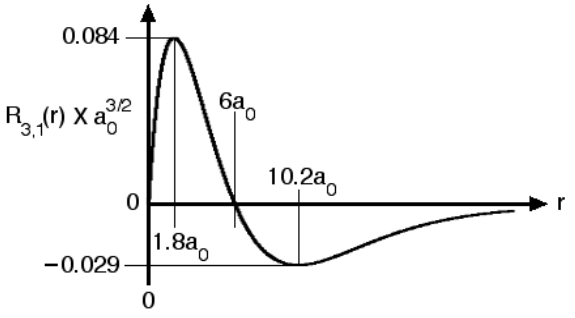

Figure 13-1e. Radial wave function for n = 3, l = 1.

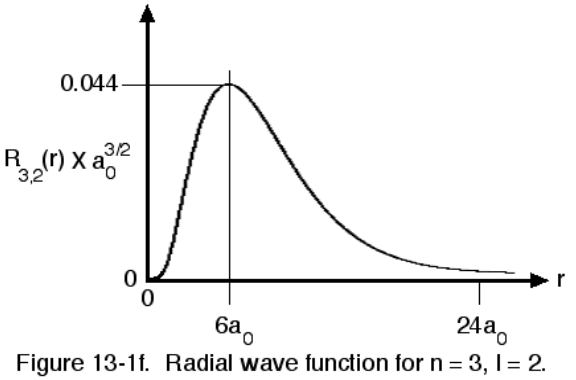

Figure 13-1f. Radial wave function for n = 3, l = 2.

Figure 13–1. The first six radial wave functions for hydrogen.

Each graph is $R(r) \times a_0^{3/2}$ versus r. The factor of $a_0^{3/2}$ is a constant so acts only to scale vertical magnitudes. The functions $R(r)$ listed in table 13–5 have dimensions of length$^{-3/2}$ so the product $R(r) \times a_0^{3/2}$ (and each vertical axis) is dimensionless. The vertical and horizontal scales are different between the six illustrations because the magnitudes and distances vary significantly, particularly between $n = 1$, $n = 2$, and $n = 3$. Many of the qualitative features, such as the basic shape of the graphs, are suppressed when they are drawn to the same scales.

13–21. (a) Find the functional description for radial probability density for $n = 3\,,\ l = 2\,.$

(b) Find the location of the maximum.

(c) Find the functional value of the maximum.

The radial wave functions are all individually normalized, so the probability is

$$<\psi(r)\,|\,\psi(r)> \;=\; <R_{n,l}(r)\,|\,R_{n,l}(r)> \;=\; \int_0^\infty R^*_{n,l}(r)\,R_{n,l}(r)\,r^2\,dr \;=\; \int_0^\infty R^2_{n,l}(r)\,r^2\,dr\,,$$

where the factor of r^2 in the integrals is from the volume element in spherical coordinates. The functions $r^2\,R^2_{n,l}(r)$ are the radial probability densities for the hydrogen atom.

Visually squaring the graph of $R_{3,2}$ from figure 13–1f, a single maximum is expected for $R^2_{3,2}\,,$ and since r is intrinsically non-negative, $r^2\,R^2_{3,2}$ should have a single maximum. Thus part (b) is a straight forward max/min calculus problem, which makes part (c) a straight forward substitution.

(a) $$R_{3,2}(r) \;=\; \frac{4}{81\sqrt{30}}a_0^{-3/2}\frac{r^2}{a_0^2}\,e^{-r/3a_0} \quad\Rightarrow\quad r^2\,R^2_{3,2} \;=\; r^2\left(\frac{4}{81\sqrt{30}}a_0^{-3/2}\frac{r^2}{a_0^2}\,e^{-r/3a_0}\right)^2$$

$$=\; \frac{16}{196,830}\,a_0^{-3}\frac{r^6}{a_0^4}\,e^{-2r/3a_0}$$

(b) The single maximum is found by setting the first derivative equal to zero, so

$$\frac{d}{dr}\,\frac{16}{196,830}\,a_0^{-3}\frac{r^6}{a_0^4}\,e^{-2r/3a_0} \;=\; \frac{16}{196,830}\,a_0^{-3}\left(\frac{6r^5}{a_0^4}\,e^{-2r/3a_0} \;+\; \frac{r^6}{a_0^4}\left(-\frac{2}{3a_0}\right)e^{-2r/3a_0}\right)$$

and setting this equal to zero,

$$\frac{16}{196,830}\,a_0^{-3}\left(\frac{6r^5}{a_0^4}\,e^{-2r/3a_0} \;+\; \frac{r^6}{a_0^4}\left(-\frac{2}{3a_0}\right)e^{-2r/3a_0}\right) \;=\; 0 \quad\Rightarrow\quad \frac{6r^5}{a_0^4} \;-\; \frac{2r^6}{3a_0^5} \;=\; 0$$

$$\Rightarrow\quad 3 \;-\; \frac{r}{3a_0} \;=\; 0 \quad\Rightarrow\quad r \;=\; 9a_0\,.$$

(c) $$\frac{16}{196,830}\,a_0^{-3}\frac{(9a_0)^6}{a_0^4}\,e^{-2(9a_0)/3a_0} \;=\; \frac{16}{196,830}\,\frac{531,441\,a_0^6}{a_0^7}\,e^{-6} \;=\; \frac{0.1071}{a_0}$$

using an electronic calculator.

13–22. Sketch the probability densities of the first six radial wave functions.

Probability density $r^2\,R^2_{n,l}(r)$ has units of inverse length which are canceled by the units of length on the differential dr in a probability integration. Multiplying $r^2\,R^2_{n,l}(r)$ by a_0 provides dimensionless functions. Thus, $r^2\,R^2_{n,l}(r)\,a_0$ are the functions sketched on the next page.

The sketches for probability density do not suffer from the same disparities of scale as the radial wave functions, thus the horizontal and vertical scales are consistent in all six illustrations. The six graphs are aligned vertically to facilitate comparisons. Maxima, minima, and appropriate functional values are indicated. The techniques of the previous problem apply, though those probability densities with more than a single maximum require solving higher degree equations, so some values are obtained numerically. The horizontal coordinate is r in all six illustrations.

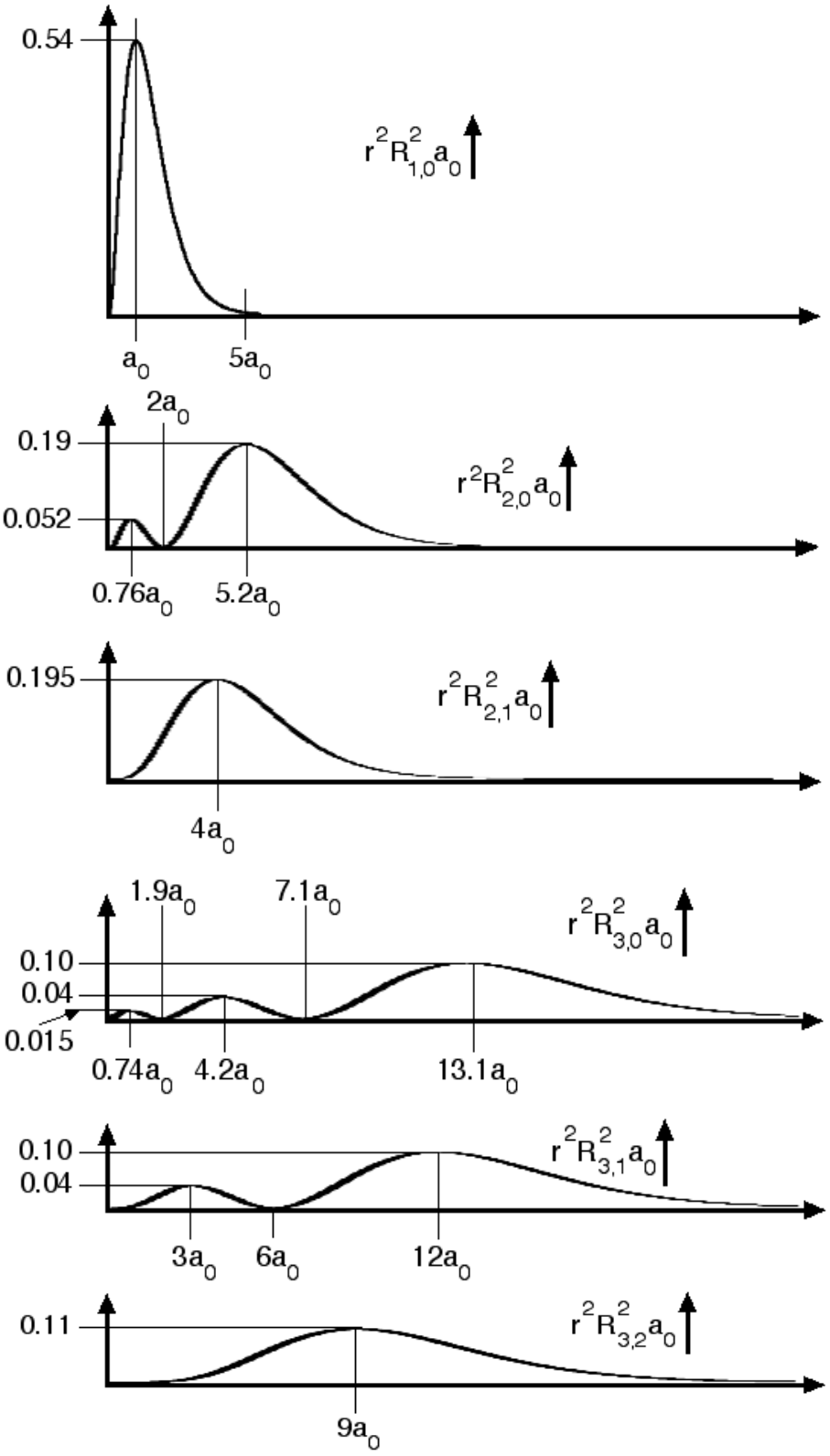

Figure 13–2. The first six radial probability densities for hydrogen.

13–23. What is $\psi_{3,1,-1}(r,\theta,\phi)$ for the hydrogen atom?

The product of the azimuthal, polar, and radial wave functions are the hydrogen wave functions. The product of the azimuthal and polar wave functions are the spherical harmonics, so the hydrogen wave functions are the product of the radial wave functions and spherical harmonics,

$$\psi_{nlm}(r,\theta,\phi) \;=\; R_{n,l}(r)\,Y_{l,m}(\theta,\phi)\,.$$

You can construct the desired hydrogen wave function by selecting the appropriate radial wave function from table 13–5, or calculating it from equation (28), and multiplying it by the appropriate spherical harmonic from table 12–1, or calculating it from equation (12). The relation

$$<r,\theta,\phi\,|\,n,l,m> \;\rightarrow\; R_{n,l}(r)\,Y_{l,m}(\theta,\phi)$$

denotes representation from Hilbert space.

From tables 13–5 and 12–1,

$$R_{3,1}(r) \;=\; \frac{8}{27\sqrt{6}}a_0^{-3/2}\left(1-\frac{r}{6a_0}\right)\frac{r}{a_0}\,e^{-r/3a_0}\,, \qquad Y_{1,-1}(\theta,\phi) \;=\; \sqrt{\frac{3}{8\pi}}\sin\theta\,e^{-i\phi}\,,$$

so

$$\begin{aligned}
\psi_{3,1,-1}(r,\theta,\phi) \;&=\; R_{3,1}(r)\,Y_{1,-1}(\theta,\phi) \\
&=\; \frac{8}{27\sqrt{6}}\;a_0^{-3/2}\left(1-\frac{r}{6a_0}\right)\frac{r}{a_0}\;e^{-r/3a_0}\sqrt{\frac{3}{8\pi}}\sin\theta\,e^{-i\phi} \\
&=\; \frac{8\sqrt{3}}{27\sqrt{6}\sqrt{8\pi}}\;a_0^{-3/2}\left(1-\frac{r}{6a_0}\right)\frac{r}{a_0}\;e^{-r/3a_0}\;\sin\theta\,e^{-i\phi} \\
&=\; \frac{2}{27\sqrt{\pi}}\;a_0^{-3/2}\left(1-\frac{r}{6a_0}\right)\frac{r}{a_0}\;\sin\theta\,e^{-r/3a_0-i\phi}\,.
\end{aligned}$$

13–24. Explain common chemistry terminology in terms of quantum numbers.

Another perspective of our development explains common chemistry terminology in terms of the quantum numbers n, l, and m. These quantum numbers apply to all atoms.

This may be slightly premature because we have not yet addressed spin. Until we add spin, we hope that is suffices to say that an electron can only be in one of two spin states, namely, **spin up** or **spin down**. The impact is that there are two quantum states for each n, l, and m. The intent is that this problem is an insight into all elements of the periodic table, given your recent appreciation of the quantum numbers n, l, and m.

The ground state of hydrogen is $n=1$, $l=0$ and $m=0$. Common chemistry designations for the ground state are the K–shell and the $1s$ subshell. Remember the K–shell may house two electrons in many electron atoms. This means the one electron in the hydrogen atom can exist in one of two possible states, though there is only one possible combination of the three quantum numbers n, l, and m. There is, however, a fourth quantum number associated with spin. For

each set of the three quantum numbers n, l, m, there is a possibility of spin up or spin down, and thus two possible states associated with the quantum numbers $n = 1$, $l = 0$, and $m = 0$, therefore two states associated with the K–shell. The point of the moment is the designation K–shell and quantum number $n = 1$ have the same meaning. The quantum number $n = 2$ is the same as the chemical designation of L–shell. The L–shell has subshells $2s$ and $2p$, where s corresponds to $l = 0$ and p corresponds to $l = 1$, which are possible quantum numbers for $n = 2$. For $l = 1$, $m = -1$, 0, or 1 so there are three states possible in the p subshell. Each of the four L–shell states may have spin up or spin down, so there are eight possible eigenstates in the L–shell. The M–shell corresponds to $n = 3$, the N–shell corresponds to $n = 4$, and the O–shell corresponds to $n = 5$. As the quantum number n becomes larger, the quantum number l can take on a greater range of values. The quantum number $l = 0$ corresponds to the s–subshell, the quantum number $l = 1$ corresponds to the p–subshell, the quantum number $l = 2$ corresponds to the d–subshell, the quantum number $l = 3$ corresponds to the f–subshell, and the quantum number $l = 4$ corresponds to the g–subshell. Each subshell has $2l + 1$ states. The total states in each shell is n^2. Figure 13–3 summarizes this discussion.

	shell							total n^2
	O	$n = 5$	$\underline{5s}_1$	$\underline{5p}_3$	$\underline{5d}_5$	$\underline{5f}_7$	$\underline{5g}_9$	25
	N	$n = 4$	$\underline{4s}_1$	$\underline{4p}_3$	$\underline{4d}_5$	$\underline{4f}_7$		16
$\uparrow$	M	$n = 3$	$\underline{3s}_1$	$\underline{3p}_3$	$\underline{3d}_5$			9
E	L	$n = 2$	$\underline{2s}_1$	$\underline{2p}_3$				4
	K	$n = 1$	$\underline{1s}_1$					1
			$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$	

Figure 13 – 3. Quantum Number, Chemical Designation Correspondence.

The subscripts on the underbars of the subshells indicate the number of states $2l + 1$ in that subshell.

Postscript: Since the energy, to this point, depends only on n, the quantum numbers l and m having no effect on energy, we have an n^2–fold degeneracy in energy using this picture. A magnetic field removes this degeneracy, the same magnetic field that will define the z-axis and provide orientation to the scheme. This was explored by Pieter Zeeman, so is known as the Zeeman effect. Pragmatically, a magnetic field is necessary if the orientation is to make sense.

Accepting that each state has a possibility of spin up or spin down, the number of states in each shell is $2n^2$ when spin is considered. The sum of the total number of states is 55 for $n \leq 5$ from figure 13–3 without spin, but is 110 with spin. Of course, $n > 5$ are possible. Hydrogen is the only element that can be treated as a purely central potential, though once ionized helium or twice ionized lithium (or other hydrogen-like ions) may be so addressed. Nevertheless, the correspondence between common chemical designations and quantum numbers is intriguing.

The last eight problems refer to the $t = 0$ state vector of a hydrogen atom

$$\Psi(r, \theta, \phi) \;=\; 2\,\psi_{1,0,0} \;+\; \psi_{2,1,0}\,. \tag{31}$$

13–25. Does equation (31) make any sense?

Why does equation (31) make sense? What postulate? What does equation (31) mean?

Yes, equation (31) is a possible state vector. The state vector postulate indicates that the state vector can be any linear combination of eigenstates. The state function is a superposition of 2 parts ground state, $\psi_{1,0,0}$, and 1 part of the first excited state, $\psi_{2,1,0}$. The orbital angular momentum and magnetic moment quantum numbers are consistent with the limitations $l_{\max} = n - 1$ and $-l \le m \le l$. We expect a system's state vector to be a linear combination of eigenstates until a measurement establishes the state vector as one of the eigenstates.

13–26. Normalize equation (31).

The probability postulate is of diminished use unless the state vector is normalized. There is a wide variety of techniques possible to accomplish the normalization.

The state function is composed of 2 parts ground state and 1 part of the first excited state, so we can write

$$\Psi(r, \theta, \phi) \;=\; 2\begin{pmatrix}1\\0\end{pmatrix} \;+\; \begin{pmatrix}0\\1\end{pmatrix} \;=\; \begin{pmatrix}2\\1\end{pmatrix}$$

which is an abstract statement of the orthonormality of eigenstates. The normalization condition can be written

$$1 \;=\; A^*\begin{pmatrix}2, & 1\end{pmatrix} A \begin{pmatrix}2\\1\end{pmatrix} \;=\; |A|^2(4+1) \qquad \Rightarrow \qquad A \;=\; \frac{1}{\sqrt{5}}$$

$$\Rightarrow \qquad \Psi(r, \theta, \phi) \;=\; \frac{2}{\sqrt{5}}\,\psi_{1,0,0} \;+\; \frac{1}{\sqrt{5}}\,\psi_{2,1,0}$$

is the properly normalized wave function or state vector.

Postscript: Easiest is to proceed as shown or using another statement of $< i \,|\, j > \;=\; \delta_{i,j}$, such as $< n, l, m \,|\, n', l', m' > \;=\; \delta_{nlm,\,n'l'm'}$. Other methods to normalize the state function for a hydrogen atom is to represent it in position space,

$$\Psi(r, \theta, \phi) \;=\; 2\,\psi_{1,0,0} \;+\; \psi_{2,1,0} \;=\; 2\,R_{1,0}\,Y_{0,0} \;+\; R_{2,1}\,Y_{1,0}\,.$$

The radial wave functions are not orthonormal, but they are normalized. This means

$$\int_0^\infty R_{i,j}\,R_{i,j}r^2\,dr \;=\; 1\,.$$

If integrated over solid angle, the indices must be identical or the integral is zero because

$$\int Y_{i,j}\, Y_{k,l}\, d\Omega \;=\; \delta_{i,k}\, \delta_{j,l}\,,$$

meaning the spherical harmonics are orthonormal, which actually ensures the orthonormality of eigenstates for hydrogen.

The most obvious method may be the most laborious. Represent the hydrogen wave functions for the eigenstates in position space and do the integrations explicitly. This method is not prohibitive, and it will work, but is mentioned solely to encourage you to favor the abstract arguments.

13–27. What are the possible results of individual measurements of energy, orbital angular momentum, and the z–component of orbital angular momentum?

The eigenvalue postulate contains the answers to these questions.

The possible results are the eigenvalues. For

$$\Psi(r,\theta,\phi) \;=\; \frac{2}{\sqrt{5}}\,\psi_{1,0,0} \;+\; \frac{1}{\sqrt{5}}\,\psi_{2,1,0}$$

we could measure a state with a principal quantum number of $n = 1$ or $n = 2$. The corresponding eigenenergies are

$$E_n \;=\; -\,\frac{13.6\,eV}{n^2} \qquad \Rightarrow \qquad E_1 \;=\; -13.6\,eV, \qquad \text{or} \qquad E_2 \;=\; -\,\frac{13.6\,eV}{4} \;=\; -3.4\,eV$$

are the possible results of a measurement of energy. For a measurement of angular momentum, we could measure a state with orbital angular momentum quantum number of $l = 0$ or $l = 1$, so anticipate a measurement of

$$\sqrt{0(0+1)}\,\hbar \;=\; 0 \qquad \text{or} \qquad \sqrt{1(1+1)}\,\hbar \;=\; \sqrt{2}\,\hbar$$

because the eigenvalues of the square of orbital angular momentum, $\mathcal{L}^2$, are $l\,(l+1)\,\hbar^2$, so a measurement of $\mathcal{L}$ is the square root. The eigenvalues of the z–component of angular momentum are $m\hbar$, and both eigenstates of the state vector have $m = 0$, so the only possibility of a measurement of the z–component of angular momentum is $0\,\hbar \;=\; 0$.

13–28. What are the probabilities of the possible results of individual measurements of energy, orbital angular momentum, and the z–component of orbital angular momentum?

The probability postulate is featured in these calculations.

The probabilities are $|<\psi\,|\,\Psi>|^2$, so the probability of measuring $E_1 = -13.6\,eV$, corresponding to measuring the eigenstate with $n = 1$, and the probability of measuring orbital angular momentum of 0, corresponding to measuring the eigenstate with $l = 0$, is

$$\begin{aligned} P\big(E = -13.6\,eV\big) \;=\; P\big(\mathcal{L} = \sqrt{\mathcal{L}^2} = 0\big) \;&=\; \left| <\psi_{1,0,0}\,| \left(\frac{2}{\sqrt{5}}\,|\,\psi_{1,0,0}> \;+\; \frac{1}{\sqrt{5}}\,|\,\psi_{2,1,0}> \right) \right|^2 \\ &=\; \left| \frac{2}{\sqrt{5}} <\psi_{1,0,0}\,|\,\psi_{1,0,0}> \;+\; \frac{1}{\sqrt{5}} <\psi_{1,0,0}\,|\,\psi_{2,1,0}> \right|^2 \\ &=\; \left| \frac{2}{\sqrt{5}}(1) \;+\; 0 \right|^2 \;=\; \frac{4}{5} \end{aligned}$$

where we have used the orthonormality of eigenstates in Dirac notation as an efficient method. Similarly, the probability of measuring $E_2 = -3.4\,eV$, corresponding to measurement of the eigenstate with $n = 2$, and the probability of measuring orbital angular momentum of $\sqrt{2}\,\hbar$, corresponding to measuring the eigenstate with $l = 1$, is

$$\begin{aligned} P\big(E = -3.4\,eV\big) \;=\; P\big(\mathcal{L} = \sqrt{\mathcal{L}^2} = \sqrt{2}\,\hbar\big) \;&=\; \left| <\psi_{2,1,0}\,| \left(\frac{2}{\sqrt{5}}\,|\,\psi_{1,0,0}> \;+\; \frac{1}{\sqrt{5}}\,|\,\psi_{2,1,0}> \right) \right|^2 \\ &=\; \left| \frac{2}{\sqrt{5}} <\psi_{2,1,0}\,|\,\psi_{1,0,0}> \;+\; \frac{1}{\sqrt{5}} <\psi_{2,1,0}\,|\,\psi_{2,1,0}> \right|^2 \\ &=\; \left| 0 \;+\; \frac{1}{\sqrt{5}}(1) \right|^2 \;=\; \frac{1}{5}\,. \end{aligned}$$

The use of the normalized state vector is a practical necessity, though the bra serves only to identify the eigenstate being used for the calculation.

Lastly, there is but one possibility for z–component of angular momentum, corresponding to $m = 0$ in both eigenstates, so we can conclude $P\big(\mathcal{L}_z = 0\big) = 1$ without calculation. Just to illustrate a calculation for which two eigenstates have the same eigenvalue, $P\big(\mathcal{L}_z = 0\big)$ is

$$\begin{aligned} &\left| <\psi_{1,0,0}\,| \left(\frac{2}{\sqrt{5}}\,|\,\psi_{1,0,0}> \;+\; \frac{1}{\sqrt{5}}\,|\,\psi_{2,1,0}> \right) \right|^2 \;+\; \left| <\psi_{2,1,0}\,| \left(\frac{2}{\sqrt{5}}\,|\,\psi_{1,0,0}> \;+\; \frac{1}{\sqrt{5}}\,|\,\psi_{2,1,0}> \right) \right|^2 \\ &\qquad =\; \left| \frac{2}{\sqrt{5}} <\psi_{1,0,0}\,|\,\psi_{1,0,0}> \right|^2 \;+\; \left| \frac{1}{\sqrt{5}} <\psi_{2,1,0}\,|\,\psi_{2,1,0}> \right|^2 \\ &\qquad\qquad =\; \left| \frac{2}{\sqrt{5}}\,(1) \right|^2 \;+\; \left| \frac{1}{\sqrt{5}}\,(1) \right|^2 \;=\; \frac{4}{5} \;+\; \frac{1}{5} \;=\; 1\,. \end{aligned}$$

13–29. What are the expectation values of energy, orbital angular momentum, and the z–component of orbital angular momentum?

Expectation values follow from the probability postulate.

$$< E > \; = \; \sum_i P(E_i)\, E_i \; = \; \frac{4}{5}\left(-13.6\, eV\right) \; + \; \frac{1}{5}\left(-3.4\, eV\right) \; = \; -10.88\, eV \, - \, 0.68\, eV \; = \; -11.56\, eV.$$

$$< \mathcal{L} > \; = \; < \sqrt{\mathcal{L}^2} > \; = \; \sum_i P(\alpha_i)\, \alpha_i \; = \; \frac{4}{5}\left(0\right) \; + \; \frac{1}{5}\left(\sqrt{2}\,\hbar\right) \; = \; \frac{\sqrt{2}\,\hbar}{5}\,.$$

The expectation value of the z–component of angular momentum is 0, since that is the only possible result of a measurement of $\mathcal{L}_z$.

13–30. What are the uncertainties of energy, orbital angular momentum, and the z–component of angular momentum?

Uncertainties also follow from the probability postulate.

$$\begin{aligned}
\triangle E \; &= \; \sqrt{\sum_i P(E_i)\left(E_i - < E > \right)^2} \\
&= \; \left[\frac{4}{5}\left(-13.6\, eV \, - \, -11.56\, eV\right)^2 \; + \; \frac{1}{5}\left(-3.4\, eV \, - \, -11.56\, eV\right)^2\right]^{1/2} \\
&= \; \left[\frac{4}{5}\left(-2.04\right)^2 \; + \; \frac{1}{5}\left(8.16\right)^2\right]^{1/2} eV \; = \; \left[\frac{4}{5}\left(4.16\right) \; + \; \frac{1}{5}\left(66.59\right)\right]^{1/2} eV \\
&= \; \left[3.33 \; + \; 13.32\right]^{1/2} eV \; = \; \left[16.65\right]^{1/2} eV \\
&= \; 4.08\, eV\,.
\end{aligned}$$

$$\begin{aligned}
\triangle \sqrt{\mathcal{L}^2} \; &= \; \left[\frac{4}{5}\left(0 - \frac{\sqrt{2}\,\hbar}{5}\right)^2 \; + \; \frac{1}{5}\left(\sqrt{2}\,\hbar - \frac{\sqrt{2}\,\hbar}{5}\right)^2\right]^{1/2} \\
&= \; \left[\frac{4}{5}\left(-\frac{\sqrt{2}}{5}\right)^2 \; + \; \frac{1}{5}\left(\frac{4\sqrt{2}}{5}\right)^2\right]^{1/2} \hbar \\
&= \; \left[\frac{4}{5}\left(\frac{2}{5^2}\right) \; + \; \frac{1}{5}\left(\frac{16\cdot 2}{5^2}\right)\right]^{1/2} \hbar \; = \; \left[\frac{8}{5^3} \; + \; \frac{32}{5^3}\right]^{1/2} \hbar \; = \; \left[\frac{40}{5^3}\right]^{1/2} \hbar \\
&= \; \frac{2\sqrt{2}}{5}\,\hbar\,.
\end{aligned}$$

The uncertainty in the z–component of angular momentum is 0, since there is only one possibility.

13–31. Express the $t = 0$ wave function in terms of r, θ, and ϕ explicitly.

The state vector is composed of 2 parts ground state and one part of the excited state $\psi_{2,1,0}$. Remembering that $\Psi_{n,l,m}(r,\ \theta,\ \phi) = R_{n,l}(r)\,Y_{l,m}(\theta,\ \phi)$ for the hydrogen atom, the intent is to obtain the radial parts from table 13–5, the angular parts from table 12–1, and multiply them together appropriately to obtain the eigenstates and then add them while including the normalization constants to obtain the desired hydrogen wave function.

$$\begin{aligned}
\psi_{1,0,0} \quad &\rightarrow \quad R_{1,0}(r)\,Y_{0,0}(\theta,\ \phi) \;=\; 2\,a_0^{-3/2}\,e^{-r/a_0}\left(\frac{1}{4\pi}\right) \;=\; \frac{1}{2\pi}\,a_0^{-3/2}\,e^{-r/a_0} \\
\psi_{2,1,0} \quad &\rightarrow \quad R_{2,1}(r)\,Y_{1,0}(\theta,\ \phi) \;=\; \frac{1}{\sqrt{24}}\,a_0^{-3/2}\,\frac{r}{a_0}\,e^{-r/2a_0}\left(\sqrt{\frac{3}{4\pi}}\,\cos\theta\right) \\
&\qquad\qquad\qquad\qquad\quad = \;\frac{1}{4}\sqrt{\frac{1}{2\pi}}\,a_0^{-3/2}\,\frac{r}{a_0}\,e^{-r/2a_0}\,\cos\theta \\
\Rightarrow \qquad \Psi(r,\ \theta,\ \phi) \;&=\; \frac{2}{\sqrt{5}}\,\frac{1}{2\pi}\,a_0^{-3/2}\,e^{-r/a_0} \;+\; \frac{1}{\sqrt{5}}\,\frac{1}{4}\sqrt{\frac{1}{2\pi}}\,a_0^{-3/2}\,\frac{r}{a_0}\,e^{-r/2a_0}\,\cos\theta \\
&=\; \frac{1}{\pi\sqrt{5}}\,a_0^{-3/2}\,e^{-r/a_0} \;+\; \frac{1}{4}\sqrt{\frac{1}{10\pi}}\,a_0^{-3/2}\,\frac{r}{a_0}\,e^{-r/2a_0}\,\cos\theta
\end{aligned}$$

13–32. What is the time dependent state vector in terms of r, θ, and ϕ?

Each eigenstate will exhibit the time dependence $e^{-iE_nt/\hbar}$. We have the E_n from problem 13–27.

$$\begin{aligned}
\Psi(r,\ \theta,\ \phi,\ t) \;&=\; \frac{1}{\pi\sqrt{5}}\,a_0^{-3/2}\,e^{-r/a_0}\,e^{-i(-13.6)t/\hbar} \;+\; \frac{1}{4}\sqrt{\frac{1}{10\pi}}\,a_0^{-3/2}\,\frac{r}{a_0}\,e^{-r/2a_0}\,\cos\theta\,e^{-i(-3.4)t/\hbar} \\
&=\; \frac{1}{\pi\sqrt{5}}\,a_0^{-3/2}\,e^{-r/a_0+13.6it/\hbar} \;+\; \frac{1}{4}\sqrt{\frac{1}{10\pi}}\,\frac{r}{a_0}\,a_0^{-3/2}\,\cos\theta\;e^{-r/2a_0+3.4it/\hbar}
\end{aligned}$$

Exercises

13–33. Confirm the Legendre polynomial $P_4(x)$ from table 13–1 using the generating function immediately preceding the table.

See problem 13–10. You are required to take a fourth derivative of a polynomial. Knowing

$$(1 - x^2)^4 \;=\; x^8 - 4x^6 + 6x^4 - 4x^2 + 1$$

may help. The numerics, even for just the fourth Legendre polynomial, are not trivial. The coefficients become large enough to be inconvenient. Using symbolic multiplication and powers of prime numbers, per problem 13–19, may aid organization in many of these exercises.

13–34. Find the associated Legendre polynomials (a) $P_{4,\,0}(x)$,

(b) $P_{4,\,1}(x)$,

(c) $P_{4,\,2}(x)$, and

(d) $P_{4,\,3}(x)$, using your result from the previous exercise.

The formula desired is in problem 13–10 and is immediately above the one used to complete the last problem. Obtaining associated Legendre polynomials using the generating function are straight forward given that you already have the appropriate Legendre polynomial.

13–35. Confirm the Laguerre polynomial $L_3(x)$ in table 13–3 using the generating function immediately following the table.

This is largely an exercise in differentiation. See problem 13–12.

13–36. Calculate the associated Laguerre polynomial $L_2^1(x)$.

Use the generating function immediately following table 13–4 and your result from the previous exercise. The result is in the table. Again, see problem 13–12.

Notice that the generating function for associated Laguerre polynomials requires the Laguerre polynomial with the subscript that is the sum of the subscript and superscript of the desired associated Laguerre polynomial.

13–37. Briefly describe the roles of the associated Legendre polynomials (which lead to spherical harmonics) and the associated Laguerre polynomials in the solution to the hydrogen atom.

Briefly means three sentences, or one sentence if you use three clauses.

13–38. Briefly describe the calculations required to obtain $L_4^3(x)$ using generating functions.

Do not do any actual calculations! Rather, think about what would be required and answer in a few sentences. Just the consideration of this question may illustrate why hydrogen wave functions for $n > 3$ are rarely seen in texts and difficult to find on the internet.

13–39. Calculate the lowest five eigenenergies of hydrogen.

The eigenenergies of hydrogen are dependent only on the principal quantum number n. Use the result of problem 13–16.

13–40. Confirm $R_{3,0}(r)$ in table 13–5.

Use equation (28) from problem 13–17 per the procedure of problem 13–19.

13–41. Calculate the hydrogen wave functions for

(a) $\psi_{1,0,0}(r,\ \theta,\ \phi)$,

(b) $\psi_{2,1,-1}(r,\ \theta,\ \phi)$,

(c) $\psi_{3,1,1}(r,\ \theta,\ \phi)$, and

(d) $\psi_{3,2,-2}(r,\ \theta,\ \phi)$.

Remember $\Psi_{n,l,m}(r,\ \theta,\ \phi) = R_{n,l}(r)\, Y_{l,m}(\theta,\ \phi)$. Multiply the appropriate radial wave function from table 13–5 and the appropriate spherical harmonic from table 12–1 to obtain the desired results. That the radial wave functions and the spherical harmonics are individually normalized means that a product hydrogen wave function is normalized. See problem 13–31.

13–42. For the $t = 0$ hydrogen wave function

$$\Psi(r, \theta, \phi) = 5\,\psi_{1,0,0} + 2\,\psi_{3,1,1}$$

(a) Normalize Ψ.

(b) What are the possible results of individual measurements of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(c) What are the probabilities of the possible results of individual measurements of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(d) What are the expectation values of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(e) What are the uncertainties of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(f) Express the $t = 0$ wave function in terms of r, θ, and ϕ explicitly.

(g) What is the time dependent state vector in terms of r, θ, and ϕ?

(h) If the z-component of orbital angular momentum is measured with a result of $\hbar$, what is the time dependent state vector in terms of r, θ, and ϕ?

(i) What is the result of a subsequent measurement of the orbital angular momentum?

Problems 13–25 and beyond should be helpful. Employing the postulates is a continued emphasis. This exercise embeds all six postulates in one manner or another. Remember that the discussion concerning the hydrogen atom started with the Schrodinger postulate, so they are all here.

13–43. For the $t = 0$ hydrogen wave function

$$\Psi(r, \theta, \phi) = 6\,\psi_{1,0,0} + 3\,\psi_{2,1,-1} + \psi_{3,2,-2}$$

(a) Normalize Ψ.

(b) What are the possible results of individual measurements of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(c) What are the probabilities of the possible results of individual measurements of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(d) What are the expectation values of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(e) What are the uncertainties of energy, orbital angular momentum, and the z-component of orbital angular momentum?

(f) Express the $t = 0$ wave function in terms of r, θ, and ϕ explicitly.

(g) What is the time dependent state vector in terms of r, θ, and ϕ?

(h) If the orbital angular momentum is measured with a result of $\sqrt{2}\,\hbar$, what is the time dependent state vector in terms of r, θ, and ϕ?

(i) What is the result of an ensuing measurement of the z-component of orbital angular momentum?

The same ideas and mathematical mechanics as the last problem, except bigger, brighter, and shinier with three eigenstates composing the initial state function.

13–44. Find the associated Legendre polynomials (a) $P_{6,0}(x)$,

(b) $P_{6,1}(x)$, and

(c) $P_{6,2}(x)$

using the Legendre polynomial and the associated Legendre polynomial generating functions.

Exercises 13–33 and 13–34 cover this material for Legendre/associated Legendre polynomials with lower indices. The numerics, repeated differentiation and subsequent arithmetic, are challenging. Again, coefficients become large enough to be inconvenient if conventionally multiplied. Using symbolic multiplication and powers of prime numbers may facilitate organization.

13–45. Calculate $L_3^2(x)$ using the Laguerre polynomial and the associated Laguerre polynomial generating functions.

See problem 13–12 and exercises 13–35 and 13–36. Exercise 13–38 is intended to encourage thought into some of the difficulties of this type of calculation. Calculate $L_5(x)$ using the chain rule of differentiation. The coefficients are all 1200 or below so conventional multiplication is appropriate. Nevertheless, this exercise should provide some insight into the generation of the radial wave function of hydrogen $R_{4,3}(r)$ which would require the Laguerre polynomial $L_7(x)$.

13–46. Calculate (a) the radial wave function for hydrogen for $n = 4$ and $l = 0$, and

(b) the hydrogen wave function for $n = 4$, $l = 0$, and $m = 0$. Then

(c) find the total number of hydrogen wave functions for $n = 4$, and

(d) find the total number of hydrogen wave functions for $n = 5$.

There are a multitude of tables and graphs for the radial wave functions for hydrogen for $n \leq 3$. Information about the radial wave functions of hydrogen for $n = 4$ are difficult to find, even on the internet, and for $n \geq 5$ are genuinely challenging to locate. This exercise should partially answer the question why this is so. Realize that $l = 0$ is likely the simplest possibility for part (a), and there are three other $n = 4$ radial wave functions. Part (b) is for completeness as the real point to calculating the radial wave function is to obtain the corresponding wave function for the hydrogen atom, again $l = 0$ is likely simplest. Parts (c) and (d) hope to illuminate the breadth of calculation required should a person want to obtain a wave function of hydrogen for $n \geq 4$.

13–47. Verify the locations of the maxima and functional values for $r^2 R_{1,0}^2$ and $r^2 R_{2,1}^2$ of figure 13–2.

Both radial probability density curves have a single maximum so obtaining maxima and functional values for those maxima are straight forward using the techniques of problem 13–21. Start with the appropriate radial wave function from table 13–5. You should notice that multiplying the functional values of the maxima by a_0, which is done in figure 13–2 to obtain $r^2 R_{1,0}^2 a_0$ and $r^2 R_{2,1}^2 a_0$, yields dimensionless numbers.

Appendix A Arithmetic with Complex Numbers

A–1. What is the imaginary number?

The imaginary number is the solution to $x^2+1 = 0$ or $x^2 = -1$. The solution is usually denoted by a lower case "i" as in $i = \sqrt{-1}$. The idea is $\left(\sqrt{-1}\right)^2 = -1$, or $i^2 = -1$.

The field of electrical engineering will frequently use "j" as in $j = \sqrt{-1}$, so denoting i as the imaginary number is not universal.

A–2. Where do imaginary numbers occur?

Imaginary numbers occur in any circumstance that requires any root of a negative number, however, they are intrinsic to the values, components, and elements of quantum mechanics.

A–3. How are $\sqrt{-4}$, $\sqrt{-25}$, and $\sqrt{-7}$ expressed?

$\sqrt{-4} = \sqrt{4}\sqrt{-1} = 2i$, $\sqrt{-25} = \sqrt{25}\sqrt{-1} = 5i$, and $\sqrt{-7} = \sqrt{7}\sqrt{-1} = \sqrt{7}\,i$.

A–4. What are complex numbers?

Complex numbers are those with both a real and imaginary part, often written in a binomial form such as $2+5i$ and $6-7i$, or in general $a+bi$. Complex numbers are often denoted using the letter z.

A–5. Find the real and imaginary parts of $z_1 = 2+5i$, $z_2 = 6-7i$, and $z = a+bi$.

The real part of a complex number, denoted $\mathrm{Re}(z)$, is self explanatory. The imaginary part, denoted $\mathrm{Im}(z)$, is the coefficient of the imaginary number. Thus,

$\mathrm{Re}(2+5i) = 2$, $\mathrm{Im}(2+5i) = 5$,

$\mathrm{Re}(6-7i) = 6$, $\mathrm{Im}(6-7i) = -7$,

$\mathrm{Re}(a+bi) = a$, $\mathrm{Im}(a+bi) = b$.

A–6. Add $2+5i$ and $6-7i$, then subtract $6-7i$ from $2+5i$.

The real part and imaginary part of complex numbers are different degrees of freedom, thus add/subtract the real parts and add/subtract the imaginary parts. In general

$a+bi + (c+di) = a+c + (b+d)\,i$ and $a+bi - (c+di) = a-c + (b-d)\,i$.

$$2+5i \;+\; 6-7i \;=\; (2+6) \;+\; (5-7)\,i \;=\; 8-2i\,, \qquad \text{and}$$
$$2+5i \;-\; (6-7i) \;=\; (2-6) \;+\; (5+7)\,i \;=\; -4+12i\,.$$

A–7. Multiply $2+5i$ and $6-7i$.

The given complex numbers are in binomial form so this is binomial multiplication.

$$(a+bi\,)(c+di) \;=\; ac+adi+bci+bi(di)$$

but $bi(di) \;=\; bdi\cdot i \;=\; bd\,(-1) \;=\; -bd$, so

$$(a+bi\,)(c+di) \;=\; ac-bd+(ad+bc)\,i\,.$$

$$\begin{aligned}(2+5i\,)(6-7i) \;&=\; 2\cdot 6+2\,(-7i)+(5i)\,6+5i\,(-7i)\\ &=\; 12-14i+30i-35i^2 \;=\; 12+16i+35 \;=\; 47+16i\end{aligned}$$

where $-35i^2 \;=\; -35\,(-1) \;=\; +35$.

A–8. Form the complex conjugates of $2+5i$ and $6-7i$.

If $z \;=\; a+bi$, the complex conjugate is $z^* \;=\; a-bi$. Leave the real part the same, form the negative of the imaginary part, and that is the complex conjugate.

$$z_1 \;=\; 2+5i \quad\Rightarrow\quad z_1^* \;=\; 2-5i\,, \qquad \text{and} \qquad z_2 \;=\; 6-7i \quad\Rightarrow\quad z_2^* \;=\; 6+7i\,.$$

Postscript: The complex conjugate for z is denoted $\overline{z}$ in some texts.

A–9. Find the products $z\,z^*$ for $2+5i$ and $6-7i$.

$$z_1\,z_1^* \;=\; (2+5i)\,(2-5i) \;=\; 2\cdot 2+2\,(-5i)+5i\,(2)+5i\,(-5i) \;=\; 4-10i+10i+25 \;=\; 29\,,$$

$$z_2\,z_2^* \;=\; (6-7i)\,(6+7i) \;=\; 6\cdot 6+6\,(7i)-7i\,(6)-7i\,(7i) \;=\; 36+42i-42i+49 \;=\; 85\,.$$

Postscript: The imaginary parts sum to zero so that $z\,z^*$ is a real number in both cases.

A–10. Prove that the product $z\,z^*$ is a real number in general.

$$z\,z^* \;=\; (a+bi)\,(a-bi) \;=\; a\cdot a + a\,(-bi) + bi\,(a) + bi\,(-bi) \;=\; a^2 - abi + abi + b^2 \;=\; a^2 + b^2$$

which does not possess an imaginary part so is a real number.

Postscript: That $z\,z^* = a^2 + b^2$, the sum of the squares of the real and imaginary parts, is a general result and is a frequently used efficiency.

A–11. Divide $2+5i$ by $6-7i$, and $6-7i$ by $2+5i$.

Division of complex numbers is a form of rationalization that expresses the quotient in the form $a+bi$. Multiply the quotient by 1 in the form of the complex conjugate of the divisor and simplify.

$$\frac{2+5i}{6-7i} \;=\; \frac{2+5i}{6-7i}\,\frac{6+7i}{6+7i} \;=\; \frac{12+14i+30i-35}{36+49} \;=\; \frac{-23+44i}{85} \;=\; -\frac{23}{85} + \frac{44}{85}\,i\,,$$

$$\frac{6-7i}{2+5i} \;=\; \frac{6-7i}{2+5i}\,\frac{2-5i}{2-5i} \;=\; \frac{12-30i-14i-35}{4+25} \;=\; \frac{-23-44i}{29} \;=\; -\frac{23}{29} - \frac{44}{29}\,i\,.$$

Postscript: $\mathrm{Re}\left(-\frac{23}{85} + \frac{44}{85}\,i\right) = -\frac{23}{85}$, $\quad \mathrm{Im}\left(-\frac{23}{85} + \frac{44}{85}\,i\right) = \frac{44}{85}$, and

$\mathrm{Re}\left(-\frac{23}{29} - \frac{44}{29}\,i\right) = -\frac{23}{29}$, $\quad \mathrm{Im}\left(-\frac{23}{29} - \frac{44}{29}\,i\right) = -\frac{44}{29}$, thus, both are of the form $a+bi$.

A–12. Plot $2+5i$ and $6-7i$ on an Argand diagram.

An Argand diagram is a two dimensional graph using the horizontal axis to indicate the real part of a complex number and the vertical axis to display the imaginary part. A complex number can be pictured by drawing an arrow from the origin to the ordered pair representing that complex number, comparable to depicting a vector quantity on the $x\,y$ plane.

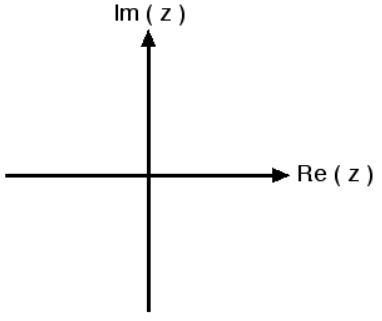

Figure A–1. Argand diagram.

Plots are seen at the right.

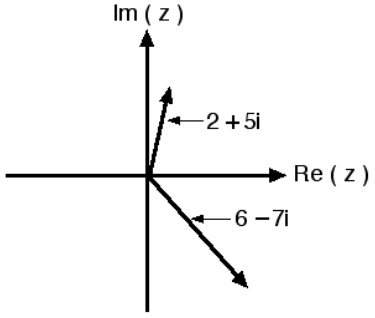

Figure A–2. $2 + 5i$ and $6 - 7i$.

Postscript: Jean-Robert Argand published his geometric interpretation of complex numbers in 1806. An Argand diagram is made in the **complex plane**, or ***z* plane**.

A–13. Find the moduli of $2 + 5i$ and $6 - 7i$

The **modulus** of a complex number is equivalent to the length of the corresponding vector on an Argand diagram. If $z = a + bi$, $\left|z\right| = \sqrt{z\,z^*} = \sqrt{(a+bi)(a-bi)} = \sqrt{a^2+b^2}$.

$$\left|2+5i\right| = \sqrt{2^2+5^2} = \sqrt{4+25} = \sqrt{29}, \qquad \text{and}$$
$$\left|6-7i\right| = \sqrt{6^2+(-7)^2} = \sqrt{36+49} = \sqrt{85}.$$

Postscript: The modulus of a complex number is also called an **absolute value** or **norm**.

A–14. What is Euler's equation?

Sometimes called **Euler's formula**, **Euler's equation** is $e^{i\,\theta} = \cos(\theta) + i\,\sin(\theta)$.

A–15. Express $2 + 5i$ and $6 - 7i$ in polar form.

Polar form, sometimes called **exponential form**, expresses a complex number as a product of its modulus and phase angle using Euler's equation. If $z = a + bi$,

$$z = r\,e^{i\,\theta} = \sqrt{a^2+b^2}\,\big(\cos(\theta) + i\,\sin(\theta)\big) \qquad \text{where} \qquad \theta = \tan^{-1}\left(\frac{b}{a}\right).$$

$$\theta_1 = \tan^{-1}\left(\frac{5}{2}\right) = 1.19 \quad \Rightarrow \quad 2+5i = \sqrt{29}\,e^{i\,1.19},$$
$$\theta_2 = \tan^{-1}\left(\frac{-7}{6}\right) = -0.86 \quad \Rightarrow \quad 6-7i = \sqrt{85}\,e^{-i\,0.86}.$$

Postscript: Imagine figure A–2 in polar coordinates. $2+5i = \sqrt{29}\, e^{i\,1.19}$ means that the magnitude is $\sqrt{29}$ rotated 1.19 radians counterclockwise from the positive horizontal axis. Similarly, $6-7i = \sqrt{85}\, e^{-i\,0.86}$ means that the magnitude is $\sqrt{85}$ rotated 0.86 radians clockwise from the positive horizontal axis.

The inverse tangent function on most calculators returns the principal value between $-\dfrac{\pi}{2}$ and $\dfrac{\pi}{2}$. Thus, phase angles for complex numbers that fall in the 2nd and 3rd quadrants on an Argand diagram require adjustment from the inverse tangent value returned by an electronic calculator.

A–16. Find the product of $z_1 = \sqrt{29}\, e^{i\,1.19}$ and $z_2 = \sqrt{85}\, e^{-i\,0.86}$. Show that the answer is consistent with problem A–7.

$$\begin{aligned} z_1\, z_2 &= \sqrt{29}\, e^{i\,1.19}\, \sqrt{85}\, e^{-i\,0.86} = \sqrt{29}\, \sqrt{85}\, e^{i\,(1.19-0.86)} = \sqrt{2465}\, e^{i\,0.33} \\ &= \sqrt{2465}\,\big(\cos(0.33) + i\,\sin(0.33)\big) = \sqrt{2465}\,\big(0.946 + i\,0.324\big) \\ &= 46.97 + 16.09\,i \approx 47 + 16i\,. \end{aligned}$$

A–17. Divide $z_1 = \sqrt{29}\, e^{i\,1.19}$ by $z_2 = \sqrt{85}\, e^{-i\,0.86}$. Show that the answer is consistent with problem A–11.

$$\frac{z_1}{z_2} = \frac{\sqrt{29}\, e^{i\,1.19}}{\sqrt{85}\, e^{-i\,0.86}} = \sqrt{\frac{29}{85}}\, e^{i\,(1.19+0.86)} = \sqrt{\frac{29}{85}}\, e^{i\,2.05} = \sqrt{\frac{29}{85}}\,\big(\cos(2.05) + i\,\sin(2.05)\big)$$

$$= \sqrt{\frac{29}{85}}\,\big(-0.461 + i\,0.887\big) = -0.269 + i\,0.518\,, \quad \text{A–11} \;\Rightarrow\; -\frac{23}{85} + \frac{44}{85}\,i \approx -0.271 + 0.518\,i\,.$$

A–18. Find the complex conjugates of $z_1 = \sqrt{29}\, e^{i\,1.19}$ and $z_2 = \sqrt{85}\, e^{-i\,0.86}$.

Just like binomial forms, change the sign of all i's with no other changes, thus

$$z_1^* = \sqrt{29}\, e^{-i\,1.19} \qquad \text{and} \qquad z_2^* = \sqrt{85}\, e^{i\,0.86}\,.$$

A–19. Show that $z\,z^* \in \mathbb{R}$ for $z_1 = \sqrt{29}\, e^{i\,1.19}$ and $z_2 = \sqrt{85}\, e^{-i\,0.86}$.

$$\begin{aligned} z_1\, z_1^* &= \sqrt{29}\, e^{i\,1.19}\, \sqrt{29}\, e^{-i\,1.19} = 29\, e^{i\,1.19-i\,1.19} = 29\, e^{0} = 29 \in \mathbb{R}\,, \\ z_2\, z_2^* &= \sqrt{85}\, e^{-i\,0.86}\, \sqrt{85}\, e^{i\,0.86} = 85\, e^{-i\,0.86+i\,0.86} = 85\, e^{0} = 85 \in \mathbb{R}\,. \end{aligned}$$

Postscript: The fact that arguments of the exponentials of the complex conjugate quantities sum to zero and $e^0 = 1$ is seen routinely in quantum mechanical probability calculations.

A–20. (a) Find the product of $z_3 = 3 - 5i$ and $z_4 = -4 + 3i$.

(b) Convert z_3 and z_4 to polar forms.

(c) Find the product of z_3 and z_4 using the polar forms of part (b).

(d) Show that the products of parts (a) and (c) are consistent.

The second remark of the postscript following problem A–15 warns that the inverse tangent function on most calculators will return values between $-\frac{\pi}{2}$ and $\frac{\pi}{2}$. Notice that z_4 will fall in the second quadrant, thus adjustment is required to obtain a proper phase angle.

(a) $z_3\, z_4 = (3 - 5i)(-4 + 3i) = -12 + 9i + 20i + 15 = 3 + 29i$.

(b) $\theta_3 = \tan^{-1}\left(\frac{-5}{3}\right) = -1.03 \quad \Rightarrow \quad z_3 = \sqrt{3^2 + (-5)^2}\, e^{i(-1.03)} = \sqrt{34}\, e^{-1.03\, i}$.

$\theta_4 = \tan^{-1}\left(\frac{3}{-4}\right) = -0.644$, which indicates the 4th quadrant rather than the 2nd, so

$\theta_4 = -0.644 + \pi = 2.498$, then $z_4 = \sqrt{(-4)^2 + 3^2}\, e^{i(2.498)} = 5\, e^{2.498\, i}$.

(c) $z_3\, z_4 = \sqrt{34}\, e^{-1.03\, i}\, 5\, e^{2.498\, i} = 29.15\, e^{1.468\, i}$.

(d) $29.15\, e^{1.468\, i} = 29.15\big(\cos 1.468 + i \sin 1.468\big)$

$= 29.15\big(0.103 + i\, 0.995\big) = 3.00 + i\, 29.00 \approx 3 + 29i$.

Postscript: The adjustment of a phase angle concerns the manner in which a calculator is used. It seems best to form a mental picture from which the manner of adjustment should be clear. This precalculus point may occur on any occasion a calculator is used to evaluate an inverse tangent.

Exercises

Use $z_1 = 2 + 5i$, $z_2 = 4 - 3i$, $z_3 = 2\,e^{i\,3\pi/4}$, $z_4 = 7\,e^{-i\,2\pi/3}$ for following exercises.

A–21. Find the real and imaginary parts of z_1 and z_2.

A–22. Find $z_1 + z_2$ and $z_1 - z_2$.

A–23. Find the products $z_1\,z_2$ and $z_3\,z_4$.

A–24. Form the complex conjugates of all four complex numbers.

A–25. Find the products $z\,z^*$ for all four complex numbers. (Notice that all are real numbers).

A–26. Divide z_1 by z_2 and z_3 by z_4.

A–27. Plot all four complex numbers on an Argand diagram. (z_3 is 2 units long and rotated $\frac{3\pi}{4}$, z_4 is 7 units long and rotated $\frac{4\pi}{3}$ or $-\frac{2\pi}{3}$. Alternately, convert the polar forms to binomial forms).

A–28. Find the moduli of all four complex numbers. (The modulus of a complex number written in polar form, such as $r\,e^{i\,\theta}$, is r).

A–29. Express z_1 and z_2 in polar form.

A–30. Show that the product of your results from A–29 is consistent with the result of A–23.

A–31. (a) Express z_3 and z_4 in binomial form.

(b) Find the product $z_3\,z_4$ using the binomial forms of part (a).

(c) Show that the product of part (b) is consistent with A–23.

A–32. (a) Find the product of $z_5 = -2 + 3i$ and $z_6 = 4 - 5i$.

(b) Convert z_5 and z_6 to polar forms.

(c) Find the product of z_5 and z_6 using the polar forms of part (b).

(d) Show that the products of parts (a) and (c) are consistent.

Postscript: Binomial and polar forms of complex numbers are most frequently used in physics, however, an ordered pair is one other notation that is used occasionally. It is understood that the second component of the ordered pair is imaginary, thus $z = a + bi$ may be written $z = (a\,,\,b)$.

Appendix B Linear Independence and the Gram-Schmidt Orthonormalization Process

Linear independence is a property of a set of vectors meaning that none of the vectors in the set can be formed using a linear combination of two or more vectors in that set. Linear independence is a sufficient condition for a set of vectors to form a basis given that the set of vectors is the same dimension as the space. Any linearly independent set of vectors can be made orthonormal using the Gram-Schmidt Orthonormalization Process.

Since all observable quantities are represented by Hermitian operators and the eigenvectors of all Hermitian operators are orthogonal so can be made orthonormal, thus inherently forming a basis set, the mathematical concept of linear independence has little consequence for our development. This appendix is included only for completeness of traditionally presented material.

B–1. (a) Are $|u_1> \rightarrow \begin{pmatrix}1\\1\\0\end{pmatrix}$, $|u_2> \rightarrow \begin{pmatrix}1\\3\\2\end{pmatrix}$, and $|u_3> \rightarrow \begin{pmatrix}-1\\0\\1\end{pmatrix}$ linearly independent?

(b) Are $|v_1> \rightarrow \begin{pmatrix}1\\1\\0\end{pmatrix}$, $|v_2> \rightarrow \begin{pmatrix}1\\0\\1\end{pmatrix}$, and $|v_3> \rightarrow \begin{pmatrix}3\\2\\1\end{pmatrix}$ linearly independent?

(c) Are $|w_1> \rightarrow \begin{pmatrix}1\\1\\0\end{pmatrix}$, $|w_2> \rightarrow \begin{pmatrix}1\\0\\1\end{pmatrix}$, and $|w_3> \rightarrow \begin{pmatrix}0\\1\\1\end{pmatrix}$ linearly independent?

A set of vectors is **linearly independent** if and only if

$$\sum_{i=1}^{n} \alpha_i |v_i> \neq |0> \qquad \text{unless all} \qquad \alpha_i = 0\,.$$

Likely the most straightforward way to determine linear independence is proof by contradiction. For example, assume the set of vectors given in part (a) is linearly independent. Then

$$\alpha_1 \begin{pmatrix}1\\1\\0\end{pmatrix} + \alpha_2 \begin{pmatrix}1\\3\\2\end{pmatrix} + \alpha_3 \begin{pmatrix}-1\\0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$$

if and only if $\alpha_1 = \alpha_2 = \alpha_3 = 0$. But the components form the simultaneous equations

$$\begin{aligned} \alpha_1 + \alpha_2 - \alpha_3 &= 0 \\ \alpha_1 + 3\alpha_2 &= 0 \\ 2\alpha_2 + \alpha_3 &= 0 \end{aligned}$$

for which $\alpha_1 = 3$, $\alpha_2 = -1$ and $\alpha_3 = 2$ is a solution. This contradicts our assumption. Therefore, the given vectors are not linearly independent, or are **linearly dependent**.

(b) Assume the vectors are linearly independent. Then

$$a_1 \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + a_3 \begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

where $a_1 = a_2 = a_3 = 0$ would be the only coefficients that could make this equation true. Performing the scalar multiplications, the above condition means

$$\begin{pmatrix} a_1 \\ a_1 \\ 0 \end{pmatrix} + \begin{pmatrix} a_2 \\ 0 \\ a_2 \end{pmatrix} + \begin{pmatrix} 3a_3 \\ 2a_3 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{array}{rcrcrcl} a_1 & + & a_2 & + & 3a_3 & = & 0 \\ a_1 & & & + & 2a_3 & = & 0 \\ & & a_2 & + & a_3 & = & 0 \end{array}$$

that is, the individual components must sum to zero. This particular system has an infinite number of solutions such that $a_i \neq 0$, for example, $a_1 = 1$, $a_2 = 1/2$, and $a_3 = -1/2$. Therefore, in contradiction to the assumption, $|v_1>$, $|v_2>$, and $|v_3>$ are linearly dependent.

(c) However, consider

$$a_1 \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + a_3 \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} a_1 \\ a_1 \\ 0 \end{pmatrix} + \begin{pmatrix} a_2 \\ 0 \\ a_2 \end{pmatrix} + \begin{pmatrix} 0 \\ a_3 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\Rightarrow \quad \begin{array}{rcl} a_1 + a_2 & = & 0 \\ a_1 + a_3 & = & 0 \\ a_2 + a_3 & = & 0 \end{array} \quad \Rightarrow \quad \begin{array}{rcl} a_1 & = & -a_2 \\ a_1 & = & -a_3 \\ a_2 & = & -a_3 \end{array} \quad \Rightarrow \quad \begin{array}{rcl} a_1 & = & -a_2 \\ -a_2 & = & -a_3 \end{array} \quad \Rightarrow \quad \begin{array}{rcl} a_2 & = & a_3 \\ a_3 & = & -a_3 \end{array}$$

The last equation can be true if and only if $a_3 = 0 \quad \Rightarrow \quad a_2 = 0 \quad \Rightarrow \quad a_1 = 0.$ Since all $a_i = 0$, $|w_1>$, $|w_2>$, and $|w_3>$ are linearly independent.

Postscript: Our definition of linear independence has an upper limit on the summation of n. The upper limit can be any number including ∞. In other words, though the vectors in this problem are in three dimensions, the concept generalizes to any including infinite dimensions.

When the number of vectors in a linearly independent set is the same as the dimension of the linear vector space, all of the other vectors in the space can be formed using a linear combination of this basic set, or set of **basis** vectors. When all other vectors in the space can be formed using a linear combination of a set of vectors, that set of vectors is said to **span** the space.

There are an infinite number of sets of vectors that will constitute a basis for any linear vector space. A vector $|v>$ exists in the Hilbert space as an abstraction. Said another way, $|v>$ is an abstract ket vector. The statements $|v> \rightarrow \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$ or $|v> \rightarrow \begin{pmatrix} -i \\ 1 \\ i \end{pmatrix}$ are representations that are **basis dependent**. A choice of basis is analogous to a choice of coordinate system and reference frame within the context of classical mechanics.

The number of components in a column or row vector effectively determines the dimension of the space. The dimension of a linear vector space is more generally defined by the number of linearly independent objects required to span the space.

B–2. Orthonormalize the vectors

$$|\,I> \;\rightarrow\; \begin{pmatrix} 1 \\ -3 \end{pmatrix} \qquad \text{and} \qquad |\,II> \;\rightarrow\; \begin{pmatrix} 3 \\ 4 \end{pmatrix},$$

and check to ensure that your resulting vectors are orthonormal.

You can make an orthonormal basis from any linearly independent set of vectors using the **Gram-Schmidt orthonormalization procedure**. Given a linearly independent basis, the Gram-Schmidt orthonormalization procedure has you

(1) choose a vector $|\,I>$ at random and normalize it to obtain the unit vector $|\,1>$.

(2) Choose a second vector $|\,II>$ and subtract its projection on the first vector meaning

$$|\,2> \;=\; |\,II> \;-\; |\,1><1|\,II> \;. \qquad \text{Normalize this vector.}$$

(3) Choose another vector $|\,III>$ and subtract its projection along the first two vectors, or

$$|\,3> \;=\; |\,III> \;-\; |\,1><1|\,III> \;-\; |\,2><2|\,III> \;. \qquad \text{Normalize this vector.}$$

(4) Repeat the procedure until you exhaust all the vectors in the linearly independent set.

$$\begin{array}{rcrcl} a_1 & + & 3a_2 & = & 0 \\ -3a_1 & + & 4a_2 & = & 0 \end{array} \quad \Rightarrow \quad 9a_2 \;+\; 4a_2 \;=\; 13a_2 \;=\; 0 \quad \Rightarrow \quad a_2 = 0 \quad \Rightarrow \quad a_1 = 0\,,$$

$$\text{so the vectors} \qquad |\,I> \;=\; \begin{pmatrix} 1 \\ -3 \end{pmatrix} \qquad \text{and} \qquad |\,II> \;=\; \begin{pmatrix} 3 \\ 4 \end{pmatrix}$$

are linearly independent. First, normalize one vector.

$$<I\,|\,\mathrm{A}^*\mathrm{A}\,|\,I> \;=\; \begin{pmatrix} 1, & -3 \end{pmatrix} \mathrm{A}^*\,\mathrm{A} \begin{pmatrix} 1 \\ -3 \end{pmatrix} \;=\; |\,\mathrm{A}\,|^2 \Big(1 + 9 \Big) \;=\; |\,\mathrm{A}\,|^2\, 10 \;=\; 1\,,$$

$$\Rightarrow \quad \mathrm{A} \;=\; \frac{1}{\sqrt{10}} \quad \Rightarrow \quad |\,1> \;=\; \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ -3 \end{pmatrix}$$

is normalized. Next subtract the projection of the second along the first,

$$\begin{aligned} |\,2> \;&=\; |\,II> \;-\; |\,1><1|\,II> \\ &=\; \begin{pmatrix} 3 \\ 4 \end{pmatrix} \;-\; \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ -3 \end{pmatrix} \left[\begin{pmatrix} 1, & -3 \end{pmatrix} \begin{pmatrix} 3 \\ 4 \end{pmatrix} \right] \frac{1}{\sqrt{10}} \\ &=\; \begin{pmatrix} 3 \\ 4 \end{pmatrix} \;-\; \frac{1}{10} \begin{pmatrix} 1 \\ -3 \end{pmatrix} (3 - 12) \;=\; \begin{pmatrix} 3 \\ 4 \end{pmatrix} \;+\; \frac{9}{10} \begin{pmatrix} 1 \\ -3 \end{pmatrix} \\ &=\; \begin{pmatrix} 3 + 9/10 \\ 4 - 27/10 \end{pmatrix} \;=\; \begin{pmatrix} 39/10 \\ 13/10 \end{pmatrix} \;=\; \frac{13}{10} \begin{pmatrix} 3 \\ 1 \end{pmatrix}, \end{aligned}$$

where the square brackets in the second line are used only to indicate that we are going to do that vector multiplication first. Normalizing this vector,

$$\frac{13}{10}\,(3,\ 1)\,\mathrm{A}^{*}\mathrm{A}\,\frac{13}{10}\begin{pmatrix}3\\1\end{pmatrix}\ =\ |\,\mathrm{A}\,|^{2}\,\frac{169}{100}\,(9+1)\ =\ |\,\mathrm{A}\,|^{2}\,\frac{169}{10}\ =\ 1$$

$$\Rightarrow\quad \mathrm{A}\ =\ \frac{\sqrt{10}}{13}\quad\Rightarrow\quad |\,2>\ =\ \frac{\sqrt{10}}{13}\,\frac{13}{10}\begin{pmatrix}3\\1\end{pmatrix}\ =\ \frac{\sqrt{10}}{10}\begin{pmatrix}3\\1\end{pmatrix}$$

is the normalized vector. Here, we have exhausted all the vectors in the linearly independent, two dimensional set, so have completed the Gram-Schmidt procedure.

Are these vectors now orthonormal? Checking

$$<1\,|\,2>\ =\ (1,\ -3)\,\frac{1}{\sqrt{10}}\,\frac{\sqrt{10}}{10}\begin{pmatrix}3\\1\end{pmatrix}\ =\ \frac{1}{10}\,(3-3)\ =\ \frac{1}{10}\,(0)\ =\ 0\,,$$

so they are orthogonal, and since they are normalized, they are also orthonormal.

B–3. (a) Show that the vectors

$$|\,I>\ \rightarrow\ \begin{pmatrix}3\\0\\0\end{pmatrix},\quad |\,II>\ \rightarrow\ \begin{pmatrix}0\\1\\2\end{pmatrix},\quad |\,III>\ \rightarrow\ \begin{pmatrix}0\\2\\5\end{pmatrix}\quad \text{are linearly independent.}$$

(b) Show that the system of three vectors in part (a) is not orthogonal.

(c) Use the Gram-Schmidt process to form an orthonormal basis from the vectors in part (a).

(d) Show that the vectors resulting from part (c) are orthonormal.

This is numerical evidence that linear independence of a set of vectors is a sufficient condition for orthonormality. Notice that orthogonality of the original set is not necessary.

Use the strategy of demonstrating linear independence seen in problem B–1 for part (a). Part (b) requires you to form inner products. This system is not orthogonal, but only one of the nine possible inner products disqualifies it. Part (c) is the Gram-Schmidt process. Part (d) answers the question "does this Gram-Schmidt process really work?" Yes it does, and you really need only check that the inner product analogous to that which was non-zero in part (b) is zero after the Gram-Schmidt process has been applied. The other properties of orthonormality are satisfied because of the nature of normalized vectors and two of the results of part (b).

(a) The condition of linear independence is

$$\sum_{i}^{n} a_i\,|\,v_i>\ \neq\ |\,0>\qquad \text{unless all}\qquad a_i\ =\ 0\,.\qquad \text{Here this means}$$

$$a_1\begin{pmatrix}3\\0\\0\end{pmatrix} + a_2\begin{pmatrix}0\\1\\2\end{pmatrix} + a_3\begin{pmatrix}0\\2\\5\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix}3a_1\\0\\0\end{pmatrix} + \begin{pmatrix}0\\a_2\\2a_2\end{pmatrix} + \begin{pmatrix}0\\2a_3\\5a_3\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$$

$$\Rightarrow \quad \begin{aligned} 3a_1 &= 0 \\ a_2 + 2a_3 &= 0 \\ 2a_2 + 5a_3 &= 0 \end{aligned} \qquad \Rightarrow \quad \begin{aligned} a_1 &= 0 \\ a_2 &= -2a_3 \\ 2a_2 &= -5a_3 \end{aligned}$$

The first line says a_1 is zero. Substituting the equation from the second line into the third line,

$$2a_2 = -5a_3 \quad \Rightarrow \quad 2(-2a_3) = -4a_3 = -5a_3\,,$$

which can be true only if $a_3 = 0$. Then since $a_2 = -2a_3$, a_2 is also zero. The unique solution for all coefficients is that all $a_i = 0$, therefore, the three vectors are linearly independent.

(b) To show the three vectors are not orthogonal, we need to show only that any inner product of different vectors does not vanish. In fact

$$<II\,|\,III> \;=\; \big(0,\ 1,\ 2\big)\begin{pmatrix}0\\2\\5\end{pmatrix} \;=\; 0+2+10 \;=\; 12 \;\neq\; 0\,,$$

so this system of three vectors is not orthogonal. By the way, $<I\,|\,II> \;=\; <I\,|\,III> \;=\; 0$.

(c) First normalize $|\,1>$,

$$<1\,|\,\mathrm{A}^*\mathrm{A}\,|\,1> \;=\; \Big(3,\ 0,\ 0\Big)\,\mathrm{A}^*\mathrm{A}\begin{pmatrix}3\\0\\0\end{pmatrix} \;=\; \big|\,\mathrm{A}\,\big|^2\Big(9+0+0\Big) \;=\; \big|\,\mathrm{A}\,\big|^2 9 \;=\; 1$$

$$\Rightarrow \quad \mathrm{A} \;=\; \frac{1}{3} \quad \Rightarrow \quad |\,1> \;=\; \frac{1}{3}\begin{pmatrix}3\\0\\0\end{pmatrix} \;=\; \begin{pmatrix}1\\0\\0\end{pmatrix}.$$

Then construct $|\,2'>$,

$$|\,2'> \;=\; \begin{pmatrix}0\\1\\2\end{pmatrix} \;-\; \begin{pmatrix}1\\0\\0\end{pmatrix}\Big(1,0,0\Big)\begin{pmatrix}0\\1\\2\end{pmatrix} \;=\; \begin{pmatrix}0\\1\\2\end{pmatrix} \;-\; \begin{pmatrix}1\\0\\0\end{pmatrix}(0+0+0) \;=\; \begin{pmatrix}0\\1\\2\end{pmatrix}$$

and then normalize $|\,2'>$ to obtain $|\,2>$,

$$<2\,|\,\mathrm{A}^*\mathrm{A}\,|\,2> \;=\; \Big(0,\ 1,\ 2\Big)\,\mathrm{A}^*\mathrm{A}\begin{pmatrix}0\\1\\2\end{pmatrix} \;=\; \big|\,\mathrm{A}\,\big|^2\Big(0+1+4\Big) \;=\; \big|\,\mathrm{A}\,\big|^2 5 \;=\; 1$$

$$\Rightarrow \quad \mathrm{A} \;=\; \frac{1}{\sqrt{5}} \quad \Rightarrow \quad |\,2> \;=\; \frac{1}{\sqrt{5}}\begin{pmatrix}0\\1\\2\end{pmatrix}.$$

Finally, construct $|\,3'>$,

$$
\begin{aligned}
|\,3'> &= \begin{pmatrix}0\\2\\5\end{pmatrix} - \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}1,0,0\end{pmatrix}\begin{pmatrix}0\\2\\5\end{pmatrix} - \begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}\left(0,\ \frac{1}{\sqrt{5}},\ \frac{2}{\sqrt{5}}\right)\begin{pmatrix}0\\2\\5\end{pmatrix} \\
&= \begin{pmatrix}0\\2\\5\end{pmatrix} - \begin{pmatrix}1\\0\\0\end{pmatrix}(0+0+0) - \begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}\left(0+\frac{2}{\sqrt{5}}+\frac{10}{\sqrt{5}}\right) \\
&= \begin{pmatrix}0\\2\\5\end{pmatrix} - \begin{pmatrix}1\\0\\0\end{pmatrix}(0) - \begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}\frac{12}{\sqrt{5}} \\
&= \begin{pmatrix}0\\2\\5\end{pmatrix} - \begin{pmatrix}0\\12/5\\24/5\end{pmatrix} = \begin{pmatrix}0\\-2/5\\1/5\end{pmatrix}
\end{aligned}
$$

and then normalize $|\,3'>$ to obtain $|\,3>$,

$$
<3\,|\,\mathrm{A}^*\mathrm{A}\,|\,3> \;=\; \left(0,\ -\frac{2}{5},\ \frac{1}{5}\right)\mathrm{A}^*\mathrm{A}\begin{pmatrix}0\\-2/5\\1/5\end{pmatrix} \;=\; |\,\mathrm{A}\,|^2\left(0+\frac{4}{25}+\frac{1}{25}\right) \;=\; |\,\mathrm{A}\,|^2\,\frac{1}{5} \;=\; 1
$$

$$
\Rightarrow \quad \mathrm{A} \;=\; \sqrt{5} \quad \Rightarrow \quad |\,3> \;=\; \sqrt{5}\begin{pmatrix}0\\-2/5\\1/5\end{pmatrix} \;=\; \begin{pmatrix}0\\-2/\sqrt{5}\\1/\sqrt{5}\end{pmatrix}.
$$

Summarizing, the application of the Gram-Schmidt procedure yields the three vectors

$$
|\,1> \;=\; \begin{pmatrix}1\\0\\0\end{pmatrix}, \qquad |\,2> \;=\; \begin{pmatrix}0\\1/\sqrt{5}\\2/\sqrt{5}\end{pmatrix}, \qquad |\,3> \;=\; \begin{pmatrix}0\\-2/\sqrt{5}\\1/\sqrt{5}\end{pmatrix}.
$$

(d) Each inner product with itself is 1 because all three vectors are normalized. Then $<I\,|\,II> \;=\; <I\,|\,III> \;=\; 0$, as before, because all inner products of the form

$$
\begin{pmatrix}a,\ 0,\ 0\end{pmatrix}\begin{pmatrix}0\\b\\c\end{pmatrix} \;=\; 0+0+0 \;=\; 0\,.
$$

However, $<II\,|\,III>$ was non-zero, but

$$
<2\,|\,3> \;=\; \begin{pmatrix}0,\ 1/\sqrt{5},\ 2/\sqrt{5}\end{pmatrix}\begin{pmatrix}0\\-2/\sqrt{5}\\1/\sqrt{5}\end{pmatrix} \;=\; -\frac{2}{5} \;+\; \frac{2}{5} \;=\; 0\,,
$$

so the three vectors in the summary of part (c) are orthonormal.

Postscript: Material of this nature is traditionally presented in QM I because linear independence of a set of vectors of appropriate dimension establishes the existence of the orthonormal basis. Once linear independence is established, orthonormality can be assumed. The validity of this assumption can be based on the Gram-Schmidt procedure, though the Gram-Schmidt process is rarely demonstrated. Our development, where the eigenvectors of a Hermitian operator are proven to be orthogonal so can be made orthonormal through the process of normalization, effectively supersedes this material for introductory quantum mechanics.

Exercises

B–4. Which of the following sets of vectors are linearly independent?

(a) $\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$

(b) $\begin{pmatrix} i \\ -1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 1 \\ -1 \\ -i \end{pmatrix}, \quad \begin{pmatrix} 1 \\ -i \\ 1 \end{pmatrix}$

(c) $\begin{pmatrix} i \\ i \\ 0 \end{pmatrix}, \quad \begin{pmatrix} i \\ i \\ i \end{pmatrix}, \quad \begin{pmatrix} i \\ 0 \\ i \end{pmatrix}$

(d) $\begin{pmatrix} -i \\ 1 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} i \\ -1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

Use the procedures of problem B–1. The vectors of parts (b) and (c) are linearly independent. The vectors of parts (a) and (d) are linearly dependent.

B–5. (a) Show that the vectors

$$|I> \rightarrow \begin{pmatrix} 0 \\ -i \\ 0 \end{pmatrix}, \quad |II> \rightarrow \begin{pmatrix} i \\ 1+i \\ 0 \end{pmatrix}, \quad |III> \rightarrow \begin{pmatrix} 1-i \\ 0 \\ 2+i \end{pmatrix} \quad \text{are linearly independent.}$$

(b) Show that the system of three vectors in part (a) is not orthogonal.

(c) Use the Gram-Schmidt process to form an orthonormal basis from the vectors in part (a).

(d) Show that the resulting vectors are orthonormal.

This problem is a complex number analogy to problem B–3. See problem B–3 for procedures. The actual value of this exercise and problem B–3 is to reinforce that linear independence is a sufficient condition for orthonormality. The Gram-Schmidt procedure is a mathematical mechanism through which an orthonormal set can be realized given a linearly independent set. Orthonormality is a practical necessity for quantum mechanical calculations. Linear independence is a property intrinsic to the eigenvectors of all Hermitian operators.

Appendix C The Gaussian Wave Packet Centered at $k = k_0$.

The normalized distribution of a plane wave within a wave packet is given to be

$$\psi(x) = \frac{e^{ik_0 x}\, e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}.$$

(a) Find the normalized distribution in wavenumber space for $k_0 \neq 0$

(b) and the wave function as a function of position and time.

(c) Show that

$$\psi(x, t) = \frac{1}{(\pi\alpha^2)^{1/4}} \left(1 + \frac{i\hbar t}{m\alpha^2}\right)^{-1/2} \exp\left[ik_0\left(x - \frac{\hbar k_0 t}{2m}\right)\right] \exp\left[\frac{-\left(x - \hbar k_0 t/m\right)^2}{2\alpha^2 + 2i\hbar t/m}\right].$$

(d) Find the wave function at $t = 0$,

(e) the probability density as a function of position and time,

(f) and the uncertainty in position as a function of time.

The normalized Gaussian distribution $\psi(x) = \dfrac{e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}}$ provides the most straightforward development of a Gaussian wave function. It has the physical limitation that the resulting distribution in wavenumber space is centered at $k = 0 \quad \Rightarrow \quad p = 0$. Thinking classically for a moment, this would mean that you are traveling with the particle. The given distribution is centered at $k = k_0$, or $p = p_0$, which is a more realistic reference frame. The amount of algebra required conspires to make this problem appear more difficult than the concepts involved.

This problem parallels the development of the Gaussian wave function centered at $k_0 = 0$. Find the Fourier transform of the given distribution which is the distribution in wavenumber, $g(k)$. Using the same integral and procedure as used in problem 7–9, you should find

$$g(k) = \frac{\alpha}{(\pi\alpha^2)^{1/4}}\, e^{-(k-k_0)^2\alpha^2/2}$$

for part (a). Multiply this by a plane wave solution $e^{i(kx-\omega t)}$, which constitutes a Gaussian wave packet. This is how time is introduced. Integrate the product over all wavenumbers using the dispersion relation $\omega = \hbar k^2/2m$ to obtain $\psi(x, t)$. Parallel problem 7–7 to find

$$\psi(x,t) = \frac{1}{(\pi\alpha^2)^{1/4}}\, e^{-\alpha^2 k_0^2/2} \left(1 + \frac{i\hbar t}{m\alpha^2}\right)^{-1/2} \exp\left[\frac{(ix + \alpha^2 k_0)^2}{2\alpha^2 + 2i\hbar t/m}\right]$$

for part (b). Part (c) is a substantial algebra problem. Reduce the amount of algebra by letting

$$b = 2\alpha^2 + \frac{2i\hbar t}{m} \qquad \text{and} \qquad c = \frac{\hbar k_0 t}{m}. \qquad \text{Express the exponentials}$$

in terms of one argument. Complete the square of that argument by multiplying by 1 in the form

$$\exp\left[\frac{2\hbar k_0 t x}{mb} - \frac{2\hbar k_0 t x}{mb} - \frac{\hbar^2 k_0^2 t^2}{m^2 b} + \frac{\hbar^2 k_0^2 t^2}{m^2 b}\right].$$

There are eight terms that form the argument of the exponential. The term in x^2 and two of the terms introduced to complete the square are $\dfrac{-\big(x-\hbar k_0 t/m\big)^2}{2\alpha^2+2i\hbar t/m}$. This is the argument of the second exponential desired for part (c). The two remaining terms that are linear in x reduce to ik_0x. The other three terms reduce to $-i\hbar k_0^2 t/2m$. These combine to be the argument of the first exponential desired for part (c). $\psi(x,0)$ is now straightforward to calculate.

(a) $\psi(x) = \dfrac{e^{ik_0x}\,e^{-x^2/2\alpha^2}}{(\pi\alpha^2)^{1/4}} \quad \Rightarrow \quad g(k) = \dfrac{1}{\sqrt{2\pi}}\dfrac{1}{(\pi\alpha^2)^{1/4}}\displaystyle\int_{-\infty}^{\infty} e^{ik_0x}\,e^{-x^2/2\alpha^2}\,e^{-ikx}\,dx$

$= \dfrac{1}{\sqrt{2\pi}}\dfrac{1}{(\pi\alpha^2)^{1/4}}\displaystyle\int_{-\infty}^{\infty} e^{-x^2/2\alpha^2}\,e^{-i(k-k_0)x}\,dx$

$\displaystyle\int_{-\infty}^{\infty} e^{-p^2x^2\pm qx}\,dx = \frac{\sqrt{\pi}}{p}\,e^{q^2/4p^2}$ so using $p^2 = \dfrac{1}{2\alpha^2}, \quad q = i\big(k-k_0\big),$

$\Rightarrow \quad g(k) = \dfrac{1}{\sqrt{2\pi}}\dfrac{1}{(\pi\alpha^2)^{1/4}}\,\alpha\sqrt{2\pi}\,e^{[i(k-k_0)]^2/4(1/2\alpha^2)} = \dfrac{\alpha}{(\pi\alpha^2)^{1/4}}\,e^{-(k-k_0)^2\alpha^2/2}$

which is a Gaussian wave packet centered at $k = k_0$.

(b) The integral over wavenumber of a plane wave weighted by the dispersion relation, which is the distribution in wavenumber from problem 7–6, yields the wave function.

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\frac{\alpha}{(\pi\alpha^2)^{1/4}}\int_{-\infty}^{\infty} e^{-(k-k_0)^2\alpha^2/2}\,e^{ikx-i\hbar k^2t/2m}\,dk \\ &= \frac{1}{\sqrt{2\pi}}\frac{\alpha}{(\pi\alpha^2)^{1/4}}\int_{-\infty}^{\infty}\exp\left[-\frac{\alpha^2}{2}k^2 + \alpha^2k_0k - \frac{\alpha^2k_0^2}{2} + ikx - \frac{i\hbar k^2t}{2m}\right]dk \\ &= \frac{1}{\sqrt{2\pi}}\frac{\alpha}{(\pi\alpha^2)^{1/4}}\,e^{-\alpha^2k_0^2/2}\int_{-\infty}^{\infty}\exp\left[-\left(\frac{\alpha^2}{2}+\frac{i\hbar t}{2m}\right)k^2 + \big(ix+\alpha^2k_0\big)k\right]dk.\end{aligned}$$

The same integral applies where $p^2 = \left(\dfrac{\alpha^2}{2}+\dfrac{i\hbar t}{2m}\right)$ and $q = ix + \alpha^2k_0,$

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\frac{\alpha}{(\pi\alpha^2)^{1/4}}\,e^{-\alpha^2k_0^2/2}\,\frac{\sqrt{\pi}}{\left(\dfrac{\alpha^2}{2}+\dfrac{i\hbar t}{2m}\right)^{1/2}}\,\exp\left[\frac{(ix+\alpha^2k_0)^2}{4\left(\dfrac{\alpha^2}{2}+\dfrac{i\hbar t}{2m}\right)}\right] \\ &= \frac{1}{(\pi\alpha^2)^{1/4}}\,e^{-\alpha^2k_0^2/2}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\exp\left[\frac{(ix+\alpha^2k_0)^2}{2\alpha^2+2i\hbar t/m}\right].\end{aligned}$$

(c) $$\psi(x,t) = \frac{1}{(\pi\alpha^2)^{1/4}}\,e^{-\alpha^2k_0^2/2}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\exp\left[\frac{-x^2 + 2i\alpha^2k_0x + \alpha^4k_0^2}{2\alpha^2 + 2i\hbar t/m}\right]. \qquad (1)$$

Simplify the notation by letting $b = 2\alpha^2 + \dfrac{2i\hbar t}{m}$ and $c = \dfrac{\hbar k_0 t}{m},$ then

$$\psi(x,t) = \frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\exp\left[-\frac{\alpha^2k_0^2}{2}\right]\exp\left[-\frac{x^2}{b} + \frac{2i\alpha^2k_0x}{b} + \frac{\alpha^4k_0^2}{b}\right].$$

Complete the square by multiplying by 1 in the form

$$\exp\left[\frac{2\hbar k_0 tx}{mb} - \frac{2\hbar k_0 tx}{mb} - \frac{\hbar^2 k_0^2 t^2}{m^2 b} + \frac{\hbar^2 k_0^2 t^2}{m^2 b}\right] = \exp\left[\frac{2cx}{b} - \frac{2cx}{b} - \frac{c^2}{b} + \frac{c^2}{b}\right].$$

The overall argument of a single exponential is the eight terms

$$-\frac{\alpha^2 k_0^2}{2} + \frac{\alpha^4 k_0^2}{b} + \frac{2i\alpha^2 k_0 x}{b} - \frac{2cx}{b} + \frac{c^2}{b} - \frac{x^2}{b} + \frac{2cx}{b} - \frac{c^2}{b}$$

$$= \left(-\frac{\alpha^2 k_0^2}{2} + \frac{\alpha^4 k_0^2}{b} + \frac{c^2}{b}\right) + \left(\frac{2i\alpha^2 k_0 x}{b} - \frac{2cx}{b}\right) + \left(-\frac{x^2}{b} + \frac{2cx}{b} - \frac{c^2}{b}\right)$$

where we have formed three groups. The last group is

$$-\frac{x^2}{b} + \frac{2cx}{b} - \frac{c^2}{b} = \frac{-(x-c)^2}{b} = \frac{-(x - \hbar k_0 t/m)^2}{2\alpha^2 + 2i\hbar t/m}. \tag{2}$$

This is the argument of the second exponential in the desired wave function. The middle group is

$$\frac{2i\alpha^2 k_0 x}{b} - \frac{2cx}{b} = \frac{2(i\alpha^2 k_0 - \hbar k_0 t/m)x}{2\alpha^2 + 2i\hbar t/m}$$

$$= \frac{(i\alpha^2 - \hbar t/m)k_0 x}{\alpha^2 + i\hbar t/m} = \frac{i(\alpha^2 + i\hbar t/m)k_0 x}{\alpha^2 + i\hbar t/m} = ik_0 x \tag{3}$$

which is a portion of the first exponential in the desired wave function. The first group is

$$\begin{aligned}
-\frac{\alpha^2 k_0^2}{2} + \frac{\alpha^4 k_0^2}{b} + \frac{c^2}{b} &= -\frac{\alpha^2 k_0^2}{2} + \frac{\alpha^4 k_0^2}{2\alpha^2 + 2i\hbar t/m} + \frac{\hbar^2 k_0^2 t^2}{m^2(2\alpha^2 + 2i\hbar t/m)} \\
&= -\frac{\alpha^2 k_0^2}{2} + \frac{\alpha^4 k_0^2 m^2}{2\alpha^2 m^2 + 2i\hbar tm} + \frac{\hbar^2 k_0^2 t^2}{2\alpha^2 m^2 + 2i\hbar tm} \\
&= \frac{-\alpha^2 k_0^2(\alpha^2 m^2 + i\hbar tm) + \alpha^4 k_0^2 m^2 + \hbar^2 k_0^2 t^2}{2\alpha^2 m^2 + 2i\hbar tm} \\
&= \frac{-\alpha^4 \cancel{k_0^2} m^2 - i\alpha^2 \hbar k_0^2 tm + \alpha^4 \cancel{k_0^2} m^2 + \hbar^2 k_0^2 t^2}{2\alpha^2 m^2 + 2i\hbar tm} \\
&= \frac{-i\hbar k_0^2 t}{2m}\left(\frac{\alpha^2 m + i\hbar t}{\alpha^2 m + i\hbar t}\right) \\
&= \frac{-i\hbar k_0^2 t}{2m}
\end{aligned} \tag{4}$$

which is the other portion of the first exponential. Adding expressions (3) and (4),

$$ik_0 x - \frac{i\hbar k_0^2 t}{2m} = ik_0\left(x - \frac{\hbar k_0 t}{2m}\right),$$

so in combination with equation (2), all the exponentials in equation (1) may be written

$$\exp\left[ik_0\left(x - \frac{\hbar k_0 t}{2m}\right)\right]\exp\left[\frac{-\left(x - \hbar k_0 t/m\right)^2}{2\alpha^2 + 2i\hbar t/m}\right].$$ Using this in equation (1) yields

$$\psi(x,t) \;=\; \frac{1}{(\pi\alpha^2)^{1/4}}\left(1+\frac{i\hbar t}{m\alpha^2}\right)^{-1/2}\exp\left[ik_0\left(x-\frac{\hbar k_0 t}{2m}\right)\right]\exp\left[\frac{-\left(x\,-\,\hbar k_0 t/m\right)^2}{2\alpha^2\,+\,2i\hbar t/m}\right].$$

Including the $e^{ik_0 x}$ term adds substantially to the algebra required which is why the Gaussian wave function was initially developed without it. The $e^{ik_0\,x}$ term centers the Gaussian wave packet at $k_0 \neq 0$ so may be essential. The algebra is insignificant compared to the concept.

(d)

$$\psi(x,0) \;=\; \frac{1}{(\pi\alpha^2)^{1/4}}(1+0)^{-1/2}\exp\left[ik_0(x-0)\right]\exp\left[\frac{-\left(x-0\right)^2}{2\alpha^2+0}\right]$$

$$=\; \frac{e^{ik_0 x}\,e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}$$

which is the initial distribution, $\psi(x)$. It will often be seen $\psi(x,0) \,=\, \psi(x) \,=\, \dfrac{e^{ip_0 x/\hbar}\,e^{-x^2/\,2\alpha^2}}{(\pi\alpha^2)^{1/4}}$.

(e) This part is similar to problem 7–8 (a) with two exceptions. The first is that the product of the first exponential and its complex conjugate is 1,

$$\exp\left[-ik_0\left(x\,-\,\frac{\hbar k_0 t}{2m}\right)\right]\exp\left[ik_0\left(x\,-\,\frac{\hbar k_0 t}{2m}\right)\right] \;=\; e^0 \;=\; 1\,,$$

so does not affect the final answer. The other is the numerator of the argument of the remaining exponential is a two-term square instead of the simpler x^2 term. All else is identical so

$$|\,\psi(x,t)\,|^{\,2} \;=\; \frac{1}{\alpha\sqrt{\pi}}\left(1+\frac{\hbar^2}{m^2\alpha^4}\,t^2\right)^{-1/2}\exp\left[\frac{-(x\,-\,\hbar k_0 t/m)^2}{\alpha^2\,+\,\dfrac{\hbar^2}{m^2\alpha^2}\,t^2}\right].$$

(f) Uncertainty is the square root of one half the denominator of the argument of the exponential

$$\triangle x \;=\; \triangle x(t) \;=\; \frac{1}{\sqrt{2}}\left(\alpha^2+\frac{\hbar^2}{m^2\alpha^2}\,t^2\right)^{1/2} \;=\; \frac{\alpha}{\sqrt{2}}\left(1+\frac{\hbar^2}{m^2\alpha^4}\,t^2\right)^{1/2}$$

per problem 7–8 (b). The uncertainty is increasing as time advances, or wave packet "spreading" is apparent for a Gaussian wave packet centered at $k \,=\, k_0$.

Appendix D Second Derivative of the Associated Laguerre Function Used for Hydrogen

$$y' \;=\; -\frac{1}{2}\,e^{-x/2}\,x^{(k+1)/2}\,v \;+\; e^{-x/2}\left(\frac{k+1}{2}\right)x^{(k-1)/2}\,v \;+\; e^{-x/2}\,x^{(k+1)/2}\,v'$$

$$\Rightarrow \quad y'' \;=\; \frac{1}{4}\,e^{-x/2}x^{(k+1)/2}\,v - \frac{1}{2}\,e^{-x/2}\left(\frac{k+1}{2}\right)x^{(k-1)/2}\,v - \frac{1}{2}\,e^{-x/2}\,x^{(k+1)/2}\,v'$$

$$- \frac{1}{2}\,e^{-x/2}\left(\frac{k+1}{2}\right)x^{(k-1)/2}\,v \;+\; e^{-x/2}\left(\frac{k+1}{2}\right)\left(\frac{k-1}{2}\right)x^{(k-3)/2}\,v \;+\; e^{-x/2}\left(\frac{k+1}{2}\right)x^{(k-1)/2}\,v'$$

$$- \frac{1}{2}\,e^{-x/2}\,x^{(k+1)/2}\,v' \;+\; e^{-x/2}\left(\frac{k+1}{2}\right)x^{(k-1)/2}\,v' \;+\; e^{-x/2}\,x^{(k+1)/2}\,v''$$

$$= \; e^{-x/2}\Bigg[\frac{1}{4}\,x^{(k+1)/2}\,v \;-\; \frac{1}{2}\left(\frac{k+1}{2x}\right)x^{(k+1)/2}\,v \;-\; \frac{1}{2}\,x^{(k+1)/2}\,v'$$

$$- \frac{1}{2}\left(\frac{k+1}{2x}\right)x^{(k+1)/2}\,v \;+\; \left(\frac{k+1}{2x}\right)\left(\frac{k-1}{2x}\right)x^{(k+1)/2}\,v \;+\; \left(\frac{k+1}{2x}\right)x^{(k+1)/2}\,v'$$

$$- \frac{1}{2}\,x^{(k+1)/2}\,v' \;+\; \left(\frac{k+1}{2x}\right)x^{(k+1)/2}\,v' \;+\; x^{(k+1)/2}\,v''\Bigg]$$

$$= \; e^{-x/2}\,x^{(k+1)/2}\Bigg[\frac{1}{4}\,v \;-\; \frac{1}{2}\left(\frac{k+1}{2x}\right)v \;-\; \frac{1}{2}\,v' \;-\; \frac{1}{2}\left(\frac{k+1}{2x}\right)v$$

$$+ \left(\frac{k+1}{2x}\right)\left(\frac{k-1}{2x}\right)v \;+\; \left(\frac{k+1}{2x}\right)v' \;-\; \frac{1}{2}\,v' \;+\; \left(\frac{k+1}{2x}\right)v' \;+\; v''\Bigg]$$

$$\Rightarrow \quad \left(e^{x/2}x^{-(k+1)/2}\right)y'' \;=\; \frac{1}{4}v - \frac{1}{2}\frac{k+1}{2x}\,v - \frac{1}{2}v' - \frac{1}{2}\frac{k+1}{2x}\,v$$

$$+ \frac{k+1}{2x}\,\frac{k-1}{2x}\,v \;+\; \frac{k+1}{2x}\,v' \;-\; \frac{1}{2}\,v' \;+\; \frac{k+1}{2x}\,v' \;+\; v''.$$

Index