MATHEMATICAL FOUNDATIONS *of* QUANTUM MECHANICS

New Edition

JOHN VON NEUMANN

Edited by NICHOLAS A. WHEELER

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John von Neumann talking shop with visiting scholars during afternoon tea at the Institute for Advanced Study. (Photo by Alfred Eisenstaedt / The LIFE Picture Collection / Getty Images.)

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OF
QUANTUM MECHANICS

by

John von Neumann

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translated from the German by

ROBERT T. BEYER

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Nicholas A. Wheeler

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1 3 5 7 9 10 8 6 4 2

CONTENTS

CHAPTER IV
Deductive Development of the Theory

CHAPTER V
General Considerations

CHAPTER VI
The Measuring Process

TRANSLATOR'S PREFACE

This translation follows closely the text of the original German edition. The translated manuscript has been carefully revised by the author so that the ideas expressed in this volume are his rather than those of the translator, and any deviations from the original text are also due to the author.

The translator wishes to express his deep gratitude to Professor von Neumann for his very considerable efforts in the rendering of the ideas of the original volume into a translation which would convey the same meanings.

Robert T. Beyer

Providence, R. I.
December, 1949

PREFACE TO THIS NEW EDITION

This book is the realization of my long-held intention to someday use the resources of TEX to produce a more easily read version of Robert T. Beyer's authorized English translation (Princeton University Press, 1955) of John von Neumann's classic *Mathematische Grundlagen der Quantenmechanik* (Springer, 1932).

I have endeavored to correct typographic errors that crept into the text and equations in the Beyer translation (a few of which were copied from the German original) and to adjust some of the transliterated sentences so that they read more easily and their meaning is easier to comprehend. But in all other respects I have adhered as closely as possible to the Beyer translation, which von Neumann reviewed and endorsed. Von Neumann wrote about his own extensive contributions to the Beyer translation in a letter (3 October 1949) addressed to Hayward Cirker, founding president of Dover Publications; that letter is reproduced on pages 91–92 of Miklós Rédei's *John von Neumann: Selected Letters* (2005).

The glorified typewriter (VariTyper, circa 1945) that was used to prepare the Beyer translation provided relatively few typographic resources, with the consequences that some of the equations are very awkwardly displayed and it is often not possible to know—except from context—the mathematical nature of the object to which a given symbol refers. Additionally, some of the symbols employed (for example, the German Gothic $\mathfrak{R}$,$\mathfrak{N}$ and certain Roman fonts) are difficult to distinguish in small type sizes. To avoid such difficulties, I have adopted the following invariable conventions:

- functions are denoted $f, g, h, \ldots$
- linear manifolds are denoted $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, $\ldots$, $\mathcal{R}$, $\mathcal{S}$, $\ldots$, $\mathcal{M}$, $\mathcal{N}$, $\ldots$
- elements of linear manifolds are denoted $\phi, \psi, \ldots$
- physical quantities are denoted $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$, $\ldots$
- operators are denoted A, B, C, $\ldots$, E, $\ldots$, P, Q, $\ldots$, U, V
- matrices are denoted $\mathbb{A}, \mathbb{B}, \mathbb{C}, \ldots, \mathbb{P}, \mathbb{Q}, \ldots$
- 3-vectors are denoted $\boldsymbol{A}, \boldsymbol{x}, \boldsymbol{y}, \ldots$

Where von Neumann invariably writes $h/2\pi$ I employ Dirac's (now universal) symbol $\hbar$.

It is my impression that von Neumann's monograph—which is today, after more than eighty years, more frequently cited than ever before—is perhaps more frequently cited than actually read, and is my certain knowledge that it contains

treasures and provides valuable insights that are too seldom appreciated. It is my hope that this edition (to which I have attached a subject index, absent from previous editions) will facilitate—and perhaps inspire—the work of a new generation of physicists.

I thank especially Marina von Neumann Whitman, Freeman Dyson and Peter Renz, and also Jeffrey Bub, Auletta Gennaro, David Griffiths, David Mermin, Miklós Rédei, Robert Rohmer, Maximilian Schlosshauer, Silvan Schweber, Veeravalli Varadarajan, Thomas Wieting and Wojciech Zurek for encouragement in this undertaking. I am greatly indebted to William Bialek of the Princeton physics faculty for his initiative, and to Vickie Kearn for her expert editorial supervision. It is with special pleasure that I thank Linda Maddux, Reed College science librarian, for assistance in preparation of the list of works cited, Paul Forman and (especially) Harvey Leff for editorial advice and assistance. The project would never have come to completion but for the wise counsel and ever-tactful patience of my attorney, William Drew, of Elliott, Ostrander & Preston, P.C. And I am—as are we all—deeply indebted to Donald Knuth for his invention of TEX.

This volume was written in Plain TEX, as implemented by Textures, an application developed here in Portland by Blue Sky Research. Textures runs, however, only on OSX systems old enough to provide Classic Mode, so the work was done on a treasured antique of an iMac.

Nicholas Wheeler

Reed College
June, 2014

By way of a

FOREWORD

In 1933, John von Neumann [28 December 1903–8 February 1957] became (together with Albert Einstein and Oswald Veblin) a member of the founding faculty (and Kurt Gödel a visiting member) of the Institute for Advanced Study, where he remained for the remainder of his life. The distinguished author of the following commemorative essay was a member in 1949 and 1952–1954, and had then an opportunity to become personally acquainted with von Neumann. The essay was taken (with permission) from volume 64, number 3, part 2 (May 1958) pages 95–99 of the Bulletin of the American Mathematical Society, the 129-page entirety of which is given over to expert surveys of von Neumann's contributions to eight different subject areas.

VON NEUMANN'S CONTRIBUTIONS TO QUANTUM THEORY

LÉON VAN HOVE

That von Neumann has been "par excellence" the mathematician of quantum mechanics is as obvious to every physicist now as it was a quarter of a century ago. Quantum mechanics was very fortunate indeed to attract, in the very first years after its discovery in 1925, the interest of a mathematical genius of von Neumann's stature. As a result, the mathematical framework of the theory was developed and the formal aspects of its entirely novel rules of interpretation were analyzed by one single man in two years time (1927–1929). Conversely, one could almost say in reciprocity, quantum mechanics introduced von Neumann into a field of mathematical investigation, operator theory, in which he achieved some of his most prominent successes.

Von Neumann's major contributions to quantum mechanics are his development of the mathematical framework of the theory and his formal study of quantum statistics, quantum measuring processes and their interrelations. Whereas the latter study was essentially complete in 1927 (except for the quantum ergodic theorem of 1929) the work on the mathematical foundations of quantum mechanics came to its culmination in 1929 with the spectral theorem

for hypermaximal symmetric operators in Hilbert space. In the next two paragraphs we shall discuss these major contributions.

The mathematical framework of quantum theory. By the time von Neumann started his investigations on the formal framework of quantum mechanics this theory was known in two different mathematical formulations: the "matrix mechanics" of Heisenberg, Born and Jordan, and the "wave mechanics" of Schrödinger. The mathematical equivalence of these formulations had been established by Schrödinger, and they had both been embedded as special cases in a general formalism, often called the "transformation theory," developed by Dirac and Jordan. This formalism, however, was rather clumsy and it was hampered by its reliance upon ill-defined mathematical objects, the famous delta-functions of Dirac and their derivatives. Although von Neumann himself attempted at first, in collaboration with Hilbert and Nordheim [1], to edify the formalism along similar lines, he soon realized that a much more natural framework was provided by the abstract, axiomatic theory of Hilbert spaces and their linear operators [2]. This mathematical formulation of quantum mechanics, whereby states of the physical system are described by Hilbert space vectors and measurable quantities by Hermitian operators acting upon them, has been very successful indeed. Unchanged in its essentials it has survived the two great extensions which quantum theory was to undergo soon: the relativistic quantum mechanics of particles (Dirac equation) and the quantum theory of fields.

One might of course remark that Dirac's delta functions and their derivatives, although poorly defined at the time of their introduction, have been recognized since as bona fide mathematical entities in L. Schwartz' theory of distributions. This is quite true and moreover these functions have been used continually by physicists throughout the development of quantum theory, in particular in the last two decades for the study of scattering processes and of quantized fields. Delta functions have established themselves as the natural tool whenever operators with continuous spectra are to be considered. This does not affect in any way, however, the fact that the axiomatically defined separable Hilbert space is the suitable framework for the quantum-mechanical formalism as we know it today, and the recognition of this fact we owe to von Neumann.

An essential feature of the Hilbert space formulation of quantum theory is that the most important physical quantities (such as position, momentum or energy) are represented by unbounded Hermitian operators. Since the theoretical prediction of measurements makes essential use of the spectral resolution of the operators representing the physical quantities, von Neumann was, in his very first invetigation [2], faced with the problem of extending to the unbounded case the known spectral theory of bounded Hermitian operators. By 1929 he had brought this problem to a complete solution [3]. He introduced the all-important concept of hypermaximal symmetric operator, being the most general Hermitian operator with a spectral resolution. This work, the results of which were reached independently by M. H. Stone [4], was for von Neumann

the start of a long series of investigations on linear operators in Hilbert space.

Still another contribution of von Neumann to the mathematical foundation of quantum theory is worth mentioning here. He established the important theorem that (in the irreducible case and after a suitable reformulation) the canonical commutation rules $Q_j P_\ell - P_\ell Q_j = \hbar i \delta_{j\ell}$ determine the operators $Q_1, \ldots, Q_n, P_1, \ldots, P_n$ uniquely except for an arbitrary transformation [5]. Although rarely quoted as such, this theorem, which was already known to Dirac and Stone [6], is really fundamental for the understanding of many quantum-mechanical investigations where the theoretical analysis is exclusively based on the canonical commutation rules or in the equivalent field-theoretical form

$$A_j A_\ell^* - A_\ell^* A_j = \hbar \delta_{j\ell}, \qquad 2^{\frac{1}{2}} A_j = P_j - iQ_j$$

Statistical aspects of quantum theory. In the course of his formulation of quantum mechanics in terms of vectors and operators of Hilbert space von Neumann also gave in complete generality the basic statistical rule of interpretation of the theory. This rule concerns the result of the measurement of a given physical quantity on a system in a given quantum state and expresses its probability distribution by means of a simple and now completely familiar formula involving the vector representing the state and the spectral resolution of the operator which represents the physical quantity [2]. This rule, originally proposed by Born in 1926, was for von Neumann the starting point of a mathematical analysis of quantum mechanics in entirely probabilistic terms. The analysis, carried out in a paper of 1927 [7], introduced the concept of statistical matrix for the description of an ensemble of systems which are not necessarily all in the same quantum state. The statistical matrix (now often called ρ-matrix although von Neumann's notation was U) has become one of the major tools of quantum statistics and it is through this contribution that von Neumann's name became familiar to even the least mathematically minded physicists.

In the same paper von Neumann also investigates a problem which is still now the subject of much discussion; viz., the theoretical description of the quantum-mechanical measuring process and of the non-causal elements which it involves. Mathematically speaking von Neumann's study of this delicate question is quite elegant. It provides a clear-cut formal framework for the numerous investigations which were needed to clarify physically the all-important implications of quantum phenomena for the nature of physical measurements, the most important of which is Neils Bohr's concept of complementarity.

The results of the paper just discussed were immediately used by the author to lay the foundation for quantum thermodynamics [8]. He gave the quantum analogue

$$S = -k \operatorname{tr}(\rho \ln \rho), \qquad \rho \text{ denotes a statistical matrix}$$

of the well known classical formula for the entropy

$$S = -k \int f \ln f \, d\omega, \qquad f \text{ denotes a distribution function in phase space.}$$

He further wrote down the density matrix for a canonical ensemble at temperature T:

$$\rho = Z^{-1} \exp(-H/kT), \qquad Z = \mathrm{tr}\big[\exp(-H/kT)\big],$$

H being the Hamiltonian operator. Two years later von Neumann came back to quantum thermodynamics with a contribution to a much more difficult problem: the formulation and proof of an ergodic theorem for quantum systems [9]. The basic principle of this work is to define quantum analogues of cells in phase space by considering sets of quantum states for which all macroscopic quantities have given values with a certain inaccuracy. One further considers the unitary transformation u relating these quantum states to the eigenstates of the Hamiltonian. The ergodicity is then established for "almost every" value of the transformation u. Although the latter restriction is a rather unsatisfactory one from a physical standpont, one must consider von Neumann's ergodic theorem as one of the very few important contributions to a most difficult subject which even now is far from complete clarification.

Most of the work we have briefly reviewed has been republished by the author, in greatly expanded form, as a book which rapidly became and still is the standard work on the mathematical foundations of quantum mechanics [10], [and of which the present volume is an English translation]. Von Neumann devoted in his book considerable attention to a point which had not been discussed in the 1927 papers and which was later the subject of much controversy. It is the question of the possible existence of "hidden variables," the consideration of which would eliminate the non-causal element involved in the measurement process. Von Neumann could show that hidden parameters with this property cannot exist if the basic structure of quantum theory is retained. Although he mentioned the latter restriction explicitly,† his result is often quoted without due reference to it, a fact which sometimes gave rise to unjustified criticism in the many discussions devoted through the years to the possibility of an entirely deterministic reformulation of quantum theory.

Other contributions. As von Neumann's complete bibilography will reveal, he wrote quite a few other papers on quantum mechanics, often in collaboration with physicists, especially with Wigner. Most of these papers deal with technical matters and the importance of the major contributions discussed above is so eminent that, in comparison, the other papers' scope is modest. There is only one broad subject which we would like to mention here, because von Neumann, obviously giving it considerable thought, returned to it several times in 1934 and 1936 (in collaboration with Jordan, Wigner and Garrett Birkhoff). It is the question of the algebraic and logical structure of quantum mechanics, where the hope has existed to reach through abstract analysis possible generalizations of the accepted theory. Nobody knows whether such a hope is justified, but it is undoubtedly a natural one and it has appealed to many other people, giving one more example of the power and originality of von Neumann's thinking.

† See, *e.g.*, [10], p. 109, line 17 *et seq* [or below: p. 132, paragraph 3].

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A "von Neumann Days" Symposium *took place on 3–7 May 2010 at Brown University's Center for Computational Molcular Biology. Remarks prepared for presentation on that occasion by Freeman Dyson—who was a member of the Institute for Advanced Study in 1948–1949 and became there a tenured faculty colleague of von Neumann in 1953—were subsequently published as "A walk through Johnny von Neumann's garden" (Notices of the AMS* ***60****, 155–161 (2013)), from which the following excerpt has (with permission) been taken.*

VON NEUMANN WORK RELATED TO QUANTUM THEORY

FREEMAN DYSON

During his Berlin years, Johnny made frequent visits to Göttingen, where Heisenberg had recently invented quantum mechanics and Hilbert was the presiding mathematician. Hilbert was intensely interested in quantum mechanics and encouraged collaboration between mathematicians and physicists. From the point of view of Hilbert, quantum mechanics was a mess. Heisenberg had no use for rigorous mathematics and no wish to learn it. Dirac made free use of his

famous delta-function, which was defined by a mathematical absurdity, being infinite at a single point and zero everywhere else. When Hilbert remarked to Dirac that the delta-function could lead to mathematical contradictions, Dirac replied, "Did I get into mathematical contradictions?" Dirac knew that his delta-function was a good tool for calculating quantum processes, and that was all that he needed. Twenty years later, Laurent Schwartz provided a rigorous basis for the delta-function and proved that Dirac was right. Meanwhile, Johnny worked with Hilbert and published a series of papers cleaning up the mess. In 1932 he published the book *Mathematical Foundations of Quantum Mechanics* [9], which occupies a substantial piece of his garden.

Johnny's book was the first exposition of quantum mechanics that made the theory mathematically respectable. The concepts were rigorously defined and the consequences rigorously deduced. Much of the work was original, especially the chapters on quantum statistics and the theory of measurement. I read the book in 1946 when I was still a pure mathematician but already intending to switch my attention to physics. I found it enormously helpful. It gave me what I needed, a mathematically precise statement of the theory, explaining the fine points that the physicists had been too sloppy to mention. From that book I learned most of what I know about quantum mechanics. But then, after I had made the transition to physics and had begun to read the current physics journals, I was surprised to discover that nobody in the physics journals ever referred to Johnny's book. So far as the physicists were concerned, Johnny did not exist. Of course, their ignorance of Johnny's work was partly a problem of language. The book was in German, and the first English translation was only published in 1955. But I think even if the book had been available in English, the physicists of the 1940s would not have found it interesting. That was a time when the culture of physics and the culture of mathematics were most widely separated. The culture of physics was dominated by people like Oppenheimer who made friends with poets and art historians but not with pure mathematicians. The culture of mathematics was dominated by the Borbaki cabal, which tried to expunge from mathematics everything that was not purely abstract. The gap between physics and mathematics was as wide as the gap between science and the humanities described by C. P. Snow in his famous lecture on the two cultures. Johnny was one of the very few people who were at home in all four cultures: in physics and mathematics, but also in science and the humanities.

The central concept in Johnny's version of quantum mechanics is the abstract Hilbert space. Hilbert space is the infinite-dimensional space in which quantum states are vectors and observable quantities are linear operators. Hilbert had defined and explored Hilbert space long before quantum mechanics made it useful. The unexpected usefulness of Hilbert space arises from the fact that the equations of quantum mechanics are exactly linear. The operators form a linear algebra, and the states can be arranged in multiplets defined by linear representations of the algebra. Johnny liked to formulate physical problems in abstract and general language, so he formulated quantum mechanics as a theory

of rings of linear operators in Hilbert space. A ring means a set of operators that can be added or subtracted or multiplied together but not divided. Any physical system obeying the rules of quantum mechanics can be described by a ring of operators. Johnny began studying rings of operators to find out how many different types of quantum systems could exist.

After Johnny published his quantum mechanics book, he continued for several years to develop the theory of rings of operators. The third volume of his collected works consists entirely of papers on rings of operators. He published seven long papers with a total of more than five hundred pages. I will not discuss these monumental papers this morning. They contain Johnny's deepest work as a pure mathematician. He proved that every ring of operators is a direct product of irreducible rings that he called factors. He discovered that there are five types of factor, of which only two were previously known. Each of the types has unique and unexpected properties. Exploring the ocean of rings of operators, he found new continents that he had no time to survey in detail. He left the study of the three new types of factor unfinished. He intended one day to publish a grand synthesis of his work on rings of operators. The grand synthesis remains an unwritten masterpiece, like the eighth symphony of Sibelius.

The quantum mechanics book is the last item on my list of flowers that Johnny published in German. It was published in 1932 when he was dividing his time equally between Berlin and Princeton. In the same year he began writing papers in English. One of his first papers to appear in English was "Proof of the quasi-ergodic hypothesis" [10], which he published in the *Proceedings of the National Academy of Sciences* to make sure that American mathematicians would read it. This paper solved an important problem in classical mechanics using the same concept of Hilbert space that he had used to solve problems in quantum mechanics. A classical dynamical system is said to be ergodic if after we put it into an initial state and then leave it alone for an infinite time, it comes arbitrarily close to any final state with probability independent of the initial state. Johnny proved that under certain clearly specified conditions, a system is ergodic if and only if there exist no constants of the motion. A constant of the motion means a quantity depending on the state of the system which does not change as the system moves forward in time. Johnny's theorem provides a firm mathematical basis for the assumptions that are customarily made by physicists using classical statistical mechanics. Translated into the sloppy language used by physicists, the theorem says that the time-average of any single trajectory of the system over a long time is equal to the statistical average of all trajectories. Even more sloppily, physicists say that time-averages are equal to ensemble averages, and we use the word ensemble to mean the set of all states of the system.

One of the American mathematicians who read Johnny's paper in the *Proceedings of the National Academy of Sciences* was Garrett Birkhoff. Garrett was the son of George Birkhoff, and both father and son were famous mathematicians. Garrett and Johnny became close friends, and Garrett came

to Princeton for frequent visits. After Johnny died, Garrett wrote a memoir about the work that Johnny did in the 1930s. Here is a sentence from Garrett's memoir: "Anyone wishing to get an unforgettable impression of the razor edge of von Neumann's mind need merely try to pursue this chain of exact reasoning for himself, realizing that often five pages of it were written down before breakfast, seated at a living room writing-table in a bathrobe."

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MATHEMATICAL FOUNDATIONS OF QUANTUM MECHANICS

INTRODUCTION

The object of this book is to present the new quantum mechanics in a unified representation which, so far as it is possible and useful, is mathematically rigorous. This new quantum mechanics has in recent years achieved in its essential parts what is presumably a definitive form: the so-called "transformation theory." Therefore the principal emphasis shall be placed on the general and fundamental questions which have arisen in connection with this theory. In particular, the difficult problems of interpretation, many of which are even now not fully resolved, will be investigated in detail. In this connection, the relation of quantum mechanics to statistics and to the classical statistical mechanics is of special importance. However, we shall as a rule omit any discussion of the application of quantum mechanical methods to particular problems, as well as any discussion of special theories derived from the general theory—at least so far as this is possible without endangering the understanding of general relationships. This seems the more advisable since several excellent treatments of these problems are either in print or in process of publication.[1]

On the other hand, a presentation of the mathematical tools necessary for the purposes of this theory will be given, *i.e.*, a theory of Hilbert space and the so-called Hermitian operators. For this end, an accurate introduction to unbounded operators is also necessary, *i.e.*, an extension of the theory beyond its classical limits (developed by D. Hilbert and E. Hellinger, F. Riesz, E. Schmidt, O. Toeplitz). The following may be said regarding the method employed in this mode of treatment: as a rule, calculations should be performed with the operators themselves (which represent physical quantities) and not with the matrices, which, after the introduction of a (special and arbitrary) coordinate system in Hilbert space, result from them. This "coordinate free," *i.e.*, invariant, method, with its strongly geometrical language, possesses noticeable formal advantages.

[1] There are, among others, the following comprehensive treatments: Sommerfeld, Supplement to the 4th edition of *Atombau und Spectrallinien*, Braunschweig, 1928; Weyl, *The Theory of Groups and Quantum Mechanics* (translated by H. P. Robertson), London, 1931; Frenkel, *Wave Mechanics*, Oxford, 1932; Born and Jordan, *Elementare Quantenmechanik*, Berlin, 1930; Dirac, *The Principles of Quantum Mechanics*, 2nd edition, Oxford, 1936.

Dirac, in several papers, as well as in his recently published book,[2] has given a representation of quantum mechanics which is scarcely to be surpassed in brevity and elegance, and which is at the same time of invariant character. It is therefore perhaps fitting to advance a few arguments on behalf of our method, which deviates considerably from that of Dirac.

The method of Dirac, mentioned above (and this is overlooked today in a great part of the quantum mechanical literature, because of the clarity and elegance of the theory) in no way satisfies the requirements of mathematical rigor—not even if these are reduced in a natural and proper fashion to the extent common elsewhere in theoretical physics. For example, the method adheres to the fiction that every self-adjoint operator can be put in diagonal form. In the case of those operators for which this is not actually the case, this requires the introduction of "improper" functions with self-contradictory properties. The insertion of such a mathematical "fiction" is frequently necessary in Dirac's approach, even though the problem at hand is merely one of calculating numerically the result of a clearly defined experiment. There would be no objection here if these concepts, which cannot be incorporated into the present-day framework of analysis, were intrinsically necessary for the physical theory. Thus, as Newtonian mechanics first brought about the development of the infinitesimal calculus, which, in its original form, was undoubtedly not self-consistent, so quantum mechanics might suggest a new structure for our "analysis of infinitely many variables"—*i.e.*, the mathematical technique would have to be changed, and not the physical theory. But this is by no means the case. It should rather be pointed out that the quantum mechanical "Transformation theory" can be established in a manner which is just as clear and unified, but which is also without mathematical objections. It should be emphasized that the correct structure need not consist in a mathematical refinement and explanation of the Dirac method, but rather that it requires a procedure differing from the very beginning, namely, the reliance on the Hilbert theory of operators.

In the analysis of fundamental questions, it will be shown how the statistical formulas of quantum mechanics can be derived from a few qualitative, basic assumptions. Furthermore, there will be a detailed discussion of the problem as to whether it is possible to trace the statistical character of quantum mechanics to an ambiguity (*i.e.*, incompleteness) in our description of nature. Indeed, such an interpretation would be a natural concomitant of the general principle that every probability statement arises from the incompleteness of our knowledge. This explanation "by hidden parameters," as well as another, related to it, which ascribes the "hidden parameter" to the observer and not to the observed system, has been proposed more than once. However, it will appear that this can scarcely succeed in a satisfactory way, or more precisely, such an explanation

[2] See Proc. Roy. Soc. London, **109** (1925) and subsequent issues, especially **113** (1926). Independently of Dirac, P. Jordan, (Z. Physik **40** (1926)) and F. London (Z. Physik **40** (1926)) gave similar foundations for the theory.

is incompatible with certain qualitative fundamental postulates of quantum mechanics.[3]

The relation of quantum statistics to thermodynamics is also considered. A closer investigation shows that the well-known difficulties of classical mechanics, which are related to the "disorder" assumptions necessary for the foundations of thermodynamics, can be eliminated here.[4]

[3] See **IV** and **VI.3**

[4] See **V**.

CHAPTER I

INTRODUCTORY CONSIDERATIONS

1. THE ORIGIN OF THE TRANSFORMATION THEORY

This is not the place to point out the great success which the quantum theory attained in the period from 1900 to 1925, a development which was dominated by the names of Planck, Einstein and Bohr.[5] At the end of this period of development, it was clear beyond doubt that all elementary processes, *i.e.,* all occurrences of an atomic or molecular order of magnitude, obey the "discontinuous" laws of quanta. There were also available quantitative, quantum theoretical methods in almost all directions, which for the most part yielded results in good or at least fair agreement with experiment. And, what was fundamentally of greater significance, was that the general opinion in theoretical physics had accepted the idea that the principle of continuity ("*natura non facit saltus*"), prevailing in the macroscopic world, is merely simulated by an averaging process in a world which in truth is discontinuous by its very nature. This simulation is such that a man generally perceives the sum of many billions of elementary processes simultaneously, so that the leveling law of large numbers completely obscures the real nature of the individual processes.

Nevertheless, up to the time mentioned there existed no mathematical-physical system of quantum theory which would have embodied everything known up to that time in a unified structure, let alone one which could have

[5] Its chief stages were: The discovery of the quantum laws by Planck for the case of black body radiation (see Planck's presentation in his book, *Theory of Heat Radiation* (translated by M. Masius), Philadelphia, 1914); the hypothesis of the corpuscular nature of light (theory of light quanta) by Einstein (Ann. Phys. **17** (1905)), wherein the first example was given of the dual form: wave-corpuscle, which, we know today, dominates all of microscopic physics; the application of these two sets of rules to the atomic model by Bohr (Phil. Mag. **26** (1913); Z. Physik **6** (1920)).

exhibited the monumental solidity of the system of mechanics, electrodynamics and relativity theory (which system was disrupted by the quantum phenomena). In spite of the claim of quantum theory to universality, which had evidently been vindicated, there was lacking the necessary formal and conceptual instrument; there was a conglomeration of essentially different, independent, heterogeneous and partially contradictory fragments. The most striking points in this respect were: the correspondence principle, belonging half to classical mechanics and electrodynamics (but which played a decisive role in the final clarification of the problem); the self-contradictory dual nature of light (wave and corpuscular, cf. Note 5 and Note 148); and finally, the existence of unquantized (aperiodic) and quantized (periodic or multiply periodic) motions.[6]

The year 1925 brought the resolution. A procedure initiated by Heisenberg was developed by Born, Heisenberg, Jordan, and a little later by Dirac, into a new system of quantum theory, the first complete system of quantum theory which physics has possessed. A little later Schrödinger developed the "wave mechanics" from an entirely different starting point. This accomplished the same ends, and soon proved to be equivalent to the Heisenberg, Born, Jordan and Dirac system (at least in a mathematical sense, cf. **3** & **4** below).[7] On the basis of the Born statistical interpretation of the quantum theoretical description[8] of nature, it was possible for Dirac and Jordan[9] to join the two theories into one, the "transformation theory," in which they make possible a grasp of physical problems which is especially simple mathematically.

It should be mentioned (although it does not belong to our particular subject) that after Goudsmit and Uhlenbeck had discovered the magnetic moment and the spin of the electron, almost all the difficulties of the earlier quantum theory disappeared, so that today we are in possession of a mechanical system which is almost entirely satisfactory. To be sure, the great unity with electrodynamics and relativity theory mentioned earlier has not yet been recovered, but at least there is a mechanics which is universally valid, where the quantum laws fit in a natural and necessary manner, and which explains

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[6] The quantum laws (added to the laws of mechanics) for multiply periodic motions were first developed by Epstein-Sommerfeld [see, for example, Sommerfeld, *Atombau und Spectrallinien*, Braunscheig (1924)]. On the other hand, it was ascertained that a freely moving mass point of a planet on an hyperbolic orbit (in contrast to those on elliptical orbits) is "unquantized." The reader will find a complete treatment of this phase of quantum theory in the books by Reiche, *The Quantum Theory* (translated by H. S. Hatfield & H. L. Brose), New York, 1922; and Landé, *Fortschritte der Quantentheorie*, Dresden, 1922.

[7] This was proved by Schrödinger, Ann Physik **79** (1926).

[8] Z. Physik **37** (1926).

[9] See the articles mentioned in Note 2. Schrödinger's papers have been published in book form, *Collected Papers on Wave Mechanics* (translated by J. F. Shearer & W. M. Deans), London, 1928.

satisfactorily the majority of our experiments.[10]

2. THE ORIGINAL FORMULATIONS OF QUANTUM MECHANICS

In order to obtain a preliminary view of the problem, let us set forth briefly the basic structure of the Heisenberg-Born-Jordan "matrix mechanics" and the Schrödinger "wave mechanics."

In both theories, a classical mechanical problem is initially proposed, which is characterized by a Hamiltonian function $H(q_1, \ldots, q_k, p_1, \ldots, p_k)$. (This means the following, as may be found in greater detail in textbooks of mechanics: Let the system have k degrees of freedom, *i.e.,* let its existing state be determined by giving that numerical values of k coordinates $q_1, \ldots, q_k$. The energy is a given function of the coordinates and their time derivatives:

$$E = L(q_1, \ldots, q_k, \dot{q}_1, \ldots, \dot{q}_k)$$

and, as a rule, is a quadratic function of the derivatives $\dot{q}_1, \ldots, \dot{q}_k$. The "conjugate momenta" $p_1, \ldots, p_k$ of the coordinates $q_1, \ldots, q_k$ are introduced by the relations

$$p_1 = \frac{\partial L}{\partial \dot{q}_1}, \ \ldots, \ p_k = \frac{\partial L}{\partial \dot{q}_k}$$

In the case of the above assumption on L, these depend linearly on the $q_1, \ldots, q_k$. If need be, we can eliminate the $\dot{q}_1, \ldots, \dot{q}_k$ from L by use of the $p_1, \ldots, p_k$, so that

$$E = L(q_1, \ldots, q_k, \dot{q}_1, \ldots, \dot{q}_k) = H(q_1, \ldots, q_k, p_1, \ldots, p_k)$$

(This H is the Hamiltonian function.) In both theories, we must now learn as much as possible from this Hamiltonian function about the true, *i.e.,* quantum mechanical, behavior of the system. Primarily, therefore, we must determine[11]

[10] The present state of affairs may be described this way, that the theory, so far as it deals with individual electrons or with electronic shells of atoms or molecules, is entirely successful, as it is also whenever it deals with electrostatic forces and with electromagnetic processes connected with the production, transmission and transformation of light. On the other hand, in problems of the atomic nucleus, and in all attempts to develop a general and relativistic theory of electromagnetism, in spite of noteworthy partial successes, the theory seems to lead to great difficulties, which apparently cannot be overcome without the introduction of wholly new ideas.

[11] Motion, according to classical mechanics, is determined (as is well known) by the Hamiltonian function, since it gives rise to the equations of motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \quad : \quad i = 1, 2, \ldots, k$$

Before the discovery of quantum mechanics, the attempt was made to explain the quantum phenomena, while retaining these equations of motion, by the

the possible energy levels, then find out the corresponding "stationary states," and calculate the "transition probabilities," etc.[12]

The directions which the matrix theory gives for the solution of this problem run as follows: We seek a system of $2k$ matrices $\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k$,[13] which in the first place satisfy the relations

$$\left.\begin{aligned} \mathbb{Q}_m\mathbb{Q}_n - \mathbb{Q}_n\mathbb{Q}_m &= \mathbb{O} \\ \mathbb{P}_m\,\mathbb{P}_n - \mathbb{P}_n\,\mathbb{P}_m &= \mathbb{O} \\ \mathbb{P}_m\,\mathbb{Q}_n - \mathbb{Q}_n\,\mathbb{P}_m &= \delta_{mn}\tfrac{h}{2\pi i}\mathbb{I} \end{aligned}\right\} \quad (m, n = 1, 2, \ldots, k)$$

and for which, in the second place, the matrix

$$\mathbb{W} = H(\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k)$$

becomes a diagonal matrix. (We shall not go into the details here of the origin of these equations, especially the first group, the so-called "commutation rules" which govern the whole non-commutative matrix calculus of this theory. The reader will find exhaustive treatments of this subject in the works cited in Note 1. The quantity h $[= 2\pi\hbar]$ is Planck's constant. The diagonal elements of $\mathbb{W}$, say

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formulation of supplementary quantum conditions (see Note 6). For each set of values of $q_1, \ldots, q_k, p_1, \ldots, p_k$, given at time $t = 0$, the equations of motion determined the further time variation, or "orbit," of the system in the $2k$ dimensional "phase space" $q_1, \ldots, q_k, p_1, \ldots, p_k$. Any additional condition, therefore, results in a limitation of all possible initial values or orbits to a certain discrete set. (Then, corresponding to the few admissible orbits, there is only a smaller number of possible energy levels.) Even though quantum mechanics has broken completely with this method, it is nevertheless clear from the outset that the Hamiltonian function must still play a great role in it. Indeed, common experience proves the validity of the Bohr correspondence principle, which asserts that the quantum theory must give results in agreement with those of classical mechanics in the so-called limiting case of large quantum numbers.

[12] The three latter concepts are taken from the old quantum theory developed principally by N. Bohr. Later we shall analyze these ideas in detail from the point of view of quantum mechanics. See the Dirac theory of radiation given in **III.6**. Their historical development can be followed in Bohr's papers on the structure of the atom, published from 1913 to 1916.

[13] As a more detailed analysis would show, this is a problem of infinite matrices. We shall not go farther here into the properties of such matrices, since we shall consider them thoroughly later on. For the moment it suffices that the formal algebraic calculation with these matrices is to be understood in the sense of the known rules of matrix addition and multiplication. By $\mathbb{O}$ and $\mathbb{I}$ we mean the null matrix and the unit matrix respectively (with all elements identically zero, and with elements equal to 1 on the main diagonal and zero everywhere else, respectively).

$w_1, w_2, \ldots$ are then the different allowed energy levels of the system. The elements of the matrices $\mathbb{Q}_1, \ldots, \mathbb{Q}_k$—$q^{(1)}_{mn}, \ldots, q^{(k)}_{mn}$—determine in a certain way the transition probabilities of the system (from the m^{th} state with energy w_m to the n^{th} state with energy w_n, $w_m > w_n$) and the radiation thereby emitted.

In addition, it should be noted that the matrix

$$\mathbb{W} = H(\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k)$$

is not completely determined by the $\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k$ and the classical Hamiltonian function

$$H(q_1, \ldots, q_k, p_1, \ldots, p_k)$$

inasmuch as the $\mathbb{Q}_i$ and $\mathbb{P}_i$ do not all commute with one another (in multiplication), while it would be meaningless to distinguish between say $p_1 q_1$ and $q_1 p_1$ for $H(q_1, \ldots, q_k, p_1, \ldots, p_k)$ in the classical mechanical sense. We must therefore determine the order of the variables q_i and p_i in the terms of H, beyond the classical meaning of this expression. This process has not been carried out with complete generality, but the appropriate arrangements are known for the most important special cases. (In the simplest case, whenever the system under investigation consists of particles, and therefore has $k = 3\nu$ coordinates $q_1, \ldots, q_{3\nu}$—such that, e.g., $q_{3\mu-2}, q_{3\mu-1}, q_{3\mu}$ are the three cartesian coordinates of the μ^{th} particle, $\mu = 1, \ldots, \nu$—in which the interaction of these particles is given by a potential energy $V(q_1, \ldots, q_{3\nu})$, there is no such doubt. The classical Hamiltonian is then

$$H(q_1, \ldots, q_{3\nu}, p_1, \ldots, p_{3\nu}) = \sum_{\mu=1}^{\nu} \frac{1}{2m_\mu}(p^2_{3\mu-2} + p^2_{3\mu-1} + p^2_{3\mu}) + V(q_1, \ldots, q_{3\nu})$$

where m_μ is the mass of the μ^{th} particle, and $p_{3\mu-2}, p_{3\mu-1}, p_{3\mu}$ are the components of its momentum. What this means after the substitution of the matrices

$$\mathbb{Q}_1, \ldots, \mathbb{Q}_{3\nu}, \mathbb{P}_1, \ldots, \mathbb{P}_{3\nu}$$

is perfectly clear; in particular, the potential energy introduces no difficulties, since all the $\mathbb{Q}_1, \ldots, \mathbb{Q}_{3\nu}$ commute with each other.) It is important that only Hermitian matrices be permitted, *i.e.*, such matrices $\mathbb{A} = \{a_{mn}\}$, for which $a_{mn} = \overline{a_{nm}}$ holds identically (the elements a_{mn} may be complex!). Therefore

$$H(\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k)$$

must be Hermitian, whenever all the $\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k$ are such. This involves a certain restriction in the problem of the order of the factors which was mentioned above. However, the restriction is not sufficient to determine the

$H(\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k)$ uniquely from the classical $H(q_1, \ldots, q_k, p_1, \ldots, p_k)$.[14]

On the other hand, the directions of wave mechanics are the following: First we form the Hamiltonian $H(q_1, \ldots, q_k, p_1, \ldots, p_k)$ and then the differential equation

$$H(q_1, \ldots, q_k, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}, \ldots, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_k})\psi(q_1, \ldots, q_k) = \lambda\psi(q_1, \ldots, q_k)$$

for an arbitrary function $\psi(q_1, \ldots, q_k)$ in the configuration space of the system (and not the phase space, *i.e.*, the $p_1, \ldots, p_k$ do not enter into ψ). In this way,

$$H(q_1, \ldots, q_k, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}, \ldots, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_k})$$

is interpreted simply as a functional operator. For example, this operator in the case mentioned above,

$$H(q_1, \ldots, q_{3\nu}, p_1, \ldots, p_{3\nu}) = \sum_{\mu=1}^{\nu} \frac{1}{2m_\mu}(p_{3\mu-2}^2 + p_{3\mu-1}^2 + p_{3\mu}^2) + V(q_1, \ldots, q_{3\nu})$$

transforms the function $\psi(q_1, \ldots, q_k)$ into

$$\sum_{\mu=1}^{\nu} \frac{1}{2m_\mu}\Big(\frac{\hbar}{i}\Big)^2\Big(\frac{\partial^2}{\partial q_{3\mu-2}^2}\psi + \frac{\partial^2}{\partial q_{3\mu-1}^2}\psi + \frac{\partial^2}{\partial q_{3\mu}^2}\psi\Big) + V\psi$$

(we have omitted the variables $q_1, \ldots, q_{3\nu}$). Since the operation

$$q_1 \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}$$

is different from the operation[15]

$$\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1} q_1$$

[14] If $\mathbb{Q}_1, \mathbb{P}_1$ are Hermitian, neither $\mathbb{Q}_1\mathbb{P}_1$ nor $\mathbb{P}_1\mathbb{Q}_1$ is necessarily Hermitian, but it is true that $\frac{1}{2}(\mathbb{Q}_1\mathbb{P}_1 + \mathbb{P}_1\mathbb{Q}_1)$ is always Hermitian. In the case of $\mathbb{Q}_1^2\mathbb{P}_1$, we should also consider $\frac{1}{2}(\mathbb{Q}_1^2\mathbb{P}_1 + \mathbb{P}_1\mathbb{Q}_1^2)$ as well as $\mathbb{Q}_1\mathbb{P}_1\mathbb{Q}_1$ (however, these two expressions happen to be equal for $\mathbb{P}_1\mathbb{Q}_1 - \mathbb{Q}_1\mathbb{P}_1 = (\hbar/i)\mathbb{I}$). In the case $\mathbb{Q}_1^2\mathbb{P}_1^2$, we should also consider $\frac{1}{2}(\mathbb{Q}_1^2\mathbb{P}_1^2 + \mathbb{P}_1^2\mathbb{Q}_1^2)$, $\mathbb{Q}_1\mathbb{P}_1^2\mathbb{Q}_1$, $\mathbb{P}_1\mathbb{Q}_1^2\mathbb{P}_1$, etc. (these expressions do not all coincide in the special case mentioned above). We shall not discuss this further at present, since the operator calculus developed later will permit these relations to be seen much more clearly.

[15] We have

$$\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}(q_1\psi) = q_1\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}\psi + \tfrac{\hbar}{i}\psi$$

Consequently

$$\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}\cdot q_1 - q_1\cdot\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1} = \tfrac{\hbar}{i}\mathsf{I}$$

where I is the identity operator (transforming ψ into itself), *i.e.*, $\frac{\hbar}{i}\frac{\partial}{\partial q_1}$ and q_1 satisfy the same commutation rules as the matrices $\mathbb{P}_1$ and $\mathbb{Q}_1$.

there is here, too, an uncertainty because of the ambiguity of the order of the terms q_i and p_i in

$$H(q_1, \ldots, q_k, p_1, \ldots, p_k)$$

However, Schrödinger has pointed out how this uncertainty can be eliminated, by reduction to a definite variational principle, in such a way that the resulting differential equation becomes self-adjoint.[16]

Now this differential equation (the "wave equation") has the character of an eigenvalue problem in which λ is to be interpreted as an eigenvalue parameter, and in which the vanishing of the eigenfunction $\psi = \psi(q_1, \ldots, q_k)$ at the boundaries of the configuration space (the space of the $q_1, \ldots, q_k$)—together with the conditions of regularity and single-valuedness—is required. In the sense of the wave theory, the eigenvalues of λ (both discrete and continuous spectra)[17] are the allowed energy levels. And even the corresponding (complex) eigenfunctions are related to the corresponding (stationary, in the Bohr sense) states of the system. For a ν-electron system ($k = 3\nu$, see above; e is the charge of the electron) the charge density of the μ^{th} electron, measured at the point x, y, x, is given by the expression

$$e \underbrace{\int \cdots \int}_{(3\nu-3)\text{fold}} |\psi(q_1 \ldots q_{3\mu-3} x y z q_{3\mu+1} \ldots q_{3\nu})|^2 dq_1 \cdots dq_{3\mu-3} dq_{3\mu+1} \cdots dq_{3\nu}$$

i.e., according to Schrödinger, this electron is to be thought of as "smeared" over the entire x, y, z ($= q_{3\mu-2}, q_{3\mu-1}, q_{3\mu}$) space. (In order that the total charge be e, ψ must be normalized by the condition

$$\underbrace{\int \cdots \int}_{(3\nu)\text{fold}} |\psi(q_1, \ldots, q_{3\nu})|^2 dq_1 \cdots dq_{3\nu} = 1$$

The integration is over all 3ν variables. The same equation obtains for each $\mu = 1, \ldots, \nu$.)

In addition, the wave mechanics can also make observations on systems which are not in Bohr stationary states,[18] in the following way: If the state is not stationary, *i.e.*, if it changes with time, then the wave function

$$\psi(q_1, \ldots, q_k; t)$$

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[16] See his first two articles, in the book mentioned in Note 9 (also Ann. Phys. **79** (1926)).

[17] See the first of the works of Schrödinger mentioned in Note 16. A precise definition of the spectrum and its parts will be given later, in **II.6** to **II.9**.

[18] In the original framework of matrix mechanics (see our presentation above), such a general state concept, of which the stationary states are special cases, was not given. Only the stationary states, arranged according to the values of the energy, were the object of that theory.

contains time t, and it varies according to the differential equation[19]

$$-H(q_1,\ldots,q_k,\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1},\ldots,\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_k})\psi(q_1,\ldots,q_k;t)=\tfrac{\hbar}{i}\tfrac{\partial}{\partial t}\psi(q_1,\ldots,q_k;t)$$

That is, ψ can be given arbitrarily for $t=t_0$, and it is then determined uniquely for all t. Even the stationary ψ are really time-dependent, as a comparison of the two Schrödinger differential equations will show, but the dependence on t is given by

$$\psi(q_1,\ldots,q_k;t)=e^{-i\lambda t/\hbar}\cdot\psi(q_1,\ldots,q_k)$$

That is, t appears only in a factor of absolute value independent of $q_1,\ldots,q_k$ (*i.e.*, constant in configuration space), so that, for example, the charge density distribution defined above does not change. (We shall suppose generally—and we shall find this confirmed later by more detailed considerations—that a factor of absolute value 1 and constant in configuration space is, in the case of ψ, essentially unobservable.)

Since the eigenfunctions of the first differential equation form a complete orthogonal set,[20] we can develop each $\psi(q_1,\ldots,q_k)$ in terms of this set of functions. If $\psi_1,\psi_2,\ldots$ are the eigenfunctions (all independent of time), and $\lambda_1,\lambda_2,\ldots$ are their respective eigenvalues, the development becomes[21]

$$\psi(q_1,\ldots,q_k)=\sum_{n=1}^{\infty}a_n\psi_n(q_1,\ldots,q_k)$$

If ψ is still time-dependent, then t is introduced in the coefficients a_n (the eigenfunctions $\psi_1,\psi_2,\ldots$ on the other hand are to be understood both here and in everything which follows as independent of time). Therefore, if the

$$\psi=\psi(q_1,\ldots,q_k)$$

at hand is actually $\psi=\psi(q_1,\ldots,q_k;t_0)$, then it follows with regard to

$$\psi=\psi(q_1,\ldots,q_k;t)=\sum_{n=1}^{\infty}a_n(t)\psi_n$$

that

$$H\psi=\sum_{n=1}^{\infty}a_n(t)H\psi_n=\sum_{n=1}^{\infty}\lambda_n a_n(t)\psi_n$$

$$\tfrac{\hbar}{i}\tfrac{\partial}{\partial t}\psi=\sum_{n=1}^{\infty}\tfrac{\hbar}{i}\dot{a}_n(t)\psi_n$$

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[19] $H=H(q_1,\ldots,q_k,p_1,\ldots,p_k)$ may also contain the time t explicitly. Naturally, there will then be in general no stationary states at all.

[20] Provided that only a discrete spectrum exists. See **II.6**.

[21] These, as also all the following series expansions, converge "in the mean." We shall consider this again in **II.2**.

and by equating the coefficients of the second differential equation:

$$\tfrac{\hbar}{i}\dot{a}_n(t) = -\lambda_n a_n(t) \quad \Longrightarrow \quad a_n(t) = c_n e^{-i\lambda_n t/\hbar}$$

i.e.,

$$a_n(t) = e^{-i\lambda_n(t-t_0)/\hbar} a_n$$

$$\psi = \psi(q_1, \ldots, q_k; t) = \sum_{n=1}^{\infty} e^{-i\lambda_n(t-t_0)/\hbar} a_n \psi_n(q_1, \ldots, q_k)$$

Therefore, if ψ is not stationary, *i.e.*, if all a_n except one do not vanish, then ψ (for variable t) no longer changes only by a space constant factor of absolute value unity. Therefore, in general, the charge densities also change, *i.e.*, real electrical oscillations occur in space.[22]

We see that the initial concepts and the practical methods of the two theories differ considerably. Nevertheless, from the beginning they have always yielded the same results, even where both gave details differing from the older concept of quantum theory.[23] This extraordinary situation was soon clarified,[24] as mentioned in **I.1**, with the proof by Schrödinger of their mathematical equivalence. We shall turn our attention to this equivalence proof, and at the same time explain the Dirac-Jordan general transformation theory (which combines the two theories).

3. THE EQUIVALENCE OF THE TWO THEORIES: The Transformation Theory

The fundamental problem of the matrix theory was to find the matrices $\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k$ such that first, the commutation rules of **I.2** (page 4) are satisfied, and second, that a certain function of these matrices,

$$H(\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k)$$

becomes a diagonal matrix. This problem had already been been divided into two parts by Born and Jordan in their first publication:

First, matrices $\bar{\mathbb{Q}}_1, \ldots, \bar{\mathbb{Q}}_k, \bar{\mathbb{P}}_1, \ldots, \bar{\mathbb{P}}_k$ were sought which have only to satisfy the commutation rules. This could easily be accomplished;[25] then, in general

$$\bar{\mathbb{H}} = H(\bar{\mathbb{Q}}_1, \ldots, \bar{\mathbb{Q}}_k, \bar{\mathbb{P}}_1, \ldots, \bar{\mathbb{P}}_k)$$

[22] That such oscillations fail to occur for the stationary states, and only for those, was one of the most important postulates of Bohr in 1913. Classical electrodynamics is in direct contradiction to this.

[23] See the second work of Schrödinger mentioned in Note 16.

[24] See Note 7.

[25] See, for example, §§20 & 23 of the book of Born and Jordan mentioned in Note 1.

would not be a diagonal matrix. Then the correct solutions were expressed in the form

$$\begin{aligned} \mathbb{Q}_1 &= \mathbb{S}^{-1}\bar{\mathbb{Q}}_1\mathbb{S} \\ &\vdots \\ \mathbb{Q}_k &= \mathbb{S}^{-1}\bar{\mathbb{Q}}_k\mathbb{S} \\ \mathbb{P}_1 &= \mathbb{S}^{-1}\bar{\mathbb{P}}_1\mathbb{S} \\ &\vdots \\ \mathbb{P}_k &= \mathbb{S}^{-1}\bar{\mathbb{P}}_k\mathbb{S} \end{aligned}$$

where $\mathbb{S}$ could be an arbitrary matrix (except that it must be one which possesses an inverse $\mathbb{S}^{-1}$ with the properties $\mathbb{S}^{-1}\mathbb{S} = \mathbb{S}\mathbb{S}^{-1} = \mathbb{I}$). Since the validity of the commutation rules for $\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k$ follows (identically in $\mathbb{S}$!) from the validity of the rules for $\bar{\mathbb{Q}}_1, \ldots, \bar{\mathbb{Q}}_k, \bar{\mathbb{P}}_1, \ldots, \bar{\mathbb{P}}_k$ and since

$$\bar{\mathbb{H}} = H(\bar{\mathbb{Q}}_1, \ldots, \bar{\mathbb{Q}}_k, \bar{\mathbb{P}}_1, \ldots, \bar{\mathbb{P}}_k)$$

goes over into[26]

$$\mathbb{H} = H(\mathbb{Q}_1, \ldots, \mathbb{Q}_k, \mathbb{P}_1, \ldots, \mathbb{P}_k) \quad \text{with} \quad \mathbb{S}^{-1}\bar{\mathbb{H}}\,\mathbb{S} = \mathbb{H}$$

the only requirement put on $\mathbb{S}$ is that $\mathbb{S}^{-1}\bar{\mathbb{H}}\,\mathbb{S}$ be a diagonal matrix where $\bar{\mathbb{H}}$ is given. (Of course, one would also have to see to it that $\mathbb{S}^{-1}\bar{\mathbb{Q}}_1\,\mathbb{S}$, etc. be Hermitian, just as the $\bar{\mathbb{Q}}_1$, etc. were. However, it can be shown upon closer examination that this additional condition on $\mathbb{S}$ can always be satisfied later, and it shall therefore not be considered in these initial observations.)

Consequently there is need of transforming a given $\bar{\mathbb{H}}$ to the diagonal form by means of the scheme $\mathbb{S}^{-1}\bar{\mathbb{H}}\,\mathbb{S}$. Let us formulate therefore precisely what this means.

Let the matrix $\mathbb{H}$ have the elements $h_{\mu\nu}$, the desired matrix $\mathbb{S}$ the elements $s_{\mu\nu}$, and the (also unknown) diagonal matrix $\mathbb{H}$ the diagonal elements w_μ, *i.e.*, the general element $w_\mu\delta_{\mu\nu}$.[27] Now $\mathbb{H} = \mathbb{S}^{-1}\bar{\mathbb{H}}\,\mathbb{S}$ is the same as $\mathbb{S}\mathbb{H} = \bar{\mathbb{H}}\mathbb{S}$, and this means (if we equate the corresponding elements to one another on both

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[26] Because

$$\mathbb{S}^{-1}\cdot\mathbb{I}\cdot\mathbb{S} = \mathbb{I} \qquad \mathbb{S}^{-1}\cdot a\mathbb{A}\cdot\mathbb{S} = a\cdot\mathbb{S}^{-1}\mathbb{A}\mathbb{S}$$
$$\mathbb{S}^{-1}\cdot(\mathbb{A}+\mathbb{B})\cdot\mathbb{S} = \mathbb{S}^{-1}\mathbb{A}\mathbb{S} + \mathbb{S}^{-1}\mathbb{B}\mathbb{S} \qquad \mathbb{S}^{-1}\cdot\mathbb{A}\mathbb{B}\cdot\mathbb{S} = \mathbb{S}^{-1}\mathbb{A}\mathbb{S}\cdot\mathbb{S}^{-1}\mathbb{B}\mathbb{S}$$

therefore, for each matrix polynomial $P(\mathbb{A}, \mathbb{B}, \ldots)$,

$$\mathbb{S}^{-1}P(\mathbb{A}, \mathbb{B}, \ldots)\mathbb{S} = P(\mathbb{S}^{-1}\mathbb{A}\mathbb{S}, \mathbb{S}^{-1}\mathbb{B}\mathbb{S}, \ldots)$$

If we choose for P the left sides of the commutation relations, their invariance follows from this; if we choose H for P, then we get $\mathbb{S}^{-1}\bar{\mathbb{H}}\,\mathbb{S} = \mathbb{H}$.

[27] $\delta_{\mu\nu} = 1$ for $\mu = \nu$ and $= 0$ for $\mu \neq \nu$ is the well-known Kronecker delta.

sides of the equation, according to the well known rules of matrix multiplication):

$$\sum_{\nu} s_{\mu\nu} \cdot w_\nu \delta_{\nu\rho} = \sum_{\nu} h_{\mu\nu} \cdot s_{\nu\rho}$$

i.e.,

$$\sum_{\nu} h_{\mu\nu} \cdot s_{\nu\rho} = w_\rho \cdot s_{\mu\rho}$$

The individual columns $s_{1\rho}, s_{2\rho}, \ldots$ $(\rho = 1, 2, \ldots)$ of the matrix $\mathbb{S}$ and the corresponding diagonal elements w_ρ of the matrix $\mathbb{H}$ are therefore solutions of the so-called eigenvalue problem, which runs as follows:

$$\sum_{\nu} h_{\mu\nu} x_\nu = \lambda \cdot x_\mu \qquad (\mu = 1, 2, \ldots)$$

(The trivial solution $x_1 = x_2 = \cdots = 0$ is naturally excluded.) In fact, $x_\nu = s_{\nu\rho}$, $\lambda = w_\rho$ is a solution. ($x_\nu \equiv 0$ *i.e.*, $s_{\nu\rho} \equiv 0$ [for all ν] is inadmissible, because then the ρ^{th} column of $\mathbb{S}$ would vanish identically, although $\mathbb{S}$ possesses an inverse $\mathbb{S}^{-1}$!) It is worth mentioning that these are essentially the only solutions.

Indeed, the above equation means the following: the transform of the vector $x = (x_1, x_2, \ldots)$ by the matrix $\bar{\mathbb{H}}$ is equal to its multiple by the number λ. We transform $x = (x_1, x_2, \ldots)$ by $\mathbb{S}^{-1}$, and there results a vector $y = (y_1, y_2, \ldots)$. If we transform y by $\mathbb{H}$, then this is the same as the transform of x by

$$\mathbb{H}\mathbb{S}^{-1} = \mathbb{S}^{-1}\bar{\mathbb{H}}\mathbb{S}\mathbb{S}^{-1} = \mathbb{S}^{-1}\bar{\mathbb{H}}$$

Hence it is a transform of λx by $\mathbb{S}^{-1}$, and therefore the result is λy. Now $\mathbb{H}y$ has the components

$$\sum_{\nu} w_\mu \delta_{\mu\nu} y_\nu = w_\mu y_\mu$$

and λy the components λy_μ. Therefore it is required that $w_\mu y_\mu = \lambda y_\mu$ for all $\mu = 1, 2, \ldots$; *i.e.*, $y_\mu = 0$ whenever $w_\mu \neq \lambda$. If we call η^ρ that vector whose ρ^{th} component is 1, but all others of which are 0, then this means: y is a linear combination of those η^ρ for which $w_\rho = \lambda$—in particular it is zero if there are none such. The value of x results from the application of $\mathbb{S}$ to y, therefore it is a linear combination of the η^ρ from before, transformed with $\mathbb{S}$. The μ^{th} component of $\mathbb{S}\eta^\rho$ is (since the ν^{th} component of η^ρ was $\delta_{\nu\rho}$)

$$\sum_{\nu} s_{\mu\nu} \delta_{\nu\rho} = s_{\mu\rho}$$

If we then interpret the ρ^{th} column $(s_{1\rho}, s_{2\rho}, \ldots)$ of $\mathbb{S}$ as a vector, then x is a linear combination of all columns for which $w_\rho = \lambda$—and in particular is zero if this does not occur. Consequentially, our original assertion has been proved: the $w_1, w_2, \ldots$ are the only eigenvalues and the $x_\nu = s_{\nu\rho}$, $\lambda = w_\rho$ are essentially the only solutions.

This is very important, because not only does the knowledge of $\mathbb{S}, \mathbb{H}$ determine all the solutions of the eigenvalue problem, but conversely, we can also determine $\mathbb{S}, \mathbb{H}$ as soon as we have solved the eigenvalue problem completely. For example, for $\mathbb{H}$: The w_μ are plainly all solutions λ, and each such λ appears in the series $w_1, w_2, \ldots$ as often as there are linearly independent solutions $x_1, x_2, \ldots$[28]—hence the $w_1, w_2, \ldots$ are already determined except for their order.[29]

The fundamental problem of the matrix theory is then the solution of the eigenvalue equation

$$\mathbf{E}_1 \qquad \sum_\nu h_{\mu\nu} x_\nu = \lambda \cdot x_\mu \qquad (\mu = 1, 2, \ldots)$$

Let us now go on to the wave theory. The fundamental equation of this theory is the "wave equation"

$$\mathbf{E}_2 \qquad \mathsf{H}\phi(q_1, \ldots, q_k) = \lambda\phi(q_1, \ldots, q_k)$$

in which H is the differential operator already discussed—we seek all solutions $\phi(q_1, \ldots, q_k)$ and λ, with the exclusion of the trivial $\phi(q_1, \ldots, q_k) \equiv 0$, λ arbitrary. This is analogous to what was required of $\mathbf{E}_1$: the sequence $x_1, x_2, \ldots$, which we can also regard as a function x_ν of the "discontinuous" variable ν (with the variable values $1, 2, \ldots$) corresponds to the function $\phi(q_1, \ldots, q_k)$ with the "continuous" variables $q_1, \ldots, q_k$; λ has the same role each time. However, the linear transformation

$$x_\mu \longrightarrow \sum_\nu h_{\mu\nu} x_\nu$$

shows little similarity to the other

$$\phi(q_1, \ldots, q_k) \longrightarrow \mathsf{H}\phi(q_1, \ldots, q_k)$$

How should such an analogy be obtained here?

We have regarded the index ν as a variable, and placed it in correspondence with the k variables $q_1, \ldots, q_k$; *i.e.*, a positive integer with the general point of the k-dimensional configuration space (which may be called Ω from now on). Therefore we should not expect that $\sum_\nu$ can be carried over as a sum into Ω. We should rather expect the integral $\int_\Omega \cdots \int_\Omega \cdots dq_1 \cdots dq_k$ (or more briefly, $\int_\Omega \cdots dv$, where dv is the volume element $dq_1 \cdots dq_k$ in Ω) to be the correct analog. To the matrix element $h_{\mu\nu}$ which depends upon two variables of the

[28] The $\mathbb{S}$ columns $s_{1\rho}, s_{2\rho}, \ldots$ of the ρ with $w_\rho = \lambda$ form a complete set of solutions, and as columns of a matrix which possesses an inverse, they must be linearly independent.

[29] Since an arbitrary permutation of the columns of $\mathbb{S}$, together with the corresponding permutation of the rows of $\mathbb{S}^{-1}$, permutes the diagonal elements of $\mathbb{H}$ in the same way, the order of the $w_1, w_2, \ldots$ is in fact indeterminate.

type of the index ν there corresponds a function

$$h(q_1, \ldots, q_k; q_1', \ldots, q_k')$$

in which the $q_1, \ldots, q_k$ and the $q_1', \ldots, q_k'$ run through the whole Ω domain independently. The transformation

$$x_\mu \longrightarrow \sum_\nu h_{\mu\nu} x_\nu \qquad \text{or} \qquad x_\nu \longrightarrow \sum_{\nu'} h_{\nu\nu'} x_{\nu'}$$

then becomes

$$\phi(q_1, \ldots, q_k) \longrightarrow \underbrace{\int \cdots \int}_{\Omega} h(q_1, \ldots, q_k; q_1', \ldots, q_k') \phi(q_1', \ldots, q_k') dq_1' \cdots dq_k'$$

and the eigenvalue problem E_1, which we can also write as

$$\mathsf{E}_1 \qquad \sum_{\nu'} h_{\nu\nu'} x_{\nu'} = \lambda \cdot x_\nu$$

becomes

$$\mathsf{E}_3 \qquad \underbrace{\int \cdots \int}_{\Omega} h(q_1, \ldots, q_k; q_1', \ldots, q_k') \phi(q_1', \ldots, q_k') dq_1' \cdots dq_k' = \lambda \cdot \phi(q_1, \ldots, q_k)$$

Eigenvalue problems of the type E_3 have been investigated extensively in mathematics, and can in fact be handled in far reaching analogy to the problem E_1. They are known as "integral equations."[30]

But, unfortunately, E_2 does not have this form, or, rather, it can only be brought to this form if a function $h(q_1, \ldots, q_k; q_1', \ldots, q_k')$ can be found for the differential operator

$$\mathsf{H} = H(q_1, \ldots, q_k, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}, \ldots, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_k})$$

such that

$$\mathsf{I} \qquad \mathsf{H}\phi(q_1, \ldots, q_k) = \underbrace{\int \cdots \int}_{\Omega} h(q_1, \ldots, q_k; q_1', \ldots, q_k') \phi(q_1', \ldots, q_k') dq_1' \cdots dq_k'$$

identically, *i.e.*, for all $\phi(q_1, \ldots, q_k)$. This $h(q_1, \ldots, q_k; q_1', \ldots, q_k')$, if it exists, is called the "kernel" of the functional operator H, and H itself is then called an "integral operator."

[30] The theory of integral equations has received its definitive form through the work of Fredholm and Hilbert. An exhaustive treatment, complete with references, is found in the book by Courant and Hilbert, *Methoden der Mathematischen Physik*, Berlin, 1931.

Now such a transformation is generally impossible, *i.e.*, differential operators H are never integral operators. Even the simplest functional operator, which transforms each ϕ into itself—this operator is called I—is not one. Let us convince ourselves of this, and for simplicity, take $k = 1$. Then let it be required that

$$\boldsymbol{\Delta}_1 \qquad \phi(q) = \int_{-\infty}^{\infty} h(q, q')\phi(q')dq'$$

We replace $\phi(q)$ by $\phi(q + q_0)$, set $q = 0$ and introduce the integration variable $q'' = q' + q_0$. Then

$$\phi(q_0) = \int_{-\infty}^{\infty} h(0, q'' - q_0)\phi(q'')dq''$$

If we replace q_0, q'' by q, q' then we see that $h(0, q' - q)$ along with $h(q, q')$ solves our problem, hence we may assume that $h(q, q')$ is only dependent upon $q' - q$. Then the requirement becomes

$$\boldsymbol{\Delta}_2 \qquad \phi(q) = \int_{-\infty}^{\infty} h(q' - q)dq' \quad : \quad h(q, q') = h(q' - q)$$

Replacing again $\phi(q + q_0)$ for $\phi(q)$, it suffices to consider $q = 0$, *i.e.*,

$$\boldsymbol{\Delta}_3 \qquad \phi(0) = \int_{-\infty}^{\infty} h(q)\phi(q)dq$$

Replacing $\phi(q)$ by $\phi(-q)$ shows that $h(-q)$ is also a solution along with $h(q)$, therefore

$$h_1(q) = \tfrac{1}{2}\big[h(q) + h(-q)\big]$$

is also, so that $h(q)$ may be considered to be an even function of q.

It is clear that these conditions are impossible of fulfillment: If we choose $\phi(q) = h(q)$ for $q \gtrless 0$, $\phi(0) = 0$, then it follows from $\boldsymbol{\Delta}_3$ that $h(q) = 0$ for $q \gtrless 0$.[31] But if we choose $\phi(q) = 1$, then we obtain

$$\int_{-\infty}^{\infty} h(q)dq = 1$$

while

$$\int_{-\infty}^{\infty} h(q)dq = 0$$

follows directly from the above.

[31] More precisely, if we take as a basis the Lebesgue concept of integral, then for $q \gtrless 0$, $h(q) = 0$ except for a set of measure 0—*i.e.*, except for such a set $h(q) = 0$ identically.

Dirac nevertheless assumes the existence of such a function

$$\mathbf{\Delta}_4 \qquad \delta(q) = 0 \ \text{ for } \ q \gtrless 0, \quad \delta(q) = \delta(-q), \quad \int_{-\infty}^{\infty} \delta(q)dq = 1$$

This would imply $\mathbf{\Delta}_3$:

$$\begin{aligned}\int_{-\infty}^{\infty} \delta(q)\phi(q)dq &= \phi(0)\int_{-\infty}^{\infty}\delta(q)dq + \int_{-\infty}^{\infty}\delta(q)[\phi(q)-\phi(0)]dq \\ &= \phi(0)\cdot 1 + \int_{-\infty}^{\infty} 0\cdot dq \\ &= \phi(0)\end{aligned}$$

therefore also $\mathbf{\Delta}_1$ and $\mathbf{\Delta}_2$. We should thus think of this function as vanishing everywhere except at the origin, and of its being so strongly infinite there that the integral still comes out to be 1 for $\delta(q)$.[32]

If we have once accepted this fiction, it is possible to represent the most varied differential operators as integral operators—provided that, in addition to $\delta(q)$, we also introduce its derivatives. Then we have

$$\begin{aligned}\frac{d^n}{dq^n}\phi(q) = \frac{d^n}{dq^n}\int_{-\infty}^{\infty}\delta(q-q')\phi(q')dq' &= \int_{-\infty}^{\infty}\frac{\partial^n}{\partial q^n}\delta(q-q')\phi(q')dq' \\ &= \int_{-\infty}^{\infty}\delta^{(n)}(q-q')\cdot\phi(q')dq' \\ q^n\phi(q) = \int_{-\infty}^{\infty}\delta(q-q')q^n\cdot\phi(q')dq'\end{aligned}$$

i.e., $\frac{d^n}{dq^n}$ and q^n have the kernels $\delta^{(n)}(q-q')$ and $\delta^{(n)}(q-q')q^n$, respectively. According to this scheme, we can investigate the kernels of rather complicated differential operators. For several variables $q_1,\ldots,q_k$ the delta functions lead to the result

$$\begin{aligned}&\underbrace{\int\cdots\int}_{\Omega}\delta(q_1-q_1')\delta(q_2-q_2')\cdots\delta(q_k-q_k')\phi(q_1',q_2'\ldots,q_k')dq_1'\cdots dq_k' \\ &=\int_{-\infty}^{\infty}\Bigg[\cdots\Bigg[\int_{-\infty}^{\infty}\Bigg[\int_{-\infty}^{\infty}\phi(q_1',q_2'\ldots,q_k')\delta(q_1-q_1')dq_1'\Bigg] \\ &\qquad\qquad\delta(q_2-q_2')dq_2'\Bigg]\cdots\Bigg]\delta(q_k-q_k')dq_k'\end{aligned}$$

[32] The area under the curve of $\delta(q)$ is then to be thought of as infinitely thin and infinitely high, for the point situated at $q=0$, and of area unity. This may be viewed as the limiting behavior for the function $\sqrt{a/\pi}e^{-aq^2}$ as $a\to\infty$ but it is nevertheless impossible.

$$= \int_{-\infty}^{\infty} \left[\cdots \left[\int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \phi(q_1, q_2' \ldots, q_k') \delta(q_2 - q_2') dq_2' \right] \cdots \right] \delta(q_k - q_k') dq_k'$$

$$\vdots$$

$$= \phi(q_1, q_2, \ldots, q_k)$$

$$\underbrace{\int \cdots \int}_{\Omega} \delta'(q_1 - q_1') \delta(q_2 - q_2') \cdots \delta(q_k - q_k') \phi(q_1', q_2' \ldots, q_k') dq_1' \cdots dq_k'$$

$$= \frac{\partial}{\partial q_1} \underbrace{\int \cdots \int}_{\Omega} \delta(q_1 - q_1') \delta(q_2 - q_2') \cdots \delta(q_k - q_k') \phi(q_1', q_2' \ldots, q_k') dq_1' \cdots dq_k'$$

$$= \frac{\partial}{\partial q_1} \phi(q_1, \ldots, q_k), \quad \text{etc.}$$

Hence the integral representation **I** can be in practice achieved for all operators.

As soon as we have achieved this representation, the analogy of problems $\mathbf{E}_1$ and $\mathbf{E}_2$ is complete. We have only to replace ν, ν', $\sum_\nu$ and x by

$$q_1, \ldots, q_k; \quad q_1', \ldots, q_k'; \quad \underbrace{\int \cdots \int}_{\Omega} \cdots dq_1' \cdots dq_k' \quad \text{and} \quad \phi$$

As the vectors x_ν correspond to the functions $\phi(q_1, \ldots, q_k)$, the kernels $h(q_1, \ldots, q_k; q_1', \ldots, q_k')$ must correspond to the matrices $h_{\nu\nu'}$; however, it is useful to regard the kernels themselves as matrices, and consequently to interpret the $q_1, \ldots, q_k$ as row- and the $q_1', \ldots, q_k'$ as column-indices, corresponding to ν and ν' respectively. We then have, in addition to the ordinary matrices $\{h_{\nu\nu'}\}$ with discrete row-column domains enumerated by the numbers $1, 2, \ldots$, others,

$$\{h(q_1, \ldots, q_k; q_1', \ldots, q_k')\}$$

(the kernels), for which each domain is characterized by k variables, varying continuously throughout the entire Ω.

This analogy may seem entirely formal, but in reality it is not so. The indices ν and ν' can also be regarded as coordinates in a state space, that is, if we interpret them as quantum numbers (in the sense of the Bohr theory: as numbers of the possible orbits in phase space which are then discrete because of the restrictions of the quantum conditions).

We do not desire to follow any further here this train of thought which was shaped by Dirac and Jordan into a unified theory of the quantum processes. The "improper" functions (such as $\delta(x), \delta'(x)$) play a decisive role in this development—they lie beyond the scope of mathematical methods generally used, and we desire to describe quantum mechanics with the help of these latter methods. We therefore pass over to the other (Schrödinger) method of unification of the two theories.

4. THE EQUIVALENCE OF THE TWO THEORIES: Hilbert Space

The method sketched in **1.3** resulted in an analogy between the "discrete" space of index values $Z = (1, 2, \ldots)$ and the continuous state space Ω of the mechanical system (Ω is k-dimensional, where k is the number of classical mechanical degrees of freedom). That this cannot be achieved without some violence to the formalism and to mathematics is not surprising. The spaces Z and Ω are very different, and every attempt to relate the two must run into great difficulties.[33]

What we do have, however, is not a relation of Z to Ω, but only a relation between the functions in these two spaces, *i.e.*, between the sequences $x_1, x_2, \ldots$ which are the functions in Z, and the wave functions $\phi(q_1, \ldots, q_k)$ which are the functions in Ω. These functions, furthermore, are the entities which enter most essentially into the problems of quantum mechanics.

In the Schrödinger theory, the integral

$$\underbrace{\int \cdots \int}_{\Omega} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k$$

plays an important role—it must equal 1 in order that ϕ can be given a physical interpretation (see **1.2**). In matrix theory, on the other hand (see problem $\mathbf{E}_1$ in **1.3**), the vector $x_1, x_2, \ldots$ plays the decisive role. The condition of finiteness $\sum_\nu |x_\nu|^2$ in the sense of the Hilbert theory of such eigenvalue problems (see reference in Note 30) is always imposed on this vector. It is also customary, having excluded the trivial solution $x_\nu \equiv 0$, to set up the normalization condition $\sum_\nu |x_\nu|^2 = 1$. It is plain in Z or Ω that this limits the field of admissible functions to those with finite

$$\sum_\nu |x_\nu|^2 \quad \text{or} \quad \underbrace{\int \cdots \int}_{\Omega} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k$$

because only with such functions can the above $\sum_\nu$ or $\int \cdots \int_\Omega$ be made equal to 1 by multiplication with a constant factor—*i.e.*, can be normalized in the

[33] Such a unification was undertaken, long before quantum mechanics, by E. H. Moore, the originator of the so-called "general analysis." See the article on this subject by Hellinger & Toeplitz in *Math. Enzyklopädie*, vol II, C, 13, Leipzig, 1927.

usual sense.[34] We call the totality of such functions F_Z and F_Ω, respectively.

Now the following theorem holds: F_Z and F_Ω are isomorphic (Fischer and F. Riesz[35]). To be precise, this means the following: It is possible to set up a one-to-one correspondence between F_Z and F_Ω; *i.e.*, to each sequence $x_1, x_2, \ldots$ with finite $\sum_\nu |x_\nu|^2$ a function $\phi(q_1, \ldots, q_k)$ with finite

$$\underbrace{\int \cdots \int}_{\Omega} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k$$

can be assigned, and conversely in such a manner that this correspondence is linear and isometric. By "linearity" this is meant: if $x_1, x_2, \ldots$ corresponds to $\phi(q_1, \ldots, q_k)$ and $y_1, y_2, \ldots$ to $\psi(q_1, \ldots, q_k)$, then $ax_1, ax_2, \ldots$ and $x_1 + y_1, x_2 + y_2, \ldots$ correspond respectively $a\phi(q_1, \ldots, q_k)$ and

$$\phi(q_1, \ldots, q_k) + \psi(q_1, \ldots, q_k)$$

By "isometry" this is meant: if $x_1, x_2, \ldots$ and $\phi(q_1, \ldots, q_k)$ correspond to one another then

$$\sum_\nu |x_\nu|^2 = \underbrace{\int \cdots \int}_{\Omega} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k$$

(The word isometric has the connotation that it is customary to regard $x_1, x_2, \ldots$ and $\phi(q_1, \ldots, q_k)$ as vectors, and to consider

$$\left(\sum_\nu |x_\nu|^2 \right)^{\frac{1}{2}}$$

and

$$\left(\underbrace{\int \cdots \int}_{\Omega} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k \right)^{\frac{1}{2}}$$

[34] It is a repeatedly observed fact in the Schrödinger theory that only the finiteness of

$$\underbrace{\int \cdots \int}_{\Omega} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k$$

is required in the case of the wave functions ϕ. So, for example, ϕ may be singular, or perhaps become infinite, if only the above integral remains finite. An instructive example for this is the hydrogen atom in the relativistic theory of Dirac; see Proc. Roy. Soc. **117** (1928); also W. Gordon, Z. Physik **48**, (1928).

[35] In the course of our discussion of Hilbert space, a proof of this theorem will be given (see **II.2** & **II.3**, especially THEOREM 5 in **II.2**). It is worth mentioning that the part of this theorem sufficient for many purposes, and easier to prove, is the isomorphism between F_Ω and an appropriate part of F_Z; this is due to Hilbert (Gött. Nachr. 1906). Thus Schrödinger's original equivalence proof (see Note 7) corresponds to just this part of the theorem.

as their "lengths.") In addition, if $x_1, x_2, \ldots$ and $y_1, y_2, \ldots$ correspond respectively to $\phi(q_1, \ldots, q_k)$ and $\psi(q_1, \ldots, q_k)$, then

$$\sum_\nu x_\nu \bar{y}_\nu = \underbrace{\int \cdots \int}_{\Omega} \phi(q_1, \ldots, q_k)\, \overline{\psi(q_1, \ldots, q_k)}\, dq_1 \ldots dq_k$$

(and both sides are absolutely convergent). On this latter point, it should be observed that one might have preferred to have quite generally

$$\sum_\nu x_\nu = \underbrace{\int \cdots \int}_{\Omega} \phi(q_1, \ldots, q_k)\, dq_1 \ldots dq_k$$

or something similar; *i.e.*, a complete analogy between addition on the one hand and integration on the other—but a closer examination shows that addition $\sum_\nu$ and integration

$$\sum_\nu x_\nu = \underbrace{\int \cdots \int}_{\Omega} \cdots dq_1 \ldots dq_k$$

are employed in quantum mechanics only in such expressions as $x_\nu \bar{y}_\nu$ or $\phi(q_1, \ldots, q_k)\, \overline{\psi(q_1, \ldots, q_k)}$, respectively.

We do not intend to pursue any investigation at this point as to how this correspondence is to be established, since this will be of great concern to us in the next chapter. But we should emphasize what its existence means: Z and Ω are very different, and to set up a direct relation between them must lead to great mathematical difficulties. On the other hand, F_Z and F_Ω are isomorphic, *i.e.*, identical in their intrinsic structure (they realize the same abstract structure in different forms)—and since they (and not Z and Ω!) are the real analytical substrata of the matrix and wave theories, this isomorphism means that the two theories must always yield the same numerical results. That is, this is the case whenever the isomorphism lets the matrix

$$\bar{\mathbb{H}} = H(\bar{\mathbb{Q}}_1, \ldots, \bar{\mathbb{Q}}_k; \bar{\mathbb{P}}_1, \ldots, \bar{\mathbb{P}}_k)$$

and the operator

$$\mathsf{H} = H(q_1, \ldots, q_k, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}, \ldots, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_k})$$

correspond to one another. Since both are obtained by the same algebraic operations from the matrices $\bar{\mathbb{Q}}_\ell, \bar{\mathbb{P}}_\ell$ $(\ell = 1, \ldots, k)$ and the functional operators $q_\ell, (\hbar/i)\frac{\partial}{\partial q_\ell}$ respectively, it suffices to show that q_ℓ corresponds to the matrix $\bar{\mathbb{Q}}_\ell$ and $(\hbar/i)\frac{\partial}{\partial q_\ell}$ to the matrix $\bar{\mathbb{P}}_\ell$. Now nothing further is required of the $\bar{\mathbb{Q}}_\ell, \bar{\mathbb{P}}_\ell$ $(\ell = 1, \ldots, k)$ than that they satisfy the commutation rules mentioned in **1.2**:

$$\left.\begin{aligned} \mathbb{Q}_m \mathbb{Q}_n - \mathbb{Q}_n \mathbb{Q}_m &= \mathbb{O} \\ \mathbb{P}_m \mathbb{P}_n - \mathbb{P}_n \mathbb{P}_m &= \mathbb{O} \\ \mathbb{P}_m \mathbb{Q}_n - \mathbb{Q}_n \mathbb{P}_m &= \delta_{mn} \tfrac{h}{2\pi i} \mathbb{I} \end{aligned}\right\} \quad (m, n = 1, 2, \ldots, k)$$

But the matrices corresponding to the $q_\ell, (\hbar/i)\frac{\partial}{\partial q_\ell}$ will certainly do this, because

the functional operators $q_\ell, (\hbar/i)\frac{\partial}{\partial q_\ell}$ possess the properties mentioned,[36] and these are not lost in the isomorphic transformation to F_Z.

Since the systems F_Z and F_Ω are isomorphic, and since the theories of quantum mechanics constructed on them are mathematically equivalent, it is to be expected that a unified theory, independent of the accidents of the formal framework selected at the time, and exhibiting only the really essential elements of quantum mechanics, will then be achieved if we do this: Investigate the intrinsic properties (common to F_Z and F_Ω) of these systems of functions, and choose these properties as a starting point.

The system F_Z is generally known as "Hilbert space." Therefore, our first problem is to investigate the fundamental properties of Hilbert space, independent of the special form of F_Z or F_Ω. The mathematical structure which is described by these properties (which in any specific special case are equivalently represented by calculations within F_Z or F_Ω, but for general purposes are easier to handle directly than by such calculations) is called "abstract Hilbert space."

We wish then to describe the abstract Hilbert space, and then to prove rigorously the following points:

1. That the abstract Hilbert space is characterized uniquely by the properties specified, *i.e.*, that it admits of no essentially different realizations.

2. That its properties belong to F_Z as well as F_Ω. (In this respect the properties discussed only qualitatively in **1.4** will be analyzed rigorously.) When this has been accomplished, we will employ the mathematical equipment thus obtained to shape the structure of quantum mechanics.

[36] We have

$$q_m \cdot q_n \cdot \phi(q_1, \ldots, q_k) = q_n \cdot q_m \cdot \phi(q_1, \ldots, q_k)$$
$$\frac{\partial}{\partial q_m}\frac{\partial}{\partial q_n}\phi(q_1, \ldots, q_k) = \frac{\partial}{\partial q_n}\frac{\partial}{\partial q_m}\phi(q_1, \ldots, q_k)$$
$$\frac{\partial}{\partial q_m} q_n \cdot \phi(q_1, \ldots, q_k) - q_n \frac{\partial}{\partial q_m} \cdot \phi(q_1, \ldots, q_k) = \delta_{mn}\phi(q_1, \ldots, q_k)$$

CHAPTER II

ABSTRACT HILBERT SPACE

1. THE DEFINITION OF HILBERT SPACE

We must now carry out the program outlined at the end of **I.4**: to define Hilbert space, which furnishes the mathematical basis for the treatment of quantum mechanics in terms of those concepts which are subsequently needed in quantum mechanics, and which have accordingly the same meaning in the "discrete" function space F_Z of the sequences x_ν ($\nu = 1, 2, \ldots$) and in the "continuous" F_Ω of the wave functions $\phi(q_1, \ldots, q_k)$ ($q_1, \ldots, q_k$ run through the entire state space Ω). These concepts are the following ones, as we have already indicated:

$\boldsymbol{\alpha}$) The "scalar product," *i.e.*, the product of a (complex) number a with an element f of Hilbert space: af. In F_Z, ax_ν is obtained from x_ν, while in F_Ω, $a\phi(q_1, \ldots, q_k)$ is obtained from $\phi(q_1, \ldots, q_k)$.

$\boldsymbol{\beta}$) The addition and subtraction of two elements f, g of Hilbert space: $f \pm g$. In F_Z, $x_\nu \pm y_\nu$ results from x_ν and y_ν; in F_Ω, $\phi(q_1, \ldots, q_k) \pm \psi(q_1, \ldots, q_k)$ results from $\phi(q_1, \ldots, q_k)$ and $\psi(q_1, \ldots, q_k)$.

$\boldsymbol{\gamma}$) The "inner product" of two elements f, g in Hilbert space. Unlike $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, this operation produces a complex number, and not an element of Hilbert space: (f, g). In F_X, $\sum_\nu x_\nu \bar{y}_\nu$ is obtained from x_ν and y_ν, while in F_Ω,

$$\underbrace{\int \cdots \int}_{\Omega} \phi(q_1, \ldots, q_k)\overline{\psi(q_1, \ldots, q_k)}\, dq_1 \ldots dq_k$$

is obtained from $\phi(q_1, \ldots, q_k)$ and $\psi(q_1, \ldots, q_k)$. (The definitions of F_Z and F_Ω are still to be completed by the appropriate convergence proofs. We shall give these proofs in **II.3**.)

In the following we shall denote the points of Hilbert space by $f, g, \ldots, \phi, \psi, \ldots$; complex numbers by $a, b, \ldots, x, y, \ldots$; and positive integers by

$k, l, m, \ldots, \mu, \nu$. We shall also refer to Hilbert space as $\mathfrak{R}_\infty$ whenever necessary (as an abbreviation for "∞-dimensional Euclidean space," analogous to the customary designation $\mathfrak{R}_n$ for "n-dimensional Euclidean space" $(n = 1, 2, \ldots)$).

The noteworthy feature of the operations af, $f \pm g$, (f, g) is that they are exactly the basic operations of the vector calculus: those which make possible the establishment of length and angle calculations in Euclidean geometry or the calculations with force and work in the mechanics of particles. The analogy becomes very clear in the case of F_Z if, in place of the $x_1, x_2, \ldots$ in $\mathfrak{R}_\infty$, we consider the ordinary points $x_1, \ldots, x_n$ of an $\mathfrak{R}_n$ (for which the operations $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ can be defined in the same way). In particular, for $n = 3$ we have the conditions of ordinary space. Under certain circumstances, it is more appropriate to regard the complexes $x_1, \ldots, x_n$ not as points but as vectors, directed from the point $0, \ldots, 0$ to the points $x_1, \ldots, x_n$.

In order to define abstract Hilbert space, we then take as a basis the fundamental vector operations af, $f \pm g$, (f, g). We shall consider all $\mathfrak{R}_n$ simultaneously with $\mathfrak{R}_\infty$, as will appear in the discussion to which we now proceed. Therefore, where we do not wish to distinguish between $\mathfrak{R}_\infty$ and the $\mathfrak{R}_n$, we shall use $\mathfrak{R}$ as the common term for the space.

First of all we postulate for $\mathfrak{R}$ the typical vector properties:[37]

A. $\mathfrak{R}$ is a linear space.

That is: an addition $f+g$ and a "scalar" multiplication af are defined in $\mathfrak{R}$ (for f, g elements of $\mathfrak{R}$, a a complex number: $f + g$ and af belong to $\mathfrak{R}$), and $\mathfrak{R}$ has a null element.[38] The well-known rules of calculation for vector algebra then hold for this space:

$$f + g = g + f \qquad \text{(commutative law of addition)}$$

$$(f + g) + h = f + (g + h) \qquad \text{(associative law of addition)}$$

$$\left.\begin{aligned} (a + b)f &= af + bf \\ a(f + g) &= af + ag \end{aligned}\right\} \qquad \text{(distributive law of multiplication)}$$

$$\left.\begin{aligned} 0f &= 0 \\ 1f &= f \end{aligned}\right\} \qquad \text{(role of 0 and 1)}$$

The rules of calculation not mentioned here follow directly from these postulates.

[37] The characterization of $\mathfrak{R}_n$ by **A**, **B**, $\mathbf{C}^{(n)}$ originated with Weyl (see *Raum, Zeit, Materie*, Berlin (1921)). If we desire to obtain $\mathfrak{R}_\infty$ instead of $\mathfrak{R}_n$, then $\mathbf{C}^{(n)}$ must naturally be replaced by $\mathbf{C}^{(\infty)}$. It is in this case only that **D** and **E** become necessary; see the discussion later in the text.

[38] Besides the origin, or the null vector of $\mathfrak{R}$, there is also the number 0, so that the same symbol is used for two things. The relations are such, however, that no confusion should arise.

For example: the role of the null vector in addition:

$$f + 0 = 1 \cdot f + 0 \cdot f = (1 + 0) \cdot f = 1 \cdot f = f$$

Or the uniqueness of subtraction: we define $-f = (-1) \cdot f$, $f - g = f + (-g)$; then

$$\left.\begin{aligned} (f - g) + g &= (f + (-g)) + g \\ &= f + ((-g) + g) \\ (f + g) - g &= (f + g) + (-g) \\ &= (f + (g + (-g))) \end{aligned}\right\} \begin{aligned} &= f + ((-1) \cdot g + 1 \cdot g) \\ &= f + ((-1) + 1) \cdot g \\ &= f + 0 \cdot g = f + 0 = f \end{aligned}$$

Or the distributive laws of multiplication with subtraction:

$$\begin{aligned} a \cdot (f - g) &= a \cdot f + a \cdot (-g) = af + a(-(1) \cdot g) = af + (a \cdot (-1)) \cdot g \\ &= af + ((-1) \cdot a) \cdot g = af + (-1) \cdot (ag) = af + (-ag) \\ &= af - ag \\ (a - b)f &= a \cdot f + (-b) \cdot f = af + ((-b)) \cdot f = af + (-1) \cdot (bf) \\ &= af + (-bf) = af - bf \end{aligned}$$

It is not worthwhile to pursue these matters any further; it ought to be clear that all the rules of the linear vector calculus are valid here.

We can therefore introduce the concept of *linear independence* for elements $f_1, \ldots, f_k$ of $\mathfrak{R}$ in the same way as this is done for vectors:

> DEFINITION 1. The elements $f_1, \ldots, f_k$ are linearly independent if it follows from $a_1 f_1 + \cdots + a_k f_k = 0$ ($a_1, \ldots, a_k$ complex numbers) that $a_1 = \cdots = a_k = 0$.

We further define the analog of the linear entities occurring in the vector calculus (the line, plane, etc., passing through the origin), the linear manifold.

> DEFINITION 2. The subset $\mathfrak{M}$ of $\mathfrak{R}$ is called a linear manifold if it contains all the linear combinations $a_1 f_1 + \cdots + a_k f_k$ of any k ($= 1, 2, \ldots$) of its elements $f_1, \ldots, f_k$.[39] If $\mathcal{A}$ is an arbitrary subset of $\mathfrak{R}$, then the set of all $a_1 f_1 + \cdots + a_k f_k$ ($k = 1, 2, \ldots$; $a_1, \ldots, a_k$ arbitrary complex numbers; $f_1, \ldots, f_k$ arbitrary elements of $\mathcal{A}$) is a linear manifold, which evidently contains $\mathcal{A}$. It is called "the linear manifold spanned by $\mathcal{A}$," and is symbolized by $\{\mathcal{A}\}$.

Before we develop this concept any further, let us formulate the next basic principle of the vector calculus, the existence of the inner product.

[39] It would be sufficient to require: if f belongs to $\mathfrak{M}$ then af also; if f, g then $f + g$ also. Then if the $f_1, \ldots, f_k$ belong to $\mathfrak{M}$, the $a_1 f_1, \ldots, a_k f_k$ do also, and hence successively the $a_1 f_1 + a_2 f_2$, $a_1 f_1 + a_2 f_2 + a_3 f_3$, ..., $a_1 f_1 + \cdots + a_k f_k$ do too.

B. An Hermitian inner product is defined in $\mathfrak{R}$.

That is: (f, g) is defined (f, g in $\mathfrak{R}$; (f, g) is a complex number), and it has the following properties:[40]

$$\begin{aligned}
(f' + f'', g) &= (f', g) + (f'', g) && \text{(distributive law for the first factor)}\\
(a \cdot f, g) &= a \cdot (f, g) && \text{(associative law for the first factor)}\\
(f, g) &= \overline{(g, f)} && \text{(Hermitian symmetry)}\\
(f, f) &\geqslant 0 && \text{(definite form)}\\
&= 0 \text{ only if } f = 0
\end{aligned}$$

In addition, the corresponding relations for the second factor follow from the two properties of the first factor, because of the Hermitian symmetry (we exchange f and g, and take the complex conjugate of both sides):

$$\begin{aligned}
(f, g' + g'') &= (f, g') + (f, g'')\\
(f, a \cdot g) &= \overline{a} \cdot (f, g)
\end{aligned}$$

This inner product is of great importance, because it makes possible the definition of length. In Euclidean space, the magnitude of a vector is defined by $\|f\| = \sqrt{(f, f)}$,[41] and the distance between two points f, g is defined by $\|f - g\|$. We shall start from this point.

DEFINITION 3. The "magnitude" of an element f of $\mathfrak{R}$ is $\|f\| = \sqrt{(f, f)}$, the distance between f, g is $\|f - g\|$.[42]

We shall see that this concept possesses all the properties of distance. For this purpose, we prove the following:

THEOREM 1. $$|(f, g)| \leqslant \|f\| \cdot \|g\|$$

PROOF: First we write

$$\begin{aligned}
\|f\|^2 + \|g\|^2 - 2\mathrm{Re}(f, g) &= (f, f) + (g, g) - (f, g) - (g, f)\\
&= (f - g, f - g) \geqslant 0
\end{aligned}$$

[40] (f, f) is a real number because of the Hermitian symmetry; indeed, for $f = g$ this gives $(f, f) = \overline{(f, f)}$.

[41] If f has the components $x_1, \ldots, x_n$, then by the observations made in $\boldsymbol{\gamma}$, **II.1** (if we restrict ourselves to a finite number of components),

$$\sqrt{(f, f)} = \left(\sum_{\nu=1}^{n} |x_\nu|^2 \right)^{\frac{1}{2}}$$

i.e., the ordinary Euclidean length.

[42] Since (f, f) is real and $\geqslant 0$, $\|f\|$ real, and the square root is chosen $\geqslant 0$. The same holds for $\|f - g\|$.

$$\mathrm{Re}(f,g) \leqslant \tfrac{1}{2}\big(\|f\|^2 + \|g\|^2\big)$$

(If $z = u + iv$ is a complex number—u, v real—then $\mathrm{Re}\, z, \mathrm{Im}\, z$ represent respectively the real and imaginary parts of z, *i.e.*, $\mathrm{Re}\, z = u, \mathrm{Im}\, z = v$.) If we replace f, g by $af, (1/a)g$ (a real, > 0) then the left side is not changed, as can easily be seen. But on the right we obtain

$$\tfrac{1}{2}\big(a^2\|f\|^2 + a^{-2}\|g\|^2\big)$$

Since this expression is $\geqslant \mathrm{Re}(f,g)$, the inequality holds in particular for its minimum, which amounts to $\|f\| \cdot \|g\|$. (This value is taken on for $f, g \neq 0$ at

$$a = \left(\frac{\|g\|}{\|f\|}\right)^{\frac{1}{2}}$$

and for $f = 0$ or $g = 0$ as $a \to +\infty$ or $a \to +0$, respectively.) Therefore

$$\mathrm{Re}(f,g) \leqslant \|f\| \cdot \|g\|$$

If we replace f, g in this by $e^{i\alpha}f, g$ (α real), then the right side of the equation does not change (because of

$$(af, ag) = a\overline{a}(f,f) = |a|^2(f,f)$$

we have

$$\|af\| = |a| \cdot \|f\|$$

therefore, for $|a| = 1$, $\|af\| = \|f\|$), while the left side goes over into

$$\mathrm{Re}\big(e^{i\alpha}(f,g)\big) = \cos\alpha\, \mathrm{Re}(f,g) - \sin\alpha\, \mathrm{Im}(f,g)$$

This clearly has a maximum

$$\sqrt{\big(\mathrm{Re}(f,g)\big)^2 + \big(\mathrm{Im}(f,g)\big)^2} = |(f,g)|$$

from which the proposition follows:

$$|(f,g)| \leqslant \|f\| \cdot \|g\|$$

COROLLARY: For the equality to hold, f, g must be identical except for a constant (complex) factor.

PROOF: For the equality to hold in the relation

$$\mathrm{Re}(f,g) \leqslant \tfrac{1}{2}\big(\|f\|^2 + \|g\|^2\big)$$

$(f - g, f - g)$ must be zero; *i.e.*, $f = g$. In the transition from this expression to $|(f,g)| \leqslant \|f\| \cdot \|g\|$, f, g are replaced by $e^{i\alpha}af, (1/a)g$ (a, α real, $a > 0$) whenever neither f nor $g = 0$. In order for the equality to hold in this case we must therefore have

$$e^{i\alpha}af = (1/a)g, \quad \textit{i.e.} \quad g = a^2e^{i\alpha}f = cf \ (c \neq 0)$$

Conversely, for f or $g = 0$, or $g = cf$ ($c \neq 0$), the equality clearly holds.

THEOREM 2. $\|f\| \geqslant 0$ and $= 0$ only if $f = 0$. Also,

$$\|a \cdot f\| = |a| \cdot \|f\|$$
$$\|f + g\| \leqslant \|f\| + \|g\|$$

always, the equality holding only if f, g are identical except for a constant, real factor $\geqslant 0$.

PROOF: We have already seen above that the first two propositions are correct. We prove the inequality of the third in the following manner:

$$\begin{aligned}(f+g, f+g) &= (f,f) + (g,g) + (f,g) + (g,f) \\ &= \|f\|^2 + \|g\|^2 + 2\mathrm{Re}(f,g) \\ &\leqslant \|f\|^2 + \|g\|^2 + 2\|f\| \cdot \|g\| \\ &= \big(\|f\| + \|g\|\big)^2 \\ \|f+g\| &\leqslant \|f\| + \|g\|\end{aligned}$$

In order that the equality hold, $\mathrm{Re}(f,g)$ must be equal to $\|f\| \cdot \|g\|$, which requires f or $g = 0$, or $g = a^2 f = cf$ (c real, > 0), by reason of the observations made in the proof of the above corollary. Conversely, it is clear in this case that the equality holds.

From THEOREM 2 it follows immediately that the distance $\|f - g\|$ has the following properties: f, g have the distance 0 for $f = g$, and never otherwise. The distance between g, f is the same as between f, g. The distance of f, h is less than or equal to the sum of the distances f, g and g, h. The equality exists only if $g = af + (1-a)h$ (a real, $0 \leqslant a \leqslant 1$).[43] The distance of af, ag is $|a|$ times the distance of f, g.

Now these are the very same properties of the concept of length which make it possible in geometry (and topology) to base the concepts of continuity, limit, limit point, etc. on the concept of length. We wish to make use of this, and define:

A function $F(f)$ in $\mathfrak{R}$ (*i.e.*, for which f is defined in $\mathfrak{R}$, and which has for values either always points in $\mathfrak{R}$ or always complex numbers) is continuous at the point f_0 (in $\mathfrak{R}$) if for each $\epsilon > 0$ there exists a $\delta > 0$ such that $\|f - f_0\| < \delta$ implies $\|F(f) - F(f_0)\| < \epsilon$ or $|F(f) - F(f_0)| < \epsilon$ (according to whether the F values are points in $\mathfrak{R}$ or complex numbers). This function is said to be bounded in $\mathfrak{R}$ or in a given subset of $\mathfrak{R}$ if always $\|F(f)\| \leqslant C$ or $|F(f)| \leqslant C$ (C a constant, suitably chosen, but fixed). Analogous definitions hold for several variables. A sequence $f_1, f_2, \ldots$ converges to f, or has the limit f, if the numbers

[43] By THEOREM 2 (which is applied here to $f-g, g-h$), $f-g=0$; *i.e.*, $g=f$ or $g-h=0$; *i.e.*, $g=h$ or $g-h=c\,(f-g)$ (c real, >0); *i.e.*, $g=\frac{c}{c+1}f+\frac{1}{c+1}h$; *i.e.*, $g=af+(1-a)h$ with a respectively equal to $1, 0, \frac{c}{c+1}$. Geometrically, this means that the point g is collinear with f, h.

$\|f_1 - f\|, \|f_2 - f\|, \ldots$ converge to zero. A point is a limit point of a set $\mathcal{A}$ (subset of $\mathcal{R}$!) if it is a limit of a sequence from $\mathcal{A}$.[44] In particular, $\mathcal{A}$ is said to be *closed* if it contains all its limit points, and it is said to be *everywhere dense* if its limit points encompass all of $\mathcal{A}$.

We have yet to prove that af, $f + g$, (f, g) are continuous in all their variables. Since

$$\|af - af'\| = |a| \cdot \|f - f'\|$$

$$\|(f + g) - (f' + g')\| = \|(f - f') + (g + g')\| \leqslant \|f - f'\| + \|g - g'\|$$

the first two propositions are clearly true. Furthermore, from

$$\|f - f'\| < \epsilon, \quad \|g - g'\| < \epsilon$$

if we substitute $f' - f = \phi$, $g' - g = \psi$, it follows that

$$\begin{aligned} |(f, g) - (f', g')| &= |(f, g) - (f + \phi, g + \psi)| \\ &= |(\phi, g) + (f, \psi) + (\phi, \psi)| \\ &\leqslant |(\phi, g)| + |(f, \psi)| + |(\phi, \psi)| \\ &\leqslant \|\phi\| \cdot \|g\| + \|f\| \cdot \|\psi\| + \|\phi\| \cdot \|\psi\| \\ &\leqslant \epsilon\big(\|f\| + \|g\| + \epsilon\big) \end{aligned}$$

As $\epsilon \to 0$ this expression approaches zero, and can be made smaller than any $\delta > 0$.

The properties **A**, **B** permit us, as we see, to state a great deal about $\mathcal{R}$, yet they are not sufficient to enable us to distinguish the $\mathcal{R}_n$ from each other and from $\mathcal{R}_\infty$. No mention has been made so far of the *number of dimensions*. This concept is clearly associated with the maximum number of linearly independent vectors. If $n = 0, 1, 2, \ldots$ then we state for this n:

> **C**$^{(n)}$. There are exactly n linearly independent vectors. That is, it is possible to specify n such vectors, but not $n + 1$.

If there exists no maximum number, then we have:

> **C**$^{(\infty)}$. There are arbitrarily many linearly independent vectors.

That is, for each $k = 1, 2, \ldots$ we can specify k such vectors.

C is then not an essentially new postulate. If **A**, **B** hold, then either **C**$^{(n)}$ or **C**$^{(\infty)}$ must hold. We obtain a different space $\mathcal{R}$ depending upon which we decide upon. We shall see that if follows from **C**$^{(n)}$ that $\mathcal{R}$ has all the properties of the n-dimensional (complex) Euclidean space. **C**$^{(\infty)}$, on the other hand, is

[44] The following definition of the limit point is also useful: for each $\epsilon > 0$ let there be an f' of $\mathcal{A}$ with $\|f - f'\| < \epsilon$. The equivalence of the two definitions can be shown exactly as in ordinary analysis.

not sufficient to guarantee the essential identity of $\mathfrak{R}$ with the Hilbert space $\mathfrak{R}_\infty$. Rather, we need two additional postulates **D**, **E**. More precisely, the situation is the following: We shall show that an $\mathfrak{R}$ with **A**, **B**, **C** has all the properties of $\mathfrak{R}_n$, in particular the **D**, **E**, which will be formulated (and which therefore follow from **A**, **B**, $\mathbf{C}^{(\infty)}$). Furthermore, we shall show that an $\mathfrak{R}$ with **A**, **B**, **C**, **D**, **E** has all the properties of $\mathfrak{R}_\infty$, but that in this case **D**, **E** are essential (*i.e.*, they do not follow from **A**, **B**, $\mathbf{C}^{(\infty)}$). We therefore proceed to the formulation of **D**, **E**, but the proof that all $\mathfrak{R}_n$, $\mathfrak{R}_\infty$ possess these properties will only be given later (see **II.3**).

D. $\mathfrak{R}$ is *complete*.[45]

That is, if a sequence $f_1, f_2, \ldots$ in $\mathfrak{R}$ satisfies the Cauchy convergence criterion (for each $\epsilon > 0$ there exists an $N = N(\epsilon)$ such that $\|f_m - f_n\| < \epsilon$ for all $m, n > N$), then it is convergent; *i.e.*, it possesses a limit f (see the definition of this concept given above).

E. $\mathfrak{R}$ is *separable*.[45]

That is, there is a sequence $f_1, f_2, \ldots$ in $\mathfrak{R}$ that is everywhere dense in $\mathfrak{R}$.

In **II.2** we shall, as we have said, develop the "geometry" of $\mathfrak{R}$ from these basic assumptions, and will be led to distinguish two cases: $\mathfrak{R}_n$ and $\mathfrak{R}_\infty$.

2. THE GEOMETRY OF HILBERT SPACE

We begin with two definitions: The first contains as much of trigonometry as is necessary for our purposes: the concept of right angle—orthogonality.

DEFINITION 4. Two f, g of $\mathfrak{R}$ are *orthogonal* if $(f, g) = 0$. Two linear manifolds $\mathfrak{M}$ and $\mathfrak{N}$ are orthogonal if each element of $\mathfrak{M}$ is orthogonal to each element of $\mathfrak{N}$. A set $\mathfrak{O}$ is called an orthonormal set if for all f, g of $\mathfrak{O}$

$$(f, g) = \begin{cases} 1 & \text{for } f = g \\ 0 & \text{for } f \neq g \end{cases}$$

(*i.e.*, each pair of elements are orthogonal and each element has the magnitude 1).[46] Furthermore, $\mathfrak{O}$ is complete if it is not a subset of any other normal set that contains additional elements.[47]

[45] We use the topological term for brevity (see Hausdorff, *Mengenlehre*, Berlin, 1927); it is explained further below in the text.

[46] Indeed, $\|f\| = \sqrt{(f, f)} = 1$.

[47] As we see, complete orthonormal sets correspond to the cartesian coordinate systems (*i.e.*, the unit vectors pointing in the directions of the axes) in $\mathfrak{R}_n$.

We observe further: That the orthonormal set is complete means obviously that no f exists, with $\|f\| = 1$, which is orthogonal to the whole $\mathfrak{O}$ (see Note 46). But if f were merely different from zero, and orthogonal to the whole set $\mathfrak{O}$, then all of the above would be satisfied for

$$f' = \frac{1}{\|f\|} \cdot f$$

(of course, $\|f\| > 0$):

$$\|f'\| = \frac{1}{\|f\|}\|f\| = 1 \quad : \quad f' \text{ orthogonal to } \mathfrak{O}$$

Therefore, the completeness of $\mathfrak{O}$ means that each f orthogonal to the entire set must vanish.

The second definition is such that it is important only in $\mathfrak{R}_\infty$, since in $\mathfrak{R}_n$ every linear manifold is of the type described by it (see the end of **II.3**). Therefore we cannot give an intuitive-geometrical picture of its meaning.

DEFINITION 5. A linear manifold which is also closed is called a *closed linear manifold*. If $\mathcal{A}$ is any set in $\mathfrak{R}$, and we add to $\{\mathcal{A}\}$ (the linear manifold spanned by $\mathcal{A}$) all its limit points, we obtain a closed linear manifold that contains $\mathcal{A}$. It is also a subset of every other closed linear manifold which contains $\mathcal{A}$.[48] We call it the closed linear manifold spanned by $\mathcal{A}$, and symbolize it by $[\mathcal{A}]$.

We now go on to the more detailed analysis of $\mathfrak{R}$, in particular of complete orthogonal sets. For theorems which require $\mathbf{C}^{(n)}$ or $\mathbf{C}^{(\infty)}$, **D**, **E** in addition to **A**, **B** we add the index $^{(n)}$ or $^{(\infty)}$ respectively. Such indices are omitted for those theorems which are common to both cases.

THEOREM $3^{(n)}$. Every orthonormal set has $\leqslant n$ elements, and is complete if and only if it has n elements.

NOTE. It follows from the first proposition that there exists a maximal value for the numbers of elements of orthonormal sets; those orthonormal sets for which this maximal value is reached are by definition complete. By virtue of this theorem, complete orthonormal sets exist in the case $\mathbf{C}^{(n)}$ and every such set has n elements.

PROOF: Each orthonormal set is (if it is finite) linearly independent. If the elements are $\phi_1, \phi_2, \ldots, \phi_m$ if follows from

$$a_1\phi_1 + \cdots + a_m\phi_m = 0$$

[48] As a linear manifold, this must contain $\{\mathcal{A}\}$, and since it is closed, also the limit points of $\{\mathcal{A}\}$.

by forming the inner product with ϕ_μ $(\mu = 1, 2, \ldots, m)$ that $a_\mu = 0$. So, by $\mathbf{C}^{(n)}$, the set cannot have $n+1$ elements. An arbitrary orthonormal set therefore can have no subsets with $n + 1$ elements. Therefore it is finite and has $\leqslant n$ elements.

A set with n elements permits no extension, and is therefore complete. But with $m < n$ elements, $\phi_1, \phi_2, \ldots, \phi_m$ is not complete. Indeed, among the linear combinations $a_1\phi_1 + \cdots + a_m\phi_m$ there cannot be $n > m$ linearly independent ones. Hence there must exist, by $\mathbf{C}^{(n)}$, an element f which differs from all $a_1\phi_1 + \cdots + a_m\phi_m$, *i.e.*, for which

$$\psi = f - a_1\phi_1 - \cdots - a_m\phi_m$$

is always different from zero. Now $(\psi, \phi_\mu) = 0$ means that $a_\mu = (f, \phi_\mu)$ $(\mu = 1, 2, \ldots, m)$. Therefore this condition can be satisfied for all $\mu = 1, 2, \ldots, m$ simultaneously, thus furnishing a ψ which shows that the set $\phi_1, \phi_2, \ldots, \phi_m$ is incomplete.

THEOREM $3^{(\infty)}$. Every orthonormal set is a finite or a countably infinite set; if it is complete then it is certainly infinite.

NOTE. We can therefore write all orthonormal sets as sequences: $\phi_1, \phi_2, \ldots$ (perhaps being terminated; *i.e.*, finite), which we shall actually do. It should be observed that the infinite number of elements of the set is necessary for its completeness, but, unlike the case $\mathbf{C}^{(n)}$, it is not sufficient.[49]

PROOF: Let $\mathfrak{O}$ be an orthonormal set, f, g two different elements belonging to it. Then

$$(f - g, f - g) = (f, f) + (g, g) - (f, g) - (g, f) = 2$$

$$\|f - g\| = \sqrt{2}$$

Now let $f_1, f_2, \ldots$ be the sequence which is everywhere dense in $\mathfrak{R}$. This sequence exists by postulate **E**. For each f of $\mathfrak{O}$ there exists an f_m of the sequence for which $\|f - f_m\| < \frac{1}{2}\sqrt{2}$. The corresponding f_m, f_n for f, g must be different, because it would follow from $f_m = f_n$ that

$$\begin{aligned} \|f - g\| &= \|(f - f_m) - (g - f_m) \\ &\leqslant \|f - f_m\| + \|g - f_m\| \\ &< \tfrac{1}{2}\sqrt{2} + \tfrac{1}{2}\sqrt{2} = \sqrt{2} \end{aligned}$$

Therefore, to each f of $\mathfrak{O}$ there corresponds an f_m of the sequence $f_1, f_2, \ldots$ with different f_m for different f. Therefore $\mathfrak{O}$ is finite or is a sequence.

[49] Let $\phi_1, \phi_2, \phi_3, \ldots$ be complete. Then $\phi_2, \phi_3, \ldots$ is not complete, but it is still infinite!

As in the proof of THEOREM $3^{(\infty)}$ we show the following: if there are $> m$ linearly independent elements in $\mathcal{R}$, a set $\phi_1, \phi_2, \ldots, \phi_m$ cannot be complete. But since by $\mathbf{C}^{(\infty)}$ this holds for all m, a complete set must be infinite.

The theorems which now follow, insofar as they are concerned with convergence, apply only to $\mathbf{C}^{(\infty)}$, but it is more desirable to formulate them generally, because of their other implications.

> THEOREM 4. Let $\phi_1, \phi_2, \ldots$ be an orthonormal set. Then all series $\sum_\nu (f, \phi_\nu)\overline{(g, \phi_\nu)}$, insofar as they have infinitely many terms, are absolutely convergent. In particular, for $f = g$, $\sum_\nu |(f, \phi_\nu)|^2 \leqslant |f|^2$.

PROOF: Let $a_\nu = (f, \phi_\nu)$, $\nu = 1, 2, \ldots, N$. Then $f - \sum_{\nu-1}^{N} a_\nu \phi_\nu = \psi$ is orthogonal to all ϕ_ν, $\nu = 1, 2, \ldots, N$ (see the proof of THEOREM $3^{(n)}$). Since $f = \sum_{\nu=1}^{N} a_\nu \phi_\nu + \psi$ then

$$\begin{aligned}(f, f) &= \sum_{\mu,\nu=1}^{N} a_\mu \overline{a}_\nu (\phi_\mu, \phi_\nu) + \sum_{\nu=1}^{N} a_\nu (\phi_\nu, \psi) + \sum_{\nu=1}^{N} \overline{a}_\nu (\psi, \phi_\nu) + (\psi, \psi) \\ &= \sum_{\nu=1}^{N} |a_\nu|^2 + (\psi, \psi) \\ &\geqslant \sum_{\nu=1}^{N} |a_\nu|^2\end{aligned}$$

i.e., $\sum_{\nu=1}^{N} |a_\nu|^2 \leqslant \|f\|^2$. If the set $\phi_1, \phi_2, \ldots$ is finite, then it follows directly that $\sum_{\nu=1}^{N} |a_\nu|^2 = \|f\|^2$; if it is infinite, then $N \to \infty$ results in the absolute convergence of $\sum_\nu |a_\nu|^2$, as well as in the fact that it is $\leqslant \|f\|^2$. This establishes the second proposition. Because of

$$|(f, \phi_\nu)\overline{(g, \phi_\nu)}| \leqslant \tfrac{1}{2}\{|(f, \phi_\nu)|^2 + |(g, \phi_\nu)|^2\}$$

the more general convergence statement of the first proposition follows from the fact of convergence just stated.

> THEOREM 5. Let $\phi_1, \phi_2, \ldots$ be an infinite orthonormal set. Then the series $\sum_{\nu=1}^{\infty} x_\nu \phi_\nu$ converges if and only if $\sum_{\nu=1}^{\infty} |x_\nu|^2$ does (the latter series has as its terms real, non-negative numbers, and is therefore convergent or else diverges to $+\infty$).

PROOF: Since this proposition has significance only for $\mathbf{C}^{(\infty)}$, we may then use $\mathbf{D}$, the Cauchy criterion for convergence. The sum $\sum_{\nu=1}^{\infty} x_\nu \phi_\nu$ then converges; *i.e.*, the sequence of partial sums $\sum_{\nu=1}^{N} x_\nu \phi_\nu$ converges as $N \to \infty$, if for each $\epsilon > 0$ such that for L, $M > N$, $\| \sum_{\nu=1}^{L} x_\nu \phi_\nu - \sum_{\nu=1}^{M} x_\nu \phi_\nu \| < \epsilon$. We assume $L > M \geqslant N$, then

$$\| \sum_{\nu=1}^{L} x_\nu \phi_\nu - \sum_{\nu=1}^{M} x_\nu \phi_\nu \| = \| \sum_{\nu=M+1}^{L} x_\nu \phi_\nu \| < \epsilon$$

$$\begin{aligned}\|\sum_{\nu=M+1}^{L} x_\nu\phi_\nu\|^2 &= \Big(\sum_{\nu=M+1}^{L} x_\nu\phi_\nu, \sum_{\nu=M+1}^{L} x_\nu\phi_\nu\Big)\\ &= \sum_{\mu,\nu=M+1}^{L} x_\mu\overline{x}_\nu(\phi_\mu,\phi_\nu)\\ &= \sum_{\nu=M+1}^{L}|x_\nu|^2\\ &= \sum_{\nu=1}^{L}|x_\nu|^2 - \sum_{\nu=1}^{M}|x_\nu|^2\end{aligned}$$

therefore

$$0 \leqslant \sum_{\nu=1}^{L}|x_\nu|^2 - \sum_{\nu=1}^{M}|x_\nu|^2 < \epsilon^2$$

But this is exactly the Cauchy convergence criterion for the sequence

$$\sum_{\nu=1}^{N}|x_\nu|^2 \quad : \quad N \to \infty$$

i.e., for the series $\sum_{\nu=1}^{\infty}|x_\nu|^2$.

> COROLLARY. For $f = \sum_\nu x_\nu\phi_\nu$, $(f,\phi_\nu) = x_\nu$ (regardless of whether the orthogonal set is finite or infinite—in the latter case, of course, convergence is assumed).

PROOF: For $N \geqslant \nu$ we have

$$\Big(\sum_{\mu=1}^{N} x_\mu\phi_\mu, \phi_\nu\Big) = \sum_{\mu=1}^{N} x_\mu(\phi_\mu,\phi_\nu) = x_\nu$$

For a finite set $\phi_1, \phi_2, \ldots$ we can set N equal to the highest index; for infinite sets $\phi_1, \phi_2, \ldots$ we can let $N \to \infty$ because of the continuity of the inner product. In either case, $(f,\phi_\nu) = x_\nu$ results.

> THEOREM 6 . Let $\phi_1, \phi_2, \ldots$ be an orthonormal set, f arbitrary. Then $f' = \sum_\nu x_\nu\phi_\nu$, $x_\nu = (f,\phi_\nu)$ $(\nu = 1, 2, \ldots)$ is always convergent if the series is infinite. The expression $f - f'$ is orthogonal to $\phi_1, \phi_2, \ldots$

PROOF: The convergence follows from THEOREMS 4 & 5, and according to the corollary of THEOREM 5

$$(f',\phi_\nu) = x_\nu = (f,\phi_\nu), \qquad (f - f',\phi_\nu) = 0$$

After these preparations, we can give the general criteria; *i.e.*, even for $\mathbf{C}^{(\infty)}$, for the completeness of an orthonormal set.

THEOREM 7. Let $\phi_1, \phi_2, \ldots$ be an orthonormal set. For completeness, each one of the following conditions is necessary and sufficient:

$\boldsymbol{\alpha}$) The closed linear manifold $[\phi_1, \phi_2, \ldots]$ spanned by $\phi_1, \phi_2, \ldots$ is equal to $\mathcal{R}$.

$\boldsymbol{\beta}$) It is always true that $f = \sum_\nu x_\nu \phi_\nu$, $x_\nu = (f, \phi_\nu)$ $(\nu = 1, 2, \ldots,$ convergence by THEOREM 6).

$\boldsymbol{\gamma}$) It is always true that

$$(f, g) = \sum_\nu (f, \phi_\nu)\overline{(g, \phi_\nu)}$$

(absolute convergence by THEOREM 4).

PROOF: If $\phi_1, \phi_2, \ldots$ is complete, then $f = \sum_\nu x_\nu \phi_\nu$ is equal to zero $(x_\nu = (f, \phi_\nu)$, $\nu = 1, 2, \ldots)$, since it is orthogonal to $\phi_1, \phi_2, \ldots$ by THEOREM 6. Then $\boldsymbol{\beta}$ is satisfied. If $\boldsymbol{\beta}$ holds, then each f is the limit of its partial sums $\sum_{\nu=1}^{N} x_\nu \phi_\nu$ $N \to \infty$ (if N is infinite) and therefore belongs to $[\phi_1, \phi_2, \ldots]$. Therefore $[\phi_1, \phi_2, \ldots] = \mathcal{R}$; *i.e.*, $\boldsymbol{\alpha}$ is satisfied. If $\boldsymbol{\alpha}$ holds, then we may argue as follows: If f is orthogonal to all $\phi_1, \phi_2, \ldots$ then it is also orthogonal to their linear combinations, and by reason of continuity also to their limit points; *i.e.*, to all $[\phi_1, \phi_2, \ldots]$. Therefore it is orthogonal to all $\mathcal{R}$, and hence to itself, $(f, f) = 0$, $f = 0$. Consequently, $\phi_1, \phi_2, \ldots$ is complete.

We have then the logical scheme:

$$\text{completeness} \to \boldsymbol{\beta} \to \boldsymbol{\alpha} \to \text{completeness}$$

i.e., $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ have been shown to be necessary and sufficient.

From $\boldsymbol{\gamma}$ it follows that if f is orthogonal to $\phi_1, \phi_2, \ldots$, and if we set $f = g$, then we obtain $(f, f) = \sum_\nu 0 \cdot 0 = 0$, $f = 0$; *i.e.*, $\phi_1, \phi_2, \ldots$ is complete. On the other hand, from $\boldsymbol{\beta}$ (which is now equivalent to completeness),

$$\begin{aligned}(f, g) &= \lim_{N\to\infty} \Big(\sum_{\mu=1}^{N} (f, \phi_\mu) \cdot \phi_\mu \, , \sum_{\nu=1}^{N} (g, \phi_\nu) \cdot \phi_\nu \Big) \\ &= \lim_{N\to\infty} \sum_{\mu,\nu=1}^{N} (f, \phi_\mu)\overline{(g, \phi_\nu)} \cdot (\phi_\mu, \phi_\nu) \\ &= \lim_{N\to\infty} \sum_{\nu=1}^{N} (f, \phi_\nu)\overline{(g, \phi_\nu)} = \sum_{\nu=1}^{\infty} (f, \phi_\nu)\overline{(g, \phi_\nu)}\end{aligned}$$

(if the set is finite, then the limit process is unnecessary); *i.e.*, $\boldsymbol{\gamma}$ is also a necessary and sufficient condition.

THEOREM 8. To each set $f_1, f_2, \ldots$ there corresponds an orthonormal set $\phi_1, \phi_2, \ldots$ which spans the same linear manifold as the former set (both sets can be finite).

PROOF: First we replace $f_1, f_2, \ldots$ by a subset $g_1, g_2, \ldots$ which spans the same linear manifold and which consists of linearly independent elements. This may be done as follows. Let g_1 be the first f_n which is different from zero; g_2 be the first f_n which is different from $a_1 g_1$; g_3 be the first f_n which is different from all $a_1 g_1 + a_2 g_2$; ... (if for any p there exists no f_n which is different from all $a_1 f_1 + a_2 f_2 + \cdots + a_p f_p$ we terminate the set with g_p). These $g_1, g_2, \ldots$ obviously furnish the desired result.

We now form

$$\gamma_1 = g_1 \ , \qquad \phi_1 = \frac{1}{\|\gamma_1\|} \cdot \gamma_1$$

$$\gamma_2 = g_2 - (g_2, \phi_1) \cdot \phi_1 \ , \qquad \phi_2 = \frac{1}{\|\gamma_2\|} \cdot \gamma_2$$

$$\gamma_3 = g_3 - (g_3, \phi_1) \cdot \phi_1 - (g_3, \phi_2) \cdot \phi_2 \ , \qquad \phi_3 = \frac{1}{\|\gamma_3\|} \cdot \gamma_3$$

(this is the well-known Schmidt orthogonalization process). Each ϕ_p construction is actually possible; *i.e.*, the denominators $\|\gamma_p\|$ are all different from zero. For otherwise, if $\gamma_p = 0$, then g_p would be a linear combination of the $\phi_1, \ldots, \phi_{p-1}$; *i.e.*, of the $g_1, \ldots, g_{p-1}$, which is contrary to the hypothesis. Furthermore, it is clear that g_p is a linear combination of the $\phi_1, \ldots, \phi_p$ and ϕ_p is a linear combination of the $g_1, \ldots, g_p$. Therefore $g_1, \ldots, g_p$ and $\phi_1, \ldots, \phi_p$ determine the same linear manifold.

Finally, by construction $\|\phi_p\| = 1$, and for $q < p$, $(\gamma_p, \phi_q) = 0$, therefore $(\gamma_p, \gamma_q) = 0$. Since we can interchange p, q, the latter statement holds for $p \neq q$. Therefore $\phi_1, \phi_2, \ldots$ is an orthonormal set.

> THEOREM 9. Corresponding to each closed linear manifold $\mathfrak{M}$ there is an orthonormal set which spans the same $\mathfrak{M}$ as a closed linear manifold.

PROOF: In the case $\mathbf{C}^{(n)}$ this theorem is immediate: Because $\mathfrak{M}$ satisfies **A**, **B**, $\mathbf{C}^{(n)}$, each linear manifold $\mathfrak{M}$ in $\mathfrak{R}$ satisfies **A**, **B**, $\mathbf{C}^{(m)}$ with $m \leqslant n$, so that the note on THEOREM $3^{(n)}$ is applicable to $\mathfrak{M}$: There is an orthonormal set $\phi_1, \ldots, \phi_m$ which is complete in $\mathfrak{M}$. Because of THEOREM $7\boldsymbol{\alpha}$, this is exactly the proposition to be proved. (As can be seen, the premise of the closed nature of $\mathfrak{M}$ is itself unnecessary, since it is actually proved. In this case, compare the statements concerning DEFINITION 5.)

In the case $\mathbf{C}^{(\infty)}$, we recall that $\mathfrak{R}$ is separable according to **E**. We want to show that $\mathfrak{M}$ is also separable—in general, that each subset of $\mathfrak{R}$ is separable. For this purpose, we form a sequence $f_1, f_2, \ldots$ everywhere dense in $\mathfrak{R}$ (see **E** in **II.1**), and for each f_n and $m = 1, 2, \ldots$ we form the sphere $\mathfrak{S}_{n,m}$ consisting of all f with $\|f - f_m\| < \frac{1}{m}$. For each $\mathfrak{S}_{n,m}$ which contains points of $\mathfrak{M}$, we select one such point: $g_{n,m}$. For some n, m this $g_{n,m}$ may be undefined, but the defined

points form a sequence in $\mathfrak{M}$.[50] Now let f be any point in $\mathfrak{M}$ and $\epsilon > 0$. Then there exists an m with $\frac{1}{m} < \frac{1}{2}\epsilon$, and an f_n with $\|f_n - f\| < \frac{1}{m}$. Since $\mathfrak{S}_{n,m}$ then contains a point of $\mathfrak{M}$ (namely f), g_{nm} is defined, and $\|f_n - g_{nm}\| < \frac{1}{m}$, therefore $\|f - g_{nm}\| < \frac{2}{m} < \epsilon$. Consequently, f is the limit point of the g_{nm} thus defined; hence this sequence yields the desired result.

We shall denote by $f_1, f_2, \ldots$ the sequence from $\mathfrak{M}$, everywhere dense in $\mathfrak{M}$. The closed linear manifold determined by it, $[f_1, f_2, \ldots]$, contains all its limit points, and hence all $\mathfrak{M}$; but, since $\mathfrak{M}$ is a closed linear manifold, and $f_1, f_2, \ldots$ belong to it, therefore $[f_1, f_2, \ldots]$ is a part of $\mathfrak{M}$—therefore it is equal to $\mathfrak{M}$. We now choose the orthonormal set $\phi_1, \phi_2, \ldots$ by THEOREM 8. Then

$$\{\phi_1, \phi_2, \ldots\} = \{f_1, f_2, \ldots\}$$

and if we add the limit points to both sides we obtain

$$[\phi_1, \phi_2, \ldots] = [\, f_1, f_2, \ldots] = \mathfrak{M}$$

But this was our proposition.

We now need only put $\mathfrak{M} = \mathfrak{R}$ in THEOREM 9 and we have by THEOREM 7α a complete orthonormal set $\phi_1, \phi_2, \ldots$ So we see: There are complete orthonormal sets. On the basis of this we can now show that $\mathfrak{R}$ is an $\mathfrak{R}_n$ or an $\mathfrak{R}_\infty$ (according to whether $\mathsf{C}^{(n)}$ or $\mathsf{C}^{(\infty)}$ holds); *i.e.*, all its properties are completely determined.

It is only necessary to show that $\mathfrak{R}$ allows a one-to-one mapping on the set of all $\{x_1, \ldots, x_n\}$ or of all $\{x_1, x_2, \ldots\}$ ($\sum_{\nu=1}^{\infty} |x_\nu|^2$ finite) respectively, in such a way that

$$1^\circ \quad af \longleftrightarrow \{ax_1, ax_2, \ldots\} \qquad \text{follows from} \quad f \longleftrightarrow \{x_1, x_2, \ldots\}$$

$$2^\circ \quad f + g \longleftrightarrow \{x_1 + y_1, x_2 + y_2, \ldots\} \qquad \text{follows from} \quad \begin{cases} f \longleftrightarrow \{x_1, x_2, \ldots\} \\ g \longleftrightarrow \{y_1, y_2, \ldots\} \end{cases}$$

$$3^\circ \quad (f, g) = \sum_{\nu=1}^{n \text{ or } \infty} x_\nu \overline{y}_\nu \qquad \text{follows from} \quad \begin{cases} f \longleftrightarrow \{x_1, x_2, \ldots\} \\ g \longleftrightarrow \{y_1, y_2, \ldots\} \end{cases}$$

(In the infinite case in 3° the absolute convergence must be shown.) We now specify the mapping $f \longleftrightarrow \{x_1, x_2, \ldots\}$.

Let $\phi_1, \phi_2, \ldots$ be a complete orthonormal set; in case $\mathsf{C}^{(n)}$ it terminates with ϕ_n, in case $\mathsf{C}^{(\infty)}$ is infinite (THEOREMS $3^{(n)}$ & $3^{(\infty)}$). We set

$$f = \sum_{\nu=1}^{n \text{ or } \infty} x_\nu \phi_\nu$$

By THEOREM 5 this series converges even in the infinite case (since $\sum_{\nu=1}^{\infty} |x_\nu|^2$ is finite); *i.e.*, the elements of either $\mathfrak{R}_n$ or $\mathfrak{R}_\infty$ are exhausted. By THEOREM 7β

[50] It should be recalled that a double sequence g_{nm} $(n, m = 1, 2, \ldots)$ can also be written as a simple sequence: $g_{11}, g_{12}, g_{21}, g_{13}, g_{22}, g_{31}, \ldots$

and because

$$\sum_{\nu=1}^{n \text{ or } \infty} |(f, \phi_\nu)|^2$$

is finite (THEOREM 4) the elements of $\mathcal{R}$ are also exhausted ($x_\nu = (f, \phi_\nu)$ is to be substituted). It is clear that only one f corresponds to each $\{x_1, x_2, \ldots\}$, while the converse follows from the corollary to THEOREM 5.

Statements 1°, 2° are obviously satisfied, while 3° follows from THEOREM 7$\boldsymbol{\gamma}$.

3. DIGRESSION ON THE CONDITIONS A–E [51]

We must still verify the proposition 2 at the end of **1.4**: That F_Z, F_Ω actually satisfy the conditions **A–E**. For this purpose, it is sufficient to consider F_Ω, because we have already shown in **II.2** that an $\mathcal{R}$ with **A–E** must be identical in all properties with $\mathcal{R}_\infty$; *i.e.*, with F_Ω, so that **A–E** must be valid for F_Z also. Moreover, we shall show the independence of the conditions **D**, **E** from **A–C**$^{(n)}$, mentioned in **II.2**, as well as the fact that they follow from **A–C**$^{(n)}$; *i.e.*, that they hold in $\mathcal{R}_n$. These three purely mathematical questions form the subject matter of this section.

We begin with the verification of **A–E** in F_Ω. For this we must rely upon the Lebesgue concept of the integral, for whose foundations reference should be made to special works on the subject.[52] (The Lebesgue integral is of importance to us only upon this occasion, and a knowledge of it is not necessary for the later chapters).

In **I.4** we had introduced Ω as the k-dimensional space of the $q_1, \ldots, q_k$ and F_Ω as the totality of all functions $f(q_1, \ldots, q_k)$ with finite

$$\underbrace{\int \cdots \int}_{\Omega} |f(q_1, \ldots, q_k)|^2 \, dq_1 \ldots dq_k$$

We now allow all the $q_1, \ldots, q_k$ to vary from $-\infty$ to $+\infty$. All our deductions would of course remain valid, and even the proofs would be carried over for the most part verbatim, if we were to limit the range of the $q_1, \ldots, q_k$ (so that Ω would be, for example, a half space, or the inside of a cube, or the inside of a sphere, or the outside of these figures, etc.)—indeed even if we were to choose Ω as a curved surface (e.g., as the surface of a sphere, etc.). But in order not to become lost in unnecessary complications (whose discussion can be carried out without difficulty by the reader himself, with the aid of our typical proof)

[51] This section is not necessary for the understanding of the later portions of the text.

[52] For example, Carathéodory, *Vorlesungen über reelle Functionen*, Leipzig, 1927, in particular pp. 237-274; Kamke, *Das Lebesguesche Integral*, Leipzig, 1925.

we limit ourselves to the simplest case just mentioned. We shall now go through **A–E** consecutively.

For A: We must show: If f, g belong to F_Ω then af, $f+g$ belong to it; *i.e.*, if

$$\int_\Omega |f|^2\,, \quad \int_\Omega |g|^2$$

(we abbreviate

$$\underbrace{\int\cdots\int}_{\Omega} |f(q_1,\ldots,q_k)|^2\,dq_1\ldots,dq_k\,, \quad \underbrace{\int\cdots\int}_{\Omega} |g(q_1,\ldots,q_k)|^2\,dq_1\ldots,dq_k$$

since no confusion can result) are finite, then

$$\int_\Omega |af|^2 = |a|^2 \int_\Omega |f|^2 \quad \text{and} \quad \int_\Omega |f \pm g|^2$$

are also finite. The first case is trivial, while the second is established, because of $|f+g|^2 = |f|^2 + |g|^2 \pm 2\mathrm{Re}\,(f\bar{g})$,[53] as soon as the finite nature of

$$\int_\Omega |f\cdot\bar{g}| = \int_\Omega |f||g|$$

is ascertained. But since $|f||g| \leqslant \frac{1}{2}\big(|f|^2 + |g|^2\big)$, this follows directly from the hypothesis.

For B: We define (f,g) as $\int_\Omega f\bar{g}$. This integral is, as we have already seen, absolutely convergent. All properties postulated in **B** are apparent except the last: That $(f,f)=0$ implies $f\equiv 0$. Now $(f,f)=0$ means that $\int_\Omega |f|^2 = 0$, so the set of points for which $|f|^2 > 0$, *i.e.*, $f(q_1,\ldots,q_k)\neq 0$, must have Lebesgue measure 0. If we now consider two functions f, g for which $f\neq g$ (*i.e.*, $f(q_1,\ldots,q_k)\neq g(q_1,\ldots,q_k)$) holds only on a $q_1,\ldots,q_k$ set of Lebesgue measure 0 as not being essentially different,[54] then we can assert that $f\equiv 0$.

For C: Let $O_1,\ldots,O_n$ be n domains in Ω, no two of which have a point in common, and let the Lebesgue measure of all be greater than zero, but finite. Let $f_\ell(q_1,\ldots,q_k)$ be 1 in O_ℓ and zero elsewhere. Since $\int_\Omega |f_\ell|^2$ is equal to the measure of O_ℓ it belongs to F_Ω $(\ell = 1,\ldots,n)$. These $f_1,\ldots,f_n$ are linearly independent. For $a_1f_1+\cdots+a_nf_n\equiv 0$ means that the function on the left fails to vanish only in a set of measure 0. It therefore has roots in each O_ℓ, but since it is a constant a_ℓ in O_ℓ, then $a_\ell = 0$; $\ell = 1,\ldots,n$. This construction holds for all n, so that $\mathbf{C}^{(\infty)}$ holds.

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[53] In general

$$\begin{aligned}|x+y|^2 = (x+y)(\bar{x}+\bar{y}) &= x\bar{x} + y\bar{y} + (x\bar{y}+\bar{x}y)\\ &= |x|^2 + |y|^2 + 2\mathrm{Re}\,(x\bar{y})\end{aligned}$$

[54] This is customary in the theory of the Lebesgue integral.

For D: Let the sequence $f_1, f_2, \ldots$ satisfy the Cauchy criterion; *i.e.*, for each $\epsilon > 0$ there exists an $N = N(\epsilon)$ such that $\int_\Omega |f_m - f_n|^2 < \epsilon$ whenever $m, n \geqslant N$. We chose $n_1 = N(\frac{1}{8})$; $n_2 = N(\frac{1}{8^2}) \geqslant n_1$; $n_3 = N(\frac{1}{8^3}) \geqslant n_1, n_2$; $\ldots$. Then $n_1 \leqslant n_2 \leqslant \cdots \leqslant n_\nu = N(\frac{1}{8^\nu}) \leqslant n_{\nu+1}$, hence

$$\int_\Omega |f_{n_{\nu+1}} - f_{n_\nu}|^2 < \frac{1}{8^\nu}$$

Let us now consider the set $P^{(\nu)}$ of all points for which

$$|f_{n_{\nu+1}} - f_{n_\nu}| > \frac{1}{2^\nu}$$

If its Lesbegue measure is $\mu^{(\nu)}$ then

$$\int_\Omega |f_{n_{\nu+1}} - f_{n_\nu}|^2 \geqslant \mu^{(\nu)} \Big(\frac{1}{2^\nu}\Big)^2 = \frac{\mu^{(\nu)}}{4^\nu} < \frac{1}{8^\nu} \implies \mu^{(\nu)} < \frac{1}{2^\nu}$$

Let us also consider the set $Q^{(\nu)}$ which consists of the union of $P^{(\nu)}, P^{(\nu+1)}, P^{(\nu+2)}, \ldots$. Its Lesbegue measure is

$$\leqslant \mu^{(\nu)} + \mu^{(\nu+1)} + \mu^{(\nu+2)} + \cdots < \frac{1}{2^\nu} + \frac{1}{2^{\nu+1}} + \frac{1}{2^{\nu+2}} + \cdots = \frac{1}{2^{\nu-1}}$$

Outside of $Q^{(\nu)}$ it is true that

$$\begin{aligned} |f_{n_{\nu+1}} - f_{n_\nu}| &< \frac{1}{2^\nu} \\ |f_{n_{\nu+2}} - f_{n_{\nu+1}}| &< \frac{1}{2^{\nu+1}} \\ |f_{n_{\nu+3}} - f_{n_{\nu+2}}| &< \frac{1}{2^{\nu+2}} \\ &\vdots \end{aligned}$$

Therefore, in general, for $\nu \leqslant \nu' \leqslant \nu''$

$$\begin{aligned} |f_{n_{\nu''}} - f_{n_{\nu'}}| \leqslant\ & |f_{n_{\nu'+1}} - f_{n_{\nu'}}| \\ & + |f_{n_{\nu'+2}} - f_{n_{\nu'+1}}| + \cdots + |f_{n_{\nu''}} - f_{n_{\nu''-1}}| \\ & < \frac{1}{2^{\nu'}} + \frac{1}{2^{\nu'+1}} + \cdots + \frac{1}{2^{\nu''-1}} \\ & < \frac{1}{2^{\nu'-1}} \end{aligned}$$

As $\nu' \longrightarrow \infty$ this approaches zero independently of ν''; *i.e.*, the sequence $f_{n_1}, f_{n_2}, \ldots$ fulfills the Cauchy criterion in the case that the $q_1, \ldots, q_k$ do not lie in $Q^{(\nu)}$. Since we are dealing with numbers (for fixed $q_1, \ldots, q_k$), this sequence also converges. Therefore we can say conversely: If the $f_{n_1}, f_{n_2}, \ldots$ sequence does not converge for a certain $q_1, \ldots, q_k$ then this lies in $Q^{(\nu)}$. Let the set of

all $q_1, \ldots, q_k$ for which convergence does not occur be Q. Then Q is a subset of $Q^{(\nu)}$, its measure is therefore not larger than that of $Q^{(\nu)}$; *i.e.*, $< \frac{1}{2^{\nu-1}}$. This must be true for all ν, although Q is defined independently of ν. Therefore Q has the Lebesgue measure 0. Consequently, nothing is changed if we, for example, set all f_n in Q equal to zero (see Note 54). But then $f_{n_1}, f_{n_2}, \ldots$ converges also in Q, and hence everywhere.

We have thus specified a subsequence $f_{n_1}, f_{n_2}, \ldots$ of $f_1, f_2, \ldots$ which converges at all points $q_1, \ldots, q_k$ (this need not be the case for $f_1, f_2, \ldots$). Let the limit of $f_{n_1}, f_{n_2}, \ldots$ be $f(q_1, \ldots, q_k)$. We must then prove: 1. f belongs to F_Ω; *i.e.*, $\int_\Omega |f|^2$ is finite; 2. f is the limit of $f_{n_1}, f_{n_2}, \ldots$ not only in the sense of convergence for each $q_1, \ldots, q_k$ but also in the sense of "length convergence" of Hilbert space; *i.e.*, $\|f - f_{n_2}\| \to 0$ or $\int_\Omega |f - f_{n_2}|^2 \to 0$; 3. In this sense it is also the limit of the entire sequence $f_1, f_2, \ldots$; *i.e.*, $\|f - f_n\| \to 0$ or $\int_\Omega |f - f_n|^2 \to 0$.

Let $\epsilon > 0$, and let ν_0 be chosen with $n_{\nu_0} \geqslant N(\epsilon)$ (for example, $\frac{1}{8^{\nu_0}} \leqslant \epsilon$), and $\nu \geqslant \nu_0$, $n \geqslant N(\epsilon)$. Then $\int_\Omega |f_{n_\nu} - f_n|^2 < \epsilon$. If we set $\nu \to \infty$ then the integrand approaches $|f - f_n|^2$, therefore $\int_\Omega |f - f_n|^2 \leqslant \epsilon$ (according to the convergence theorem of Lebesgue integrals: see Note 52). Consequently, first, $\int_\Omega |f - f_n|^2$ is finite; *i.e.*, $f - f_n$ in F_Ω; also, since f_n belongs to F_Ω, f does likewise: 1. is then proved. Second, it follows from the above inequality that $\int_\Omega |f - f_n|^2 \to 0$ as $n \to \infty$; *i.e.*, 2. and 3. are proved.

For E: We must specify a function sequence $f_1, f_2, \ldots$ everywhere dense in F_Ω.

Let $\Omega_1, \Omega_2, \ldots$ be a sequence of regions in Ω, each of which has a finite measure, and which cover the entire Ω. (For example, let Ω_N be a sphere of radius N about the origin. Let $f = f(q_1, \ldots, q_k)$ be any element of F_Ω. We define an $f_N = f_N(q_1, \ldots, q_k)$ for each $N = 1, 2, \ldots$:

$$f_N(q_1, \ldots, q_k) = \begin{cases} f(q_1, \ldots, q_k) & \begin{cases} \text{if } q_1, \ldots, q_k \text{ are in } \Omega_N \\ \text{and } |f(q_1, \ldots . q_k)| \leqslant N \end{cases} \\ 0 & \text{otherwise} \end{cases}$$

As $N \to \infty$, $f_N(q_1, \ldots, q_k) \to f(q_1, \ldots, q_k)$ (from a certain N on, equality is obtained), therefore $|f - f_N|^2 \leqslant f^2$. The integrals

$$\int_\Omega |f - f_N|^2$$

are therefore dominated by $\int_\Omega |f|^2$ (finite). Since the integrands approach zero, the integrals do likewise (see the convergence theorem cited above).

Let the class of all functions $g = g(q_1, \ldots, q_k)$ for which the set of all points with $g \neq 0$ has finite measure, and which satisfies an inequality $|g| \leqslant C$ throughout all space, with arbitrary but fixed C, be called G. The above f_N all belong to G. Therefore C is everywhere dense (in F_Ω).

Let g belong to G, $\epsilon > 0$. Let the measure of the $g \neq 0$ set be M, and the upper bound for $|g|$ be C. We chose a series of rational numbers

$$-C < \rho_1 < \rho_2 < \cdots < \rho_t < C$$

such that

$$\rho_1 < -C + \epsilon,\ \rho_2 < \rho_1 + \epsilon,\ \ldots,\ \rho_t < \rho_{t-1} + \epsilon,\ C < \rho_t + \epsilon$$

which can easily be done. We now change each $\operatorname{Re} g(q_1, \ldots, q_k)$ value into the nearest ρ_s $(s = 1, 2, \ldots, t)$, only we let zero remain zero. Then a new function $h_1(q_1, \ldots, q_k)$ is obtained which differs from $\operatorname{Re} g$ everywhere by less than ϵ. In the same way, we construct an $h_2(q_1, \ldots, q_k)$ for $\operatorname{Im} g$. Then for $h = h_1 + ih_2$

$$\begin{aligned} \int_\Omega |g - h|^2 &= \int_\Omega |\operatorname{Re} g - h_1|^2 + \int_\Omega |\operatorname{Im} g - h_2|^2 \\ &\leqslant M\epsilon^2 + M\epsilon^2 = 2M\epsilon^2 \\ \|g - h\| &\leqslant \sqrt{2M}\,\epsilon \end{aligned}$$

If $\delta > 0$ is given, then we set $\epsilon < \delta/\sqrt{2M}$ and then $\|g - h\| < \delta$.

Let the class of all functions $h = h(q_1, \ldots, q_k)$ which take on only a finite number of different values, actually only those of the form $\rho + i\sigma$, ρ, σ rational, and each such value, except zero, only on sets of measure 0, be called H. The above h belong to H, therefore H is everywhere dense in G, and therefore in F_Ω also.

Let Π be a set of finite Lebesgue measure. We define a function $f_\Pi = f_\Pi(q_1, \ldots, q_k)$:

$$f_\Pi(q_1, \ldots, q_k) = \begin{cases} 1 & \text{in } \Pi \\ 0 & \text{elsewhere} \end{cases}$$

The class H obviously consists of all

$$\sum_{s=1}^{t} (\rho_s + i\sigma_s) f_{\Pi_s} \quad (t = 1, 2, \ldots;\ \rho_s, \sigma_s \text{ rational})$$

We now seek a Π-set sequence $\Pi^{(1)}, \Pi^{(2)}, \ldots$ with the following property: for each $\epsilon > 0$ there exists a $\Pi^{(n)}$ such that the measure of all points which belong to Π but not to $\Pi^{(n)}$, or to $\Pi^{(n)}$ but not to Π, is $< \epsilon$ (this set is known as the difference set $\Pi^{(n)}$ of Π). If we have such a sequence, then the

$$\sum_{s=1}^{t} (\rho_s + i\sigma_s) f_{\Pi^{(n_s)}}$$

$(t = 1, 2, \ldots;\ \rho_s, \sigma_s \text{ rational};\ n_s = 1, 2, \ldots)$ are everywhere dense in H, because

if we choose for each Π_s the $\Pi^{(n_s)}$ according to the above discussion, then

$$\begin{aligned}
&\sqrt{\int_\Omega \Big|\sum_{s=1}^{t}(\rho_s+i\sigma_s)f_{\Pi_s}-\sum_{s=1}^{t}(\rho_s+i\sigma_s)f_{\Pi^{(n_s)}}\Big|^2}\\
&\quad\leqslant\sum_{s=1}^{t}\sqrt{\int_\Omega\big|(\rho_s+i\sigma_s)f_{\Pi_s}-(\rho_s+i\sigma_s)f_{\Pi^{(n_s)}}\big|^2}\\
&\quad=\sum_{s=1}^{t}\sqrt{(\rho_s^2+\sigma_s^2)\int_\Omega\big|f_{\Pi_s}-f_{\Pi^{(n_s)}}\big|^2}\\
&\quad=\sum_{s=1}^{t}\sqrt{(\rho_s^2+\sigma_s^2)\cdot\text{measure of the difference set }\big(\Pi_s,\Pi^{(n_s)}\big)}\\
&\quad<\sum_{s=1}^{t}\sqrt{(\rho_s^2+\sigma_s^2)\cdot\epsilon}=\Big(\sum_{s=1}^{t}\sqrt{\rho_s^2+\sigma_s^2}\Big)\sqrt{\epsilon}
\end{aligned}$$

If a $\delta>0$ is given, then

$$\epsilon=\delta^2\Big/\Big(\sum_{s=1}^{t}\sqrt{\rho_s^2+\sigma_s^2}\Big)^2$$

supplies the result

$$\Big\|\sum_{s=1}^{t}(\rho_s+i\sigma_s)f_{\Pi_s}-\sum_{s=1}^{t}(\rho_s+i\sigma_s)f_{\Pi^{(n_s)}}\Big\|<\delta$$

But the

$$\sum_{s=1}^{t}(\rho_s+i\sigma_s)f_{\Pi^{(n_s)}}$$

form a sequence, if we order them appropriately. This can be done in the following way: Let the common denominator of all $\rho_1,\sigma_1,\ldots,\rho_t,\sigma_t$ be τ, and the new numerators be $\rho'_1,\sigma'_1,\ldots,\rho'_t,\sigma'_t$, then the relation becomes

$$\tfrac{1}{\tau}\sum_{s=1}^{t}(\rho'_s+i\sigma'_s)f_{\Pi^{(n_s)}}$$

in which we have $t,\tau=1,2,\ldots;\ \rho'_s,\sigma'_s=0,\pm1,\pm2,\ldots;\ n_s=1,2,\ldots$ for $s=1,\ldots,t$. To order these functions as a sequence is the identical problem as doing the same thing for the integers $t,\tau,\rho'_1,\sigma'_1,\ldots,\rho'_t,\sigma'_t,n_1,\ldots,n_t$. Among these complexes of numbers group together those for which the positive integer

$$I=t+\tau+|\rho'_1|+|\sigma'_1|+\cdots+|\rho'_t|+|\sigma'_t|+n_1+\cdots n_t$$

has the same value. Then arrange these groups in the order of increase of their indices I. Each one of these groups (with fixed I) consists obviously of a finite

number of the complexes in question. If we now arrange each one of these finite sets in any order, we have in fact obtained a simple sequence containing all the complexes.

In order to be able to specify the set sequence $\Pi^{(1)}, \Pi^{(2)}, \ldots$ mentioned, we make use of the fact that for each set Π with finite Lebesgue measure M, and for each $\delta > 0$, there exists an open point set Π' which covers Π, but whose measure exceeds it by $< \delta$ (see the references of Note 52 and Note 45, where the concept "open point set" has been defined). For each open Π' and a $\delta > 0$, there obviously exists a set Π'' consisting of a finite number of cubes, which is contained in Π', and whose measure is less than that of Π' by $< \delta$. Clearly the lengths of the edges of these cubes and their center coordinates can all be chosen rational. We now easily recognize that the "difference set" of Π, Π'', as defined above, has measure $< \delta + \delta = 2\delta$ and therefore for $\delta = \frac{1}{2}\epsilon$ a measure $< \epsilon$. We have then accomplished our purpose, if we can order a sequence of sets of cubes of the type just described.

These sets of cubes are now characterized by the number of their cubes $n = 1, 2, \ldots$, together with the lengths of their edges $\kappa^{(\nu)}$ and the coordinates of their center points $\xi_1^{(\nu)}, \ldots, \xi_k^{(\nu)}$ $(\nu = 1, \ldots, n)$. The $\kappa^{(\nu)}, \xi_1^{(\nu)}, \ldots, \xi_k^{(\nu)}$ are rational. Let their common denominator (for all $\nu = 1, \ldots, n$) be $\eta = 1, 2, \ldots$, their numerators

$$\kappa'^{(\nu)} = 1, 2, \ldots ; \quad \xi'^{(\nu)}_1, \ldots, \xi'^{(\nu)}_k = 0, \pm 1, \pm 2, \ldots$$

Then our sets of cubes are characterized by the complexes of numbers

$$n, \eta, \kappa'^{(1)}, \xi'^{(1)}_1, \ldots, \xi'^{(1)}_k, \ldots, \kappa'^{(n)}, \xi'^{(n)}_1, \ldots, \xi'^{(n)}_k$$

If we arrange these in the order of increase of the positive integers

$$n + \eta + \kappa'^{(1)} + |\xi'^{(1)}_1| + \cdots + |\xi'^{(n)}_k| + \cdots + \kappa'^{(n)} + |\xi'^{(n)}_1| + \cdots + |\xi'^{(n)}_k|$$

then we obtain a simple sequence, exactly as in the earlier analogous case of the linear combinations of functions.

Before we continue, let us answer the following question: Given an $\mathcal{R}$ satisfying **A–E** (with $\mathbf{C}^{(\infty)}$), in which subsets $\mathcal{M}$ of $\mathcal{R}$ are **A–E** again satisfied (with unchanged definitions of af, $f \pm g$ as well as (f, g))?

In order that **A** hold, $\mathcal{M}$ must be a linear manifold. **B** is valid of itself. We postpone **C** momentarily; in any case a $\mathbf{C}^{(n)}$ or a $\mathbf{C}^{(\infty)}$ holds. **D** means: if a sequence in $\mathcal{M}$ satisfies the Cauchy convergence criterion, then it has a limit in $\mathcal{M}$. Since such a sequence will certainly possess a limit in $\mathcal{R}$, **D** means simply that this limit also belongs to $\mathcal{M}$. That is, $\mathcal{M}$ must be closed. The condition **E** always holds, as we saw in thee proof of THEOREM 9. Therefore, we may summarize thus: $\mathcal{M}$ must be a closed linear manifold. We call the orthonormal linear set which spans $\mathcal{M}$ (THEOREM 9) $\phi_1, \phi_2, \ldots$. If it is infinite, then $\mathbf{C}^{(\infty)}$ obviously

holds, and $\mathcal{M}$ is isomorphic to $\mathcal{R}_\infty$, therefore to $\mathcal{R}$ itself; if it terminates at ϕ_n then $\mathbf{C}^{(n)}$ holds (e.g., because of THEOREM $3^{(n)}$); *i.e.*, $\mathcal{M}$ is isomorphic to $\mathcal{R}_n$.

But since $\mathbf{D}, \mathbf{E}$ are valid in $\mathcal{M}$ in any case, they are valid in each $\mathcal{R}_n$. Therefore they also follow from $\mathbf{A}$–$\mathbf{C}^{(n)}$.

As we see, we have avoided the direct verification of $\mathbf{A}$–$\mathbf{E}$ (with $\mathbf{C}^{(n)}$ or $\mathbf{C}^{(\infty)}$) in $\mathcal{R}_n$ or $\mathcal{R}_\infty$. This was achieved by indirect, logical devices. However, a direct, analytical demonstration causes no essential difficulties either. It may be left to the reader for proof.

It still remains to show that $\mathbf{D}$ and $\mathbf{E}$ are independent of $\mathbf{A}$–$\mathbf{C}^{(\infty)}$. As we have seen previously, every linear manifold in $\mathcal{R}_\infty$ satisfies $\mathbf{A}, \mathbf{B}, \mathbf{E}$ as well as $\mathbf{C}^{(n)}$ or $\mathbf{C}^{(\infty)}$, but if it is not closed then $\mathbf{D}$ is not fulfilled. In this case $\mathbf{C}^{(\infty)}$ must hold in it, because $\mathbf{D}$ follows from $\mathbf{C}^{(n)}$. Now it is not difficult to exhibit such a non-closed linear manifold. Let $\phi_1, \phi_2, \ldots$ be an orthonormal set. Then the

$$\sum_{\nu=1}^{N} x_\nu \phi_\nu \quad : \quad N = 1, 2, \ldots; \;\; x_1, \ldots, x_N \text{ arbitrary}$$

form a linear manifold, but one which is not closed, because

$$\sum_{\nu=1}^{\infty} \tfrac{1}{\nu} \phi_\nu$$

($\sum_{\nu=1}^{\infty} (\frac{1}{\nu})^2$ is infinite!) is a limiting point, but not an element of the manifold.

$$\left(\sum_{\nu=1}^{N} \tfrac{1}{\nu} \phi_\nu \longrightarrow \sum_{\nu=1}^{\infty} \tfrac{1}{\nu} \phi_\nu \quad \text{as} \quad N \longrightarrow \infty \right)$$

Consequently, $\mathbf{D}$ is independent of $\mathbf{A}$–$\mathbf{C}^{(\infty)}, \mathbf{E}$.

Let us consider next all complex functions $x(\alpha)$ whose parameter α is continuous: $-\infty < \alpha < +\infty$. Moreover, suppose that it is possible to write $x(\alpha) \neq 0$ in a series, such that the sum $\sum_\alpha |x(\alpha)|^2$ extended over these terms is finite.[55] All these functions $x(\alpha)$ form a space $\mathcal{R}_{\text{cont}}$. Since for any two points $x(\alpha), y(\alpha)$ of the latter space, $x(\alpha)$ or $y(\alpha) \neq 0$ only for two α-sequences, and since we can join these two sequences into a single one, $x(\alpha) = y(\alpha) = 0$ except for a certain α-sequence $\alpha_1, \alpha_2, \ldots$. Therefore we need discuss only the values $x_n = x(\alpha_n)$, $y_n = y(\alpha_n)$ for all $n = 1, 2, \ldots$. These all behave the same as in $\mathcal{R}_\infty$, as long as only two $\mathcal{R}_{\text{cont}}$ points appear. Hence $\mathbf{A}, \mathbf{B}$ hold in $\mathcal{R}_{\text{cont}}$ exactly as in $\mathcal{R}_\infty$.[56] The same follows for k $(= 1, 2, \ldots)$ $\mathcal{R}_{\text{cont}}$ points, therefore $\mathbf{C}^{(\infty)}$ holds also. Moreover, this is even true for a sequence of $\mathcal{R}_{\text{cont}}$ points. Consider

[55] Although α varies continuously, this is a sum and not an integral, since only a sequence of the α appears in the sum!

[56] We naturally define $\big(x(\alpha), y(\alpha)\big)$ as $\sum_\alpha x(\alpha)\overline{y(\alpha)}$.

$x_1(\alpha), x_2(\alpha), \ldots$; the α with $x_n(\alpha) \neq 0$ for a sequence for each $n = 1, 2, \ldots$: $\alpha_1^{(1)}, \alpha_2^{(1)}, \alpha_1^{(2)}, \alpha_2^{(2)}, \alpha_1^{(3)}, \ldots$. Consequently, **D** holds in $\mathfrak{R}_{\text{cont}}$ as well as in $\mathfrak{R}_\infty$. It is otherwise with **E**. In that case, all points of $\mathfrak{R}$ play a role (all must be limit points of an appropriate sequence), therefore we must reason from $\mathfrak{R}_\infty$ to $\mathfrak{R}_{\text{cont}}$. Also, the condition is actually not satisfied, because one deduction from it is invalid: there exists an orthonormal set which cannot be written as a sequence (contrary to THEOREM $3^{(\infty)}$).

Let

$$x_\beta(\alpha) = \begin{cases} 1 & \text{for} \quad \alpha = \beta \\ 0 & \text{for} \quad \alpha \neq \beta \end{cases}$$

for each β; $x_\beta(\alpha)$ is an element of $\mathfrak{R}_{\text{cont}}$, and the $x_\beta(\alpha)$ form an orthonormal set. But they could be written as a sequence only if it were possible for all β: $-\infty < \beta < +\infty$, which is well known not to be the case.[57] Therefore, **E** is also independent of **A–C**$^{(\infty)}$, **D**.

(In addition, the fundamental difference between the function space of the $f(x)$ with finite

$$\int_{-\infty}^{+\infty} |f(x)|^2 \, dx$$

and that of the $x(\alpha)$ with finite $\sum_\alpha |x(\alpha)|^2$ should be noted. We could just as well characterize the former as the space of all $x(\alpha)$ with finite

$$\int_{-\infty}^{+\infty} |x(\alpha)|^2 \, d\alpha \; !$$

The entire difference is the replacing of $\int_{-\infty}^{+\infty} \ldots d\alpha$ by $\sum_\alpha \ldots$, and yet the first named space is F_Ω, therefore satisfies **A–E** and is isomorphic to $\mathfrak{R}_\infty$, while the latter, $\mathfrak{R}_{\text{cont}}$, violates **E** and is essentially different from $\mathfrak{R}_\infty$. Nevertheless the two spaces are identical except for their differing definitions of magnitude!)

4. CLOSED LINEAR MANIFOLDS

The § **II.2** is of importance for us not only because of the proof of isomorphism, but also because several theorems on orthonormal sets were proved therein. We now desire to go further into the geometric analysis of Hilbert space, and to investigate in detail the closed linear manifolds which play in $\mathfrak{R}_\infty$ a role analogous to that played by straight lines, planes, etc. in $\mathfrak{R}_n$ (*i.e.*, the $\mathfrak{R}_m$, $m \leqslant n$).

We first recall the DEFINITIONS 2 & 5: if $\mathcal{A}$ is any set in $\mathfrak{R}$, then $\{\mathcal{A}\}$ or $[\mathcal{A}]$ is the linear manifold spanned by $\mathcal{A}$ or the closed linear manifold respectively; *i.e.*, smallest representant of either type which contains $\mathcal{A}$.

[57] This is the set theoretical theorem on the "Non-denumerability of the Continuum." See, for example, the book of Hausdorff mentioned in Note 45.

Now we extend this notation so that by

$$\{\mathcal{A}, \mathcal{B}, \ldots, f, g, \ldots\} \quad \text{or} \quad [\mathcal{A}, \mathcal{B}, \ldots, f, g, \ldots]$$

(if $\mathcal{A}$, $\mathcal{B}$, ... are any subsets and $f, g, \ldots$ any elements of $\mathcal{R}$) we understand respectively the linear manifold or the closed linear manifold spanned by that set which results from the combination of the $\mathcal{A}$, $\mathcal{B}$, ... and the $f, g, \ldots$.

If, in particular, $\mathcal{M}$, $\mathcal{N}$, ... (finite or infinite in number) are closed linear manifolds, then we designate the closed linear manifold $[\mathcal{M}, \mathcal{N}, \ldots]$ by $\mathcal{M}+\mathcal{N}+\cdots$. The linear manifold $\{\mathcal{M}, \mathcal{N}, \ldots\}$ clearly consists of all sums $f+g+\cdots$ (f running through $\mathcal{M}$, g running through $\mathcal{N}, \ldots$), while $[\mathcal{M}, \mathcal{N}, \ldots] = \mathcal{M}+\mathcal{N}+\cdots$ is obtained from this by the addition of the limit points. If only a finite number of sets $\mathcal{M}$, $\mathcal{N}$ are present, and each element of one is orthogonal to all elements of the others, then, as we shall soon see, these two representations are equal to each other, which is not necessarily the case in general.

If $\mathcal{M}$ is a subset of $\mathcal{N}$, then we consider the totality of elements of $\mathcal{N}$ which are orthogonal to all elements of $\mathcal{M}$. This also is obviously a closed linear manifold, which may be called $\mathcal{N} - \mathcal{M}$. THEOREM 14 will clarify the reason for denoting this as subtraction. The set $\mathcal{N} - \mathcal{M}$ of all f orthogonal to the entire $\mathcal{M}$ is of special importance. This is called the closed linear manifold complementary to $\mathcal{M}$.

Finally, we select three particularly simple closed linear manifolds: first, $\mathcal{R}$ itself; second, the set $\{0\} = [0]$ consisting of zero alone; and third, the set of all af (f a given element of $\mathcal{R}$, a variable), which is clearly a closed linear manifold, and therefore simultaneously $= \{f\} = [f]$.

We now introduce the concept of "projection," one which is completely analogous to that term in Euclidean geometry:

> THEOREM 10. Let $\mathcal{M}$ be a closed linear manifold. Then each f can be resolved in one and only one way into two components, $f = g+h$, g from $\mathcal{M}$, h from $\mathcal{R} - \mathcal{M}$.
>
> NOTE. We call g the projection of f in $\mathcal{M}$, h (which is orthogonal to all $\mathcal{M}$) the normal from f onto $\mathcal{M}$. We introduce the notation $\mathsf{P}_{\mathcal{M}} f$ for g.

PROOF: Let $\phi_1, \phi_2, \ldots$ be the orthonormal set, existing by reason of THEOREM 9, spanning the closed manifold $\mathcal{M}$. We write $g = \sum_n (f, \phi_n) \cdot \phi_n$. By THEOREM 6, this series converges (even when infinite), its sum g obviously belonging to $\mathcal{M}$. Furthermore, by THEOREM 6, $h = f - g$ is orthogonal to all $\phi_1, \phi_2, \ldots$. But since the vectors orthogonal to h form a closed linear manifold, along with $\phi_1, \phi_2, \ldots$ all $\mathcal{M}$ is also orthogonal to h; *i.e.*, h belongs to $\mathcal{R} - \mathcal{M}$.

If there were still another resolution $f = g' + h'$, g' from $\mathcal{M}$, h' from $\mathcal{R} - \mathcal{M}$, then $g + h = g' + h'$, $g - g' = h - h' = j$. The j would have to belong simultaneously to $\mathcal{M}$ and $\mathcal{R} - \mathcal{M}$, and would therefore be orthogonal to itself. Therefore $(j, j) = 0$, $j = 0$ and consequently $g = g'$, $h = h'$.

The operation $\mathsf{P}_{\mathcal{M}}f$ is therefore one which assigns to each f of $\mathcal{R}$ its projection in $\mathcal{M}$, $\mathsf{P}_{\mathcal{M}}f$. In the next section we shall define: an operator R is a function defined in a subset of $\mathcal{R}$ with values from $\mathcal{R}$; *i.e.*, a correspondence which assigns to certain f of $\mathcal{R}$ certain $\mathsf{R}f$ of $\mathcal{R}$. (Not necessarily for all f. For other f of $\mathcal{R}$ the operation may be undefined; *i.e.*, "meaningless.") $\mathsf{P}_{\mathcal{M}}$ is then an operator defined everywhere in $\mathcal{R}$ and is known as the *projection operator* of $\mathcal{M}$, or merely the projection of $\mathcal{M}$.

THEOREM 11. The operator $\mathsf{P}_{\mathcal{M}}$ has the following properties:

$$\begin{aligned}\mathsf{P}_{\mathcal{M}}(a_1f_1+\cdots+a_nf_n) &= a_1\mathsf{P}_{\mathcal{M}}f_1+\cdots+a_n\mathsf{P}_{\mathcal{M}}f_n\\ (\mathsf{P}_{\mathcal{M}}f,g) &= (f,\mathsf{P}_{\mathcal{M}}g)\\ \mathsf{P}_{\mathcal{M}}(\mathsf{P}_{\mathcal{M}}f) &= \mathsf{P}_{\mathcal{M}}f\end{aligned}$$

$\mathcal{M}$ is the set of all values of $\mathsf{P}_{\mathcal{M}}$; *i.e.*, the set of all $\mathsf{P}_{\mathcal{M}}f$. But it can also be characterized as the set of all solutions of $\mathsf{P}_{\mathcal{M}}f=f$, while $\mathcal{R}-\mathcal{M}$ is the set of all solutions of $\mathsf{P}_{\mathcal{M}}f=0$.

NOTE. In the succeeding sections we shall see that the first property determines the so-called linear operators, and the second the so-called Hermitian operators. The third expresses the following: double application of $\mathsf{P}_{\mathcal{M}}$ has the same effect as single application. The customary symbolic representation of this is

$$\mathsf{P}_{\mathcal{M}}\mathsf{P}_{\mathcal{M}}=\mathsf{P}_{\mathcal{M}} \quad \text{or} \quad \mathsf{P}_{\mathcal{M}}^2=\mathsf{P}_{\mathcal{M}}$$

PROOF: From $f_1=g_1+h_1,\ldots,f_n=g_n+h_n$

$$\begin{pmatrix} g_1,\ldots,g_n & \text{from} & \mathcal{M} \\ h_1,\ldots,h_n & \text{from} & \mathcal{R}-\mathcal{M}\end{pmatrix}$$

it follows that

$$a_1f_1+\ldots+a_nf_n=(a_1g_1+\ldots+a_ng_n)+(a_1h_1+\ldots+a_nh_n)$$

$$\begin{pmatrix} a_1g_1+\ldots+a_ng_n & \text{from} & \mathcal{M} \\ a_1h_1+\ldots+a_nh_n & \text{from} & \mathcal{R}-\mathcal{M}\end{pmatrix}$$

Therefore

$$\begin{aligned}\mathsf{P}_{\mathcal{M}}(a_1f_1+\ldots+a_nf_n) &= a_1g_1+\ldots+a_ng_n\\ &= a_1\mathsf{P}_{\mathcal{M}}f_1+\cdots+a_n\mathsf{P}_{\mathcal{M}}f_n\end{aligned}$$

This is the first assertion.

In the second case, let

$$f = g' + h', \;\; g = g'' + h'' \quad : \quad \begin{cases} g', g'' & \text{from} \quad \mathfrak{R} \\ h', h'' & \text{from} \quad \mathfrak{R} - \mathfrak{M} \end{cases}$$

Then g', g'' are orthogonal to h', h''. Therefore

$$(g', g) = (g', g'' + h'') = (g', g'') = (g' + h', g'') = (f, g'')$$

i.e., $(\mathsf{P}_{\mathfrak{M}} f, g) = (f, \mathsf{P}_{\mathfrak{M}} g)$. This is the second assertion.

Finally, $\mathsf{P}_{\mathfrak{M}} f$ belongs to $\mathfrak{M}$, therefore $\mathsf{P}_{\mathfrak{M}} f = \mathsf{P}_{\mathfrak{M}} f + 0$ is the resolution into components guaranteed by THEOREM 10 for $\mathsf{P}_{\mathfrak{M}} f$; *i.e.*, $\mathsf{P}_{\mathfrak{M}}(\mathsf{P}_{\mathfrak{M}} f) = \mathsf{P}_{\mathfrak{M}} f$. This is the third assertion.

The relations $\mathsf{P}_{\mathfrak{M}} f = f$ or 0 signify that in the resolution $f = g + h$ (g from $\mathfrak{M}$, h from $\mathfrak{R} - \mathfrak{M}$: THEOREM 10) either $f - g, h = 0$ or $g = 0, f = h$; *i.e.*, that f belongs either to $\mathfrak{M}$ or to $\mathfrak{R} - \mathfrak{M}$. These are the fifth and sixth assertions. All $\mathsf{P}_{\mathfrak{M}} f$ belong to $\mathfrak{M}$ by definition, and each f' of $\mathfrak{M}$ is equal to a $\mathsf{P}_{\mathfrak{M}} f$: e.g., according to the statements just made, to $\mathsf{P}_{\mathfrak{M}} f$. This is the fourth assertion.

We observe next that the second and third assertions imply this:

$$(\mathsf{P}_{\mathfrak{M}} f, \mathsf{P}_{\mathfrak{M}} g) = (f, \mathsf{P}_{\mathfrak{M}} \mathsf{P}_{\mathfrak{M}} g) = (f, \mathsf{P}_{\mathfrak{M}} g) = (\mathsf{P}_{\mathfrak{M}} f, g)$$

We now want to characterize the projection operators independently of the $\mathfrak{M}$.

THEOREM 12. An operator E, defined everywhere (see the discussion preceding THEOREM 11) is a projection; *i.e.*, $\mathsf{E} = \mathsf{P}_{\mathfrak{M}}$ for a closed linear manifold $\mathfrak{M}$, if and only if it has the following properties:

$$(\mathsf{E} f, g) = (f, \mathsf{E} g), \qquad \mathsf{E}^2 = \mathsf{E}$$

(see the note on THEOREM 11). In this case, $\mathfrak{M}$ is uniquely determined by E (according to THEOREM 11).

PROOF: The necessity of this condition as well as the determination of $\mathfrak{M}$ by E is obvious from THEOREM 11. We then have only to show that if E possesses the above properties, then there is a closed linear manifold $\mathfrak{M}$ with $\mathsf{E} = \mathsf{P}_{\mathfrak{M}}$.

Let $\mathfrak{M}$ be the closed manifold spanned by all $\mathsf{E} f$. Then $g - \mathsf{E} g$ is orthogonal to all $\mathsf{E} f$:

$$(\mathsf{E} f, g - \mathsf{E} g) = (\mathsf{E} f, g) - (\mathsf{E} f, \mathsf{E} g) = (\mathsf{E} f, g) - (\mathsf{E}^2 f, g) = 0$$

The elements orthogonal to $g - \mathsf{E} g$ of $\mathfrak{R}$ form a closed linear manifold; therefore they include $\mathfrak{M}$ along with $\mathsf{E} f$, so $g - \mathsf{E} g$ belongs to $\mathfrak{R} - \mathfrak{M}$. The resolution of g for $\mathfrak{M}$, in the sense of THEOREM 10, is then $g = \mathsf{E} g + (g - \mathsf{E} g)$, hence $\mathsf{P}_{\mathfrak{M}} g = \mathsf{E} g$, where g is arbitrary. Therefore the entire theorem is proved.

If $\mathcal{M} = \mathcal{R}$ or $[0]$ then $\mathcal{R} - \mathcal{M} = [0]$ or $\mathcal{R}$ respectively, therefore $f = f + 0$ or $0 + f$ is the resolution, by THEOREM 11; hence $\mathsf{P}_{\mathcal{M}} f = f$ or 0 respectively. We call I the operator defined (everywhere!) by $\mathsf{R}f = f$, and O the operator defined by $\mathsf{R}f = 0$. Hence $\mathsf{P}_{\mathcal{R}} = \mathsf{I}$, $\mathsf{P}_{[0]} = \mathsf{O}$. Furthermore, it is clear that the resolution $f = g + h$ (g from $\mathcal{M}$, h from $\mathcal{R} - \mathcal{M}$) belonging to $\mathcal{M}$ is also useful for $\mathcal{R} - \mathcal{M}$ in the form $f = h + g$ (h from $\mathcal{R} - \mathcal{M}$, g from $\mathcal{M}$). (For, since g belongs to $\mathcal{M}$, it is orthogonal to each element of $\mathcal{R} - \mathcal{M}$ and therefore belongs to $\mathcal{R} - (\mathcal{R} - \mathcal{M})$). Therefore $\mathsf{P}_{\mathcal{M}} f = g, \mathsf{P}_{\mathcal{R}-\mathcal{M}} f = h = f - g$; *i.e.*, $\mathsf{P}_{\mathcal{R}-\mathcal{M}} f = f - \mathsf{P}_{\mathcal{M}} f$. This fact, $\mathsf{P}_{\mathcal{R}-\mathcal{M}} f = \mathsf{I}f - \mathsf{P}_{\mathcal{M}} f$, we express symbolically as $\mathsf{P}_{\mathcal{R}-\mathcal{M}} = \mathsf{I} - \mathsf{P}_{\mathcal{M}}$ (for the addition, subtraction and multiplication of operators, see the discussion in THEOREM 14).

The following should be noted: A short time ago we easily recognized that $\mathcal{M}$ is a subset of $\mathcal{R} - (\mathcal{R} - \mathcal{M})$. It is difficult to prove directly that both sets are equal. But this equality follows immediately from

$$\mathsf{P}_{\mathcal{R}-(\mathcal{R}-\mathcal{M})} = \mathsf{I} - \mathsf{P}_{\mathcal{R}-\mathcal{M}} = \mathsf{I} - (\mathsf{I} - \mathsf{P}_{\mathcal{M}}) = \mathsf{P}_{\mathcal{M}}$$

Moreover, it follows from the above that if E is a projection, $\mathsf{I} - \mathsf{E}$ is also a projection, and because $\mathsf{I} - (\mathsf{I} - \mathsf{E}) = \mathsf{E}$ the converse is also true.

THEOREM 13. It is always true that

$$\|\mathsf{E}f\|^2 = (\mathsf{E}f, f), \qquad \|\mathsf{E}f\| \leqslant \|f\|$$

$\|\mathsf{E}f\| = 0$ or $= \|f\|$ is characteristic for the f of $\mathcal{R} - \mathcal{M}$ and $\mathcal{M}$ respectively.

NOTE. In particular, therefore,

$$\|\mathsf{E}f - \mathsf{E}g\| = \|\mathsf{E}(f - g)\| \leqslant \|f - g\|$$

i.e., the operator E is continuous (see the discussion after THEOREM 2 in **II.1**).

PROOF: We have (see the discussion after THEOREM 11)

$$\|\mathsf{E}f\|^2 = (\mathsf{E}f, \mathsf{E}f) = (\mathsf{E}f, f)$$

Since $\mathsf{I} - \mathsf{E}$ is also a projection,

$$\begin{aligned} \|\mathsf{E}f\|^2 + \|f - \mathsf{E}f\|^2 &= \|\mathsf{E}f\|^2 + \|(\mathsf{I} - \mathsf{E})f\|^2 \\ &= (\mathsf{E}f, f) + ((\mathsf{I} - \mathsf{E})f, f) \\ &= (f, f) = \|f\|^2 \end{aligned}$$

Since both components are $\geqslant 0$, they are also $\leqslant \|f\|^2$; in particular $\|\mathsf{E}f\|^2 \leqslant \|f\|^2$, $\|\mathsf{E}f\| \leqslant \|f\|$. That $\|\mathsf{E}f\| = 0$, $\mathsf{E}f = 0$ expresses the fact that f belongs to $\mathcal{R} - \mathcal{M}$ we know from THEOREM 11. Because of the above relation, $\|\mathsf{E}f\| = \|f\|$ means that $\|f - \mathsf{E}f\| = 0$, $\mathsf{E}f = f$ and therefore, by THEOREM 11, that f belongs to $\mathcal{M}$.

If R and S are two operators, then we understand by $\mathsf{R}\pm\mathsf{S}$, $a\mathsf{R}$ (a a complex number) and RS the operators defined by

$$(\mathsf{R}\pm\mathsf{S})f=\mathsf{R}f\pm\mathsf{S}f,\quad (a\mathsf{R})f=a(\mathsf{R}f),\quad (\mathsf{RS})f=\mathsf{R}(\mathsf{S}f)$$

and we use the then natural notation

$$\mathsf{R}^0=\mathsf{I},\quad \mathsf{R}^1=\mathsf{R},\quad \mathsf{R}^2=\mathsf{RR},\quad \mathsf{R}^3=\mathsf{RRR},\quad \ldots$$

The rules of calculation which are valid here can be discussed rather easily. For $\mathsf{R}\pm\mathsf{S}$, $a\mathsf{R}$ we can verify without difficulty all elementary laws of calculation valid for numbers, but such is not the case for RS. The distributive law holds, as can easily be verified: $(\mathsf{R}\pm\mathsf{S})\mathsf{T}=\mathsf{RT}\pm\mathsf{ST}$ and $\mathsf{R}(\mathsf{S}\pm\mathsf{T})=\mathsf{RS}\pm\mathsf{RT}$ (for the latter the linearity of R is of course necessary; see the note on THEOREM 11 and the discussion in the following paragraph). The associative law also holds: $(\mathsf{RS})\mathsf{T}=\mathsf{R}(\mathsf{ST})=\mathsf{RST}$, but the commutative law $\mathsf{RS}=\mathsf{SR}$ is not generally valid. [$(\mathsf{RS})f=\mathsf{R}(\mathsf{S}f)$ and $(\mathsf{SR})f=\mathsf{S}(\mathsf{R}f)$ need not equal each other!] If this law does hold for two particular R,S they are said to *commute*. Hence, for example, O and I commute with all R which are defined everywhere:

$$\mathsf{RO}=\mathsf{OR}=\mathsf{O},\qquad \mathsf{RI}=\mathsf{IR}=\mathsf{R}$$

Also, R^m and R^n commute, since $\mathsf{R}^m\mathsf{R}^n=\mathsf{R}^{m+n}$, and therefore does not depend upon the order of m,n.

> THEOREM 14. Let E,F project onto closed linear manifolds $\mathcal{M}$ and $\mathcal{N}$. Then EF is also a projection if and only if E,F commute; *i.e.*, if and only if $\mathsf{EF}=\mathsf{FE}$. Also, EF belongs to the closed linear manifold $\mathcal{P}$ which consists of the elements common to $\mathcal{M}$ and $\mathcal{N}$. The operator $\mathsf{E}+\mathsf{F}$ is a projection if and only if $\mathsf{EF}=\mathsf{O}$ (or equally: $\mathsf{FE}=\mathsf{O}$). This means that all $\mathcal{M}$ is orthogonal to all $\mathcal{N}$; $\mathsf{E}+\mathsf{F}$ then belongs to $\mathcal{M}+\mathcal{N}=[\mathcal{M},\mathcal{N}]$, which in this case $=\{\mathcal{M},\mathcal{N}\}$. The operator $\mathsf{E}-\mathsf{F}$ is a projection if and only if $\mathsf{EF}=\mathsf{F}$ (or equally: if $\mathsf{FE}=\mathsf{F}$). This means that $\mathcal{N}$ is a subset of $\mathcal{M}$, and $\mathsf{E}-\mathsf{F}$ belongs to $\mathcal{M}-\mathcal{N}$.

PROOF: For EF we must re-examine the two conditions of THEOREM 12:

$$(\mathsf{EF}f,g)=(f,\mathsf{EF}g),\qquad (\mathsf{EF})^2=\mathsf{EF}$$

Because $(\mathsf{EF}f,g)=(\mathsf{F}f,\mathsf{E}g)=(f,\mathsf{FE}g)$, the first signifies that

$$(f,\mathsf{EF}g)=(f,\mathsf{FE}g),\qquad (f,(\mathsf{EF}-\mathsf{FE})g)=0$$

Since this holds for all f, $(\mathsf{EF}-\mathsf{FE})g=0$, and since this holds for all g, $\mathsf{EF}-\mathsf{FE}=\mathsf{O}$, $\mathsf{EF}=\mathsf{FE}$. Commutativity is therefore necessary and sufficient for the first condition, but it also has the second one as a consequence:

$$(\mathsf{EF})^2=\mathsf{EFEF}=\mathsf{EEFF}=\mathsf{E}^2\mathsf{F}^2=\mathsf{EF}$$

Since $\mathsf{E}+\mathsf{F}$ always satisfies the first condition $((\mathsf{E}+\mathsf{F})f,g)=(f,(\mathsf{E}+\mathsf{F})g)$ (because E,F do so) only the second condition $(\mathsf{E}+\mathsf{F})^2=\mathsf{E}+\mathsf{F}$ remains to be proved. Since

$$(\mathsf{E}+\mathsf{F})^2=\mathsf{E}^2+\mathsf{F}^2+\mathsf{EF}+\mathsf{FE}=(\mathsf{E}+\mathsf{F})+(\mathsf{EF}+\mathsf{FE})$$

this means simply that $\mathsf{EF}+\mathsf{FE}=\mathsf{O}$. Now for $\mathsf{EF}=\mathsf{O}$, EF is a projection. Therefore, by the above proof, $\mathsf{EF}=\mathsf{FE}$, therefore $\mathsf{EF}+\mathsf{FE}=\mathsf{O}$. Conversely, from $\mathsf{EF}+\mathsf{FE}=\mathsf{O}$ it follows that

$$\mathsf{E}(\mathsf{EF}+\mathsf{FE})=\mathsf{E}^2\mathsf{F}+\mathsf{EFE}=\mathsf{EF}+\mathsf{EFE}=\mathsf{O}$$

therefore $\mathsf{EFE}=\mathsf{O}$, and therefore $\mathsf{EF}=\mathsf{O}$. Consequently, $\mathsf{EF}=\mathsf{O}$ is necessary and sufficient, and, since E and F play identical roles, $\mathsf{FE}=\mathsf{O}$ too is necessary and sufficient.

$\mathsf{E}-\mathsf{F}$ is a projection if and only if $\mathsf{I}-(\mathsf{E}-\mathsf{F})=(\mathsf{I}-\mathsf{E})+\mathsf{F}$ is one, and since $\mathsf{I}-\mathsf{E},\mathsf{F}$ are projections, by the same argument, $(\mathsf{I}-\mathsf{E})\mathsf{F}=\mathsf{O}$, $\mathsf{F}-\mathsf{EF}=\mathsf{O}$, $\mathsf{EF}=\mathsf{F}$ are characteristic of this, or equally, $\mathsf{F}(\mathsf{I}-\mathsf{E})=\mathsf{O}$, $\mathsf{F}-\mathsf{FE}=\mathsf{O}$, $\mathsf{FE}=\mathsf{F}$.

We have yet to prove the propositions on $\mathfrak{M}$, $\mathfrak{N}$ ($\mathsf{E}=\mathsf{P}_{\mathfrak{M}}$, $\mathsf{F}=\mathsf{P}_{\mathfrak{N}}$). First, let $\mathsf{EF}=\mathsf{FE}$. Then each $\mathsf{EF}f=\mathsf{FE}f$ belongs to both $\mathfrak{M}$ and $\mathfrak{N}$, and therefore to $\mathfrak{P}$. And, for each g of $\mathfrak{P}$, $\mathsf{E}g=\mathsf{F}g=g$, therefore $\mathsf{EF}g=\mathsf{F}g=g$; *i.e.*, it has the form $\mathsf{EF}f$. Consequently, $\mathfrak{P}$ is the totality of the values of EF, hence, by THEOREM 11, $\mathsf{EF}=\mathsf{P}_{\mathfrak{P}}$. Second, let $\mathsf{EF}=\mathsf{O}$ (therefore also $\mathsf{FE}=\mathsf{O}$). Each $(\mathsf{E}+\mathsf{F})f=\mathsf{E}f+\mathsf{F}f$ belongs to $\{\mathfrak{M},\mathfrak{N}\}$, and each g of $\{\mathfrak{M},\mathfrak{N}\}$ is equal to $h+j$ (h from $\mathfrak{M}$, j from $\mathfrak{N}$). Therefore $\mathsf{E}h=h,\mathsf{F}h=\mathsf{FE}f=0,\mathsf{F}j=j,\mathsf{E}j=\mathsf{EF}j=0$. Therefore

$$(\mathsf{E}+\mathsf{F})(h+j)=\mathsf{E}h+\mathsf{F}h+\mathsf{E}j+\mathsf{F}j=h+j,\qquad(\mathsf{E}+\mathsf{F})g=g$$

Then g has the form $(\mathsf{E}+\mathsf{F})f$. Consequently $\{\mathfrak{M},\mathfrak{N}\}$ is the totality of values of $\mathsf{E}+\mathsf{F}$, but since $\mathsf{E}+\mathsf{F}$ is a projection, $\{\mathfrak{M},\mathfrak{N}\}$ is the corresponding closed linear manifold (THEOREM 11). Since $\{\mathfrak{M},\mathfrak{N}\}$ is closed, it $=[\mathfrak{M},\mathfrak{N}]=\mathfrak{M}+\mathfrak{N}$. Third, let $\mathsf{EF}=\mathsf{F}$ (therefore $\mathsf{FE}=\mathsf{F}$ also). Then $\mathsf{E}=\mathsf{P}_{\mathfrak{M}},\mathsf{I}-\mathsf{F}=\mathsf{P}_{\mathfrak{R}-\mathfrak{N}}$, therefore $\mathsf{E}-\mathsf{F}=\mathsf{E}-\mathsf{EF}=\mathsf{E}(\mathsf{I}-\mathsf{F})$, equaling $\mathsf{P}_{\mathfrak{P}}$, where $\mathfrak{P}$ is the intersection of $\mathfrak{M}$ and $\mathfrak{R}-\mathfrak{N}$; *i.e.*, $\mathfrak{M}-\mathfrak{N}$.

Finally, $\mathsf{EF}=\mathsf{O}$ means that $(\mathsf{EF}f,g)=0$ always; *i.e.*, $(\mathsf{F}f,\mathsf{E}g)=0$; *i.e.*, that the entire $\mathfrak{M}$ is orthogonal to the entire $\mathfrak{N}$. And $\mathsf{EF}=\mathsf{F}$ means $\mathsf{F}(\mathsf{I}-\mathsf{E})=\mathsf{O}$; *i.e.*, all $\mathfrak{N}$ is orthogonal to $\mathfrak{R}-\mathfrak{M}$, or equally: $\mathfrak{N}$ is a subset of $\mathfrak{R}-(\mathfrak{R}-\mathfrak{M})=\mathfrak{M}$.

If $\mathfrak{N}$ is a subset of $\mathfrak{M}$, then we want also to say for $\mathsf{F}=\mathsf{P}_{\mathfrak{N}},\mathsf{E}=\mathsf{P}_{\mathfrak{M}}$ that F is a part of E: symbolically, $\mathsf{E}\geqslant\mathsf{F}$ or $\mathsf{F}\leqslant\mathsf{E}$. (This then means that $\mathsf{EF}=\mathsf{F}$ or also $\mathsf{FE}=\mathsf{F}$, and has commutativity as a consequence. This can be seen by observation of $\mathfrak{M}$, $\mathfrak{N}$ or by direct calculation. It is always true that $\mathsf{O}\leqslant\mathsf{E}\leqslant\mathsf{I}$. From $\mathsf{E}\leqslant\mathsf{F},\mathsf{F}\leqslant\mathsf{E}$ it follows that $\mathsf{E}=\mathsf{F}$. From $\mathsf{E}\leqslant\mathsf{F},\mathsf{F}\leqslant\mathsf{G}$ it follows that $\mathsf{E}\leqslant\mathsf{G}$. This possesses the characteristics of an ordering according to magnitude. It should further be observed that $\mathsf{E}\leqslant\mathsf{F},\mathsf{I}-\mathsf{E}\geqslant\mathsf{I}-\mathsf{F}$ and E orthogonal to $\mathsf{I}-\mathsf{F}$ are all equivalent. Furthermore, the orthogonality of E',F' follows from that of E,F if $\mathsf{E}'\leqslant\mathsf{E},\mathsf{F}'\leqslant\mathsf{F}$.) If $\mathfrak{M},\mathfrak{N}$ are orthogonal we say that E,F are also orthogonal. (Hence this means that $\mathsf{EF}=\mathsf{O}$ or $\mathsf{FE}=\mathsf{O}$.) Conversely, if E,F commute we say that $\mathfrak{M},\mathfrak{N}$ also commute.

THEOREM 15. The statement $\mathsf{E} \leqslant \mathsf{F}$ is equivalent to the general validity of $\|\mathsf{E}f\| \leqslant \|\mathsf{F}f\|$.

PROOF: From $\mathsf{E} \leqslant \mathsf{F}$ it follows that $\mathsf{E} = \mathsf{EF}$, therefore $\|\mathsf{E}f\| = \|\mathsf{EF}f\| \leqslant \|\mathsf{F}f\|$ (see THEOREM 13). Conversely, this theorem has the following consequence: If $\mathsf{F}f = 0$ then $\|\mathsf{E}f\| \leqslant \|\mathsf{F}f\| = 0$, $\mathsf{E}f = 0$. Now, because of $\mathsf{F}(\mathsf{I}-\mathsf{F})f = (\mathsf{F}-\mathsf{F}^2)f = 0$ we have $\mathsf{E}(\mathsf{I}-\mathsf{F})f = 0$ identically; *i.e.*, $\mathsf{E}(\mathsf{I}-\mathsf{F}) = \mathsf{E}-\mathsf{EF} = \mathsf{O}$, $\mathsf{E} = \mathsf{EF}$, therefore $\mathsf{E} \leqslant \mathsf{F}$.

THEOREM 16. Let $\mathsf{E}_1, \ldots, \mathsf{E}_k$ be projections. Then $\mathsf{E}_1 + \cdots + \mathsf{E}_k$ is a projection if and only if all $\mathsf{E}_m, \mathsf{E}_\ell$ $(m, \ell = 1, \ldots, k;\ m \neq \ell)$ are mutually orthogonal. Another necessary and sufficient condition is

$$\|\mathsf{E}_1 f\|^2 + \cdots + \|\mathsf{E}_k f\|^2 \leqslant \|f\|^2 \qquad \text{for all } f$$

Moreover, $\mathsf{E}_1 + \cdots + \mathsf{E}_k$, $(\mathsf{E}_1 = \mathsf{P}_{\mathfrak{M}_1}, \ldots, \mathsf{E}_k = \mathsf{P}_{\mathfrak{M}_k})$ is then the projection of $\mathfrak{M}_1 + \cdots + \mathfrak{M}_k = [\mathfrak{M}_1, \ldots, \mathfrak{M}_k]$, which in this case $= \{\mathfrak{M}_1, \ldots, \mathfrak{M}_k\}$.

PROOF: The last proposition obtains by repeated application of THEOREM 14. And so does the sufficiency of the first criterion. If the second criterion is satisfied, then the first one is too. For $m \neq \ell$, $\mathsf{E}_m f = f$

$$\|\mathsf{E}_1 f\|^2 + \cdots + \|\mathsf{E}_k f\|^2 = \|f\|^2 + \sum_{\ell \neq m} \|\mathsf{E}_\ell f\|^2 \leqslant \|f\|^2$$

$$\|\mathsf{E}_\ell f\|^2 = 0, \quad \mathsf{E}_\ell f = 0 \quad : \quad \ell \neq m$$

But since $\mathsf{E}_m(\mathsf{E}_m f) = \mathsf{E}_m f$ holds identically, $\mathsf{E}_\ell(\mathsf{E}_m f) = 0$; *i.e.*, $\mathsf{E}_\ell \mathsf{E}_m = \mathsf{O}$. Finally, the second condition is necessary: If $\mathsf{E}_1 + \cdots + \mathsf{E}_k$ is a projection, then (THEOREM 13)

$$\begin{aligned} \|\mathsf{E}_1 f\|^2 + \cdots + \|\mathsf{E}_k f\|^2 &= (\mathsf{E}_1 f, f) + \cdots + (\mathsf{E}_k f, f) \\ &= ((\mathsf{E}_1 + \cdots + \mathsf{E}_k)f, f) \\ &= \|(\mathsf{E}_1 + \cdots + \mathsf{E}_k)f\|^2 \leqslant \|f\|^2 \end{aligned}$$

We have therefore the following logical scheme: $\mathsf{E}_1 + \cdots + \mathsf{E}_k$ is a projection $\Rightarrow$ second criterion $\Rightarrow$ first criterion $\Rightarrow$ $\mathsf{E}_1 + \cdots + \mathsf{E}_k$ is a projection. Therefore all three are equivalent.

In conclusion, we prove a theorem on the convergence of the projections:

THEOREM 17. Let $\mathsf{E}_1, \mathsf{E}_2, \ldots$ be an increasing or decreasing sequence of projections: $\mathsf{E}_1 \leqslant \mathsf{E}_2 \leqslant \cdots$ or $\mathsf{E}_1 \geqslant \mathsf{E}_2 \geqslant \cdots$. These converge to a projection E in the sense that for all f, $\mathsf{E}_n f \longrightarrow \mathsf{E}f$; also, all $\mathsf{E}_n \leqslant \mathsf{E}$ or $\mathsf{E}_n \geqslant \mathsf{E}$, respectively.

PROOF: It suffices to investigate the second case, since the first can be reduced to it by the substitutions $\mathsf{I}-\mathsf{E}_1, \mathsf{I}-\mathsf{E}_2, \ldots, \mathsf{I}-\mathsf{E}$ for $\mathsf{E}_1, \mathsf{E}_2, \ldots, \mathsf{E}$. Let therefore $\mathsf{E}_1 \geqslant \mathsf{E}_2 \geqslant \cdots$. By THEOREM 13, $\|\mathsf{E}_1 f\|^2 \geqslant \|\mathsf{E}_2 f\|^2 \geqslant \cdots \geqslant 0$ therefore

$\lim_{m\to\infty} \|\mathsf{E}_m f\|^2$ exists. Then for each $\epsilon > 0$ there exists an $N = N(\epsilon)$ such that for $m, \ell \geqslant N$

$$\|\mathsf{E}_m f\|^2 - \|\mathsf{E}_\ell f\|^2 < \epsilon$$

Now for $m \leqslant \ell$, $\mathsf{E}_m \geqslant \mathsf{E}_\ell$ the operator $\mathsf{E}_m - \mathsf{E}_\ell$ is a projection, therefore

$$\begin{aligned}\|\mathsf{E}_m f\|^2 - \|\mathsf{E}_\ell f\|^2 &= (\mathsf{E}_m f, f) - (\mathsf{E}_\ell f, f)\\ &= ((\mathsf{E}_m - \mathsf{E}_\ell)f, f) = \|(\mathsf{E}_m - \mathsf{E}_\ell)f\|^2\\ &= \|\mathsf{E}_m f - \mathsf{E}_\ell f\|^2\end{aligned}$$

from which it follows that $\|\mathsf{E}_m f - \mathsf{E}_\ell f\| < \sqrt{\epsilon}$. The sequence $\mathsf{E}_1 f, \mathsf{E}_2 f, \ldots$ therefore satisfies the Cauchy convergence criterion and has a limit f^* (see **D** from **II.2**!). $\mathsf{E}f = f^*$ therefore defines an operation which has meaning everywhere.

From $(\mathsf{E}_n f, g) = (f, \mathsf{E}_n g)$ it follows by transition to the limit that

$$(\mathsf{E}f, g) = (f, \mathsf{E}g)$$

and from $(\mathsf{E}_n f, \mathsf{E}_n g) = (\mathsf{E}_n f, g)$ that $(\mathsf{E}f, \mathsf{E}g) = (\mathsf{E}f, g)$. Therefore

$$(\mathsf{E}^2 f, g) = (\mathsf{E}f, g) \quad : \quad \mathsf{E}^2 = \mathsf{E}$$

Consequently E is a projection. For $\ell \geqslant m$, $\|\mathsf{E}_m f\| \geqslant \|\mathsf{E}_\ell f\|$ and as $\ell \to \infty$ we obtain $\|\mathsf{E}_m f\| \geqslant \|\mathsf{E}f\|$. Therefore $\mathsf{E}_m \geqslant \mathsf{E}$ (THEOREM 15).

If $\mathsf{E}_1, \mathsf{E}_2, \ldots$ are projections, each pair of which are mutually orthogonal, then

$$\mathsf{E}_1, \quad \mathsf{E}_1 + \mathsf{E}_2, \quad \mathsf{E}_1 + \mathsf{E}_2 + \mathsf{E}_3, \quad \ldots$$

are also projections, and form an increasing sequence. By THEOREM 17 they converge to a projection which is $\geqslant$ all of them, and which we can denote by $\mathsf{E} = \mathsf{E}_1 + \mathsf{E}_2 + \cdots$. Let $\mathsf{E}_1 = \mathsf{P}_{\mathfrak{M}_1}$, $\mathsf{E}_2 = \mathsf{P}_{\mathfrak{M}_2}, \ldots, \mathsf{E} = \mathsf{P}_{\mathfrak{M}}$. Since all $\mathsf{E}_m \leqslant \mathsf{E}$, $\mathfrak{M}_m$ is a subset of $\mathfrak{M}$, therefore $\mathfrak{M}$ also includes

$$[\mathfrak{M}_1, \mathfrak{M}_2, \ldots] = \mathfrak{M}_1 + \mathfrak{M}_2 + \cdots = \mathfrak{M}'$$

Conversely, all $\mathfrak{M}_m$ are subsets of $\mathfrak{M}'$; therefore $\mathsf{E}_m \leqslant \mathsf{P}_{\mathfrak{M}'} = \mathsf{E}'$. Consequently, by reasons of continuity (see the treatment in the proof above), $\mathsf{E} \leqslant \mathsf{E}'$. Therefore $\mathfrak{M}$ is a subset of $\mathfrak{M}'$, and hence $\mathfrak{M} = \mathfrak{M}'$, $\mathsf{E} = \mathsf{E}'$; *i.e.*, $\mathfrak{M} = \mathfrak{M}_1 + \mathfrak{M}_2 + \cdots$ or, written another way,

$$\mathsf{P}_{\mathfrak{M}_1 + \mathfrak{M}_2 + \ldots} = \mathsf{P}_{\mathfrak{M}_1} + \mathsf{P}_{\mathfrak{M}_2} + \cdots$$

With this we conclude our study of projection operators.

5. OPERATORS IN HILBERT SPACE

We have now given sufficient consideration to the geometric relations of the (Hilbert) space $\mathcal{R}_\infty$ of infinitely many dimensions that we may turn our attention to its linear operators; *i.e.*, to the linear mappings of $\mathcal{R}_\infty$ on itself. For this purpose, we must introduce several concepts which were actually anticipated, to a certain extent, in the last few sections.

In these sections, we concerned ourselves with *operators*, which we define as follows (in accord with the statements made preceding THEOREM 11):

> DEFINITION 6. An operator R is a function defined in a subset of $\mathcal{R}$ with values from $\mathcal{R}$; that is, a relation which establishes a correspondence between certain elements f of $\mathcal{R}$ and elements $\mathsf{R}f$ of $\mathcal{R}$.

(We have admitted the $\mathcal{R}_n$ here in addition to $\mathcal{R}_\infty$. It should be observed that if $\mathcal{R}_\infty$ is an F_Ω then the operator R is defined for the elements of F_Ω; *i.e.*, ordinary configuration space functions, and its values are defined likewise. The operators are then so-called "function-functions" or "functionals." See the examples of **I.2** & **4**.) The class of the f for which $\mathsf{R}f$ is defined—the domain of R—need not encompass the entire $\mathcal{R}$, but if it does so, R is said to be defined everywhere. In addition, it is not necessary that the set of all the $\mathsf{R}f$—the range of R (the mapping of its domain mediated by R)—be contained in the domain of R; *i.e.*, if $\mathsf{R}f$ has meaning, it does not necessarily follow that $\mathsf{R}(\mathsf{R}f) = \mathsf{R}^2 f$ is defined.[58]

We have already given the meaning of $\mathsf{R} \pm \mathsf{S}$, $a\mathsf{R}$, RS, R^m (R, S operators, a a complex number, $m = 0, 1, 2, \ldots$) in the preceding section:

$$(\mathsf{R} \pm \mathsf{S})f = \mathsf{R}f \pm \mathsf{S}f, \quad (a\mathsf{R})f = a \cdot \mathsf{R}f, \quad (\mathsf{RS})f = \mathsf{R}(\mathsf{S}f)$$
$$\mathsf{R}^0 = \mathsf{I}, \quad \mathsf{R}^1 = \mathsf{R}, \quad \mathsf{R}^2 = \mathsf{RR}, \quad \mathsf{R}^3 = \mathsf{RRR}, \quad \ldots$$

In determining the domains of these operators, it should be observed that

[58] For example, let $\mathcal{R}_\infty$ be an F_Ω, where Ω is the space of all real x, $-\infty < x < +\infty$. $\frac{d}{dx}$ is a functional; *i.e.*, an operator, but defined in our sense only for such $f(x)$ as, in the first place, are differentiable and which, in the second place, have finite

$$\int_{-\infty}^{+\infty} |\tfrac{d}{dx} f(x)|^2 \, dx$$

(see **II.8** where this is discussed in more detail). Naturally, in general, $\frac{d^2}{dx^2} f(x)$ will not exist, and

$$\int_{-\infty}^{+\infty} |\tfrac{d^2}{dx^2} f(x)|^2 \, dx$$

is not necessarily finite. For example, $f(x) = |x|^{\frac{3}{2}} e^{-x^2}$ behaves in this manner.

the left sides (*i.e.*, the operators $\mathsf{R} \pm \mathsf{S}$, $a\mathsf{R}$, RS) are defined only if the right sides are also defined. Therefore, for example, $\mathsf{R} \pm \mathsf{S}$ is defined only in the common parts of the domains of R and S, etc. If $\mathsf{R}f$ takes on each of its values only once, then it has an inverse R^{-1}: R^{-1} is defined if $\mathsf{R}f = g$ has a solution g, and its value is then this g. The discussion in the preceding sections was on the laws of calculation valid for $\mathsf{R} \pm \mathsf{S}$, $a\mathsf{R}$, RS; here we will only add the following with regard to their domains. The operators there designated as equal also have identical domains, while operator equations such as $\mathsf{O} \cdot \mathsf{R} = \mathsf{O}$ do not hold for the domains. $\mathsf{O}f$ always has meaning, while $(\mathsf{O} \cdot \mathsf{R})f$, by definition, only has meaning if $\mathsf{R}f$ is defined (but if both are defined, then both $= 0$). On the other hand, $\mathsf{I} \cdot \mathsf{R} = \mathsf{R} \cdot \mathsf{I} = \mathsf{R}$ hold, and also $\mathsf{R}^m \cdot \mathsf{R}^\ell = \mathsf{R}^{m+\ell}$, and the same is true for their domains.

If R, S have inverses, then RS also possesses an inverse, which is, as can easily be seen, $(\mathsf{RS})^{-1} = \mathsf{S}^{-1}\mathsf{R}^{-1}$. Furthermore, for $a \neq 0$, $(a\mathsf{R})^{-1} = \frac{1}{a}\mathsf{R}^{-1}$. If R^{-1} exists we can also form the other negative powers of R:

$$\mathsf{R}^{-2} = \mathsf{R}^{-1}\mathsf{R}^{-1}, \quad \mathsf{R}^{-3} = \mathsf{R}^{-1}\mathsf{R}^{-1}\mathsf{R}^{-1}, \quad \dots$$

After this general development, we proceed to the investigation in more detail of those special classes of operators which will be of particular importance to us.

DEFINITION 7. An operator A is said to be *linear* if its domain is a linear manifold; *i.e.*, if it contains $a_1 f_1 + \cdots + a_k f_k$ along with $f_1, \dots, f_k$, and if

$$\mathsf{A}(a_1 f_1 + \cdots + a_k f_k) = a_1 \mathsf{A} f_1 + \cdots + a_k \mathsf{A} f_k$$

In the following we shall consider only linear operators, and indeed, only those whose domains are everywhere dense.

The latter remark provides a sufficient substitute, for many purposes, for the requirement that operators be defined everywhere, which we must abandon in quantum mechanics. This circumstance is sufficiently important for us to consider it in more detail. For example, let us consider the configuration space in Schrödinger's wave mechanics which, for simplicity, we shall take as one dimensional: $-\infty < q < +\infty$. The wave functions are $\phi(x)$ with finite

$$\int_{-\infty}^{+\infty} |\phi(q)|^2 dq$$

These form a Hilbert space (see **II.3**). We also consider the operators $q\cdot$ and $\frac{\hbar}{i}\frac{d}{dq}\cdot$. They are evidently linear operators, but their domain is not the entire Hilbert space. This is not so for $q\cdot$ because

$$\int_{-\infty}^{+\infty} |q \cdot \phi(q)|^2 dq = \int_{-\infty}^{+\infty} q^2 |\phi(q)|^2 dq$$

can very well become infinite, even if $\int_{-\infty}^{+\infty}|\phi(q)|^2dq$ is finite, so that $q\cdot\phi(q)$ no longer lies in the Hilbert space. And it is not so for $\frac{\hbar}{i}\frac{d}{dq}\cdot$ because there are non-differentiable functions for which, even though $\int_{-\infty}^{+\infty}|\phi(q)|^2dq$ is finite,

$$\int_{-\infty}^{+\infty}|\tfrac{\hbar}{i}\tfrac{d}{dq}\cdot\phi(q)|^2dq=\hbar^2\int_{-\infty}^{+\infty}|\tfrac{d}{dq}\phi(q)|^2dq$$

is not finite (for example: $|q|^{\frac{1}{2}}e^{-q^2}$ or $e^{-q^2}\sin(a^{q^2})$). But the domains are everywhere dense. Both operators are certainly applicable to functions $\phi(q)$ which vanish except on a finite interval $-c<q<+c$ and which are everywhere continuously differentiable; this set of functions is everywhere dense.[59]

We further define

DEFINITION 8. Two operators A and A^* are said to be *adjoint* if they have the same domain, and in this domain

$$(\mathsf{A}f,g)=(f,\mathsf{A}^*g),\qquad(\mathsf{A}^*f,g)=(f,\mathsf{A}g)$$

By exchanging f,g and taking the complex conjugate of both sides, each of these relations follows from the other. Furthermore, it is clear that the relation A,A^* is symmetric; *i.e.*, that A^*,A are also adjoint, so that $\mathsf{A}^{**}=\mathsf{A}$.

We note further that for A only one adjoint A^* can be given; *i.e.*, if A is adjoint to A_1^* and to A_2^*, then $\mathsf{A}_1^*=\mathsf{A}_2^*$. In fact, for all g with $\mathsf{A}g$ defined,

$$(\mathsf{A}_1^*f,g)=(f,\mathsf{A}g)=(\mathsf{A}_2^*f,g)$$

and since there g are everywhere dense, $\mathsf{A}_1^*f=\mathsf{A}_2^*f$. Since this holds in general, $\mathsf{A}_1^*=\mathsf{A}_2^*$. Consequently, A determines A^* uniquely, just as A^* does A.

[59] According to the development of **II.3** (in the discussion of the condition **E**), it is sufficient if we can approximate all linear combinations of the following function arbitrarily well: $f(x)=1$ in a set consisting of a finite number of intervals, and $=0$ elsewhere. This is possible if we can approximate each one of these functions separately, and this in turn is possible if the same can be done for functions with a single unit-interval (the other functions are sums of such). For example, let the interval be $a<x<b$. The function

$$f(x)=\begin{cases}0 & \text{for } x<a-\epsilon \text{ or } x>b+\epsilon\\ \cos^2\left(\frac{\pi}{2}\frac{a-x}{\epsilon}\right) & \text{for } a-\epsilon\leqslant x\leqslant a\\ \cos^2\left(\frac{\pi}{2}\frac{x-b}{\epsilon}\right) & \text{for } b\leqslant x\leqslant b+\epsilon\\ 1 & \text{for } a<x<b\end{cases}$$

actually satisfies our requirements of regularity and approximates the given function arbitrarily well for sufficiently small ϵ.

The following can be seen immediately: O, I and, in general, all projections E are *self-adjoint* (see THEOREM 12); *i.e.*, O^*, I^* and E^* are respectively equal to O, I and E. Furthermore, $(a\mathsf{A})^* = \overline{a}\mathsf{A}^*$ and, so far as $\mathsf{A}+\mathsf{B}$ can be formed in general (*i.e.*, their domain is everywhere dense), $(\mathsf{A}\pm\mathsf{B})^* = \mathsf{A}^*\pm\mathsf{B}^*$. Finally, with limitations on the domain which can easily be ascertained, $(\mathsf{AB})^* = \mathsf{B}^*\mathsf{A}^*$ (because $(\mathsf{AB}f,g) = (\mathsf{B}f,\mathsf{A}^*g) = (f,\mathsf{A}^*\mathsf{B}^*g)$) and $(\mathsf{A}^{-1})^* = (\mathsf{A}^*)^{-1}$ by $(\mathsf{A}^{-1}f,g) = (\mathsf{A}^{-1}f,\mathsf{A}^*\mathsf{A}^{*-1}g) = (\mathsf{A}\mathsf{A}^{-1}f,\mathsf{A}^{*-1}g) = (f,\mathsf{A}^{*-1}g)$.

In particular, for the case of the Schrödinger wave mechanics (which we considered previously, but here a k-dimensional configuration space will be assumed), where the Hilbert space consists of the $\phi(q_1,\dots,q_k)$ with finite

$$\int\cdots\int_{-\infty}^{+\infty} |\phi(q_1,\dots,q_k)|^2 dq_1\dots dq_k$$

we have for the operators $q_\ell\cdot$ and $\frac{\hbar}{i}\frac{\partial}{\partial q_\ell}\cdot$

$$(q_\ell\cdot)^* = q_\ell\cdot, \qquad \Big(\frac{\hbar}{i}\frac{\partial}{\partial q_\ell}\cdot\Big)^* = \frac{\hbar}{i}\frac{\partial}{\partial q_\ell}\cdot$$

The former is clear since

$$\begin{aligned}&\int\cdots\int_{-\infty}^{+\infty} q_\ell\cdot\phi(q_1,\dots,q_k)\cdot\overline{\psi(q_1,\dots,q_k)}dq_1\dots dq_k\\ =&\int\cdots\int_{-\infty}^{+\infty}\phi(q_1,\dots,q_k)\cdot\overline{q_\ell\cdot\psi(q_1,\dots,q_k)}dq_1\dots dq_k\end{aligned}$$

The latter implies that

$$\begin{aligned}&\int\cdots\int_{-\infty}^{+\infty}\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_\ell}\phi(q_1,\dots,q_k)\cdot\overline{\psi(q_1,\dots,q_k)}dq_1\dots dq_k\\ =&\int\cdots\int_{-\infty}^{+\infty}\phi(q_1,\dots,q_k)\cdot\overline{\tfrac{\hbar}{i}\tfrac{\partial}{\partial q_\ell}\psi(q_1,\dots,q_k)}dq_1\dots dq_k\end{aligned}$$

i.e.,

$$\begin{aligned}\int\cdots\int_{-\infty}^{+\infty}\Big\{&\frac{\partial}{\partial q_\ell}\phi(q_1,\dots,q_k)\cdot\overline{\psi(q_1,\dots,q_k)}\\ &+\phi(q_1,\dots,q_k)\cdot\frac{\partial}{\partial q_k}\overline{\psi(q_1,\dots,q_k)}\Big\}dq_1\dots dq_k = 0\end{aligned}$$

$$\begin{aligned}\lim_{A,B\to+\infty}\int\cdots\int_{-\infty}^{+\infty}\Big[\phi(q_1,\dots,q_k)\overline{\psi(q_1,\dots,q_k)}\Big]_{q_\ell=-B}^{q_\ell=+A}\\ dq_1\dots dq_{\ell-1}dq_{\ell+1}\dots dq_k = 0\end{aligned}$$

The limit must exist because the convergence of all integrals

$$\int\cdots\int_{-\infty}^{+\infty}\cdots\ dq_1\dots dq_k$$

is certain (since ϕ, ψ, $\partial\phi/\partial q_\ell$, $\partial\psi/\partial q_\ell$ belong to the Hilbert space), so that it

is only its vanishing which is of importance. If it were $\neq 0$ then the limit (which certainly exists) would be $\neq 0$ for $q_\ell \to +\infty$ or for $q_\ell \to -\infty$:

$$\int \cdots \int_{-\infty}^{+\infty} \phi(q_1, \ldots, q_k)\overline{\psi(q_1, \ldots, q_k)} dq_1 \ldots dq_{\ell-1} dq_{\ell+1} \ldots dq_k$$

which is incompatible with the absolute convergence of the integral

$$\int \cdots \int_{-\infty}^{+\infty} \phi(q_1, \ldots, q_k)\overline{\psi(q_1, \ldots, q_k)} dq_1 \ldots dq_{\ell-1} dq_\ell dq_{\ell+1} \ldots dq_k$$

(ϕ, ψ belong to the Hilbert space!).

If A is the *integral operator*

$$\mathsf{A}\phi(q_q, \ldots, q_k) = \int \cdots \int_{-\infty}^{+\infty} K(q_1, \ldots, q_k; q'_1, \ldots, q'_k) dq'_1 \ldots, dq'_k$$

then the following is obtained directly: A^* is also an integral operator, only its kernel is not

$$K(q_1, \ldots, q_k; q'_1, \ldots, q'_k)$$

but

$$\overline{K(q'_1, \ldots, q'_k; q_1, \ldots, q_k)}$$

Let us now consider the situation in matrix theory, where the Hilbert space consists of all sequences $x_1, x_2, \ldots$ with finite $\sum_{\mu=1}^{\infty} |x_\mu|^2$. A linear operator A transforms $\{x_1, x_2, \ldots\}$ into $\{y_1, y_2, \ldots\}$

$$\mathsf{A}\{x_1, x_2, \ldots\} = \{y_1, y_2, \ldots\}$$

where, because of the linearity of A, the $y_1, y_2, \ldots$ must depend linearly on the $x_1, x_2, \ldots$: [60]

$$y_\mu = \sum_{\nu=1}^{\infty} a_{\mu\nu} x_\nu$$

Therefore A is characterized by the matrix $\{a_{\mu\nu}\}$. We see immediately that the

[60] The following consideration is not rigorous, since it uses linearity in the case of infinite sums, etc. But it can be perfected as follows: Let $\phi_1, \phi_2, \ldots$ be a complete orthonormal set, and let A, A^* be adjoint operators. Let

$$f = \sum_{\nu=1}^{\infty} x_\nu \phi_\nu, \qquad \mathsf{A}f = \sum_{\nu=1}^{\infty} y_\nu \phi_\nu$$

Then

$$y_\mu = (\mathsf{A}f, \phi_\mu) = (f, \mathsf{A}^*\phi_\mu) = \sum_{\nu=1}^{\infty} (f, \phi_\nu)\overline{(\mathsf{A}^*\phi_\mu, \phi_\nu)} \qquad \text{by THEOREM } 7\boldsymbol{\gamma}$$

$$= \sum_{\nu=1}^{\infty} x_\nu \overline{(\phi_\mu, \mathsf{A}\phi_\nu)} = \sum_{\nu=1}^{\infty} (\mathsf{A}\phi_\nu, \phi_\mu) x_\nu$$

matrix $\{\overline{a}_{\nu\mu}\}$ belongs to A^*.[60]

The analogy with the situation in matrix theory which has just been developed suggests introducing the concept of Hermitian operator, in a manner which we shall not expound. Simultaneously we shall introduce also two other concepts which will be important for our later purposes.

DEFINITION 9. The operator A is said to be *Hermitian* if $\mathsf{A}^* = \mathsf{A}$. It is also said to be *definite* if it is always true that $(\mathsf{A}f, f) \geqslant 0$.[61] The operator U is said to be *unitary* if $\mathsf{U}\mathsf{U}^* = \mathsf{U}^*\mathsf{U} = \mathsf{I}$.[62]

For unitary operators we thus have $\mathsf{U}^* = \mathsf{U}^{-1}$. By definition,

$$(\mathsf{U}f, \mathsf{U}g) = (\mathsf{U}^*\mathsf{U}f, g) = (f, g)$$

so, in particular (for $f = g$), $\|\mathsf{U}f\| = \|f\|$. Conversely, unitarity follows from the latter properties if U is defined everywhere and takes on every value (see Note 62). We prove this as follows: Assume it to be true that $\|\mathsf{U}f\| = \|f\|$;

If we set $a_{\mu\nu} = (\mathsf{A}\phi_\nu, \phi_\mu)$ we have the formula

$$y_\mu = \sum_{\nu=1}^{\infty} a_{\mu\nu} x_\nu$$

of the text, and absolute convergence is assured. In the Hilbert space of the sequences $x_1, x_2, \ldots$ the sequences

$$\phi_1 = 1, 0, 0, \ldots$$
$$\phi_2 = 0, 1, 0, \ldots \quad \text{etc.}$$

form a complete orthonormal set (as can easily be seen). For

$$f = \{x_1, x_2, \ldots\}, \qquad f = \sum_{\nu=1}^{\infty} x_\nu \phi_\nu$$
$$\mathsf{A}f = \{y_1, y_2, \ldots\}, \quad \mathsf{A}f = \sum_{\nu=1}^{\infty} y_\nu \phi_\nu$$

In this way complete concordance with the text is reached. If we form $a^*_{\mu\nu}$ for A^* then we see that

$$a^*_{\mu\nu} = (\mathsf{A}^*\phi_\nu, \phi_\mu) = (\phi_\nu, \mathsf{A}\phi_\mu) = \overline{a}_{\nu\mu}$$

[61] $(\mathsf{A}f, f)$ is real in any case, since it equals

$$(\mathsf{A}^*f, f) = (f, \mathsf{A}f) = \overline{(\mathsf{A}f, f)}$$

[62] Consequently, U, U^* must be defined everywhere. Furthermore, they are inverse to each other. Therefore they each take on every value once and only once.

i.e., that $(\mathsf{U}f, \mathsf{U}f) = (f, f)$, $(\mathsf{U}^*\mathsf{U}f, f) = (f, f)$. If we replace f by $\frac{1}{2}(f+g)$ and again by $\frac{1}{2}(f-g)$ and subtract, then we obtain, as may easily be calculated, $\mathrm{Re}(\mathsf{U}f, \mathsf{U}g) = \mathrm{Re}(f, g)$. If we substitute $i \cdot f$ here for f then we get Im in place of Re. Consequently it is true in general that

$$(\mathsf{U}f, \mathsf{U}g) = (f, g), \qquad (\mathsf{U}^*\mathsf{U}f, g) = (f, g)$$

For fixed f this holds for all g. Therefore $\mathsf{U}^*\mathsf{U}f = f$. Since this holds for all f, we have $\mathsf{U}^*\mathsf{U} = \mathsf{I}$. We still must show that $\mathsf{U}\mathsf{U}^* = \mathsf{I}$. For each f there is a g with $\mathsf{U}g = f$, so $\mathsf{U}\mathsf{U}^* f = \mathsf{U}\mathsf{U}^* \cdot \mathsf{U}g = \mathsf{U} \cdot \mathsf{U}^*\mathsf{U}g = \mathsf{U}g = f$. Therefore $\mathsf{U}\mathsf{U}^* = \mathsf{I}$.

Since, because of linearity,

$$\|\mathsf{U}f - \mathsf{U}g\| = \|\mathsf{U}(f-g)\| = \|f-g\|$$

each unitary operator is continuous, which is not at all necessary for Hermitian operators. For example, the operators $q\cdot$ and $\frac{\hbar}{i}\frac{\partial}{\partial q}\cdot$ so important for quantum mechanics are discontinuous.[63]

From our formal rules of calculation for A^* it follows immediately that if U, V are unitary, U^{-1} and $\mathsf{U}\mathsf{V}$ are also. Therefore, all powers of U are also unitary. If A, B are Hermitian then $\mathsf{A} \pm \mathsf{B}$ are also Hermitian. On the other hand, $a\mathsf{A}$ is Hermitian only for real a (if $\mathsf{A} \neq \mathsf{O}$), while $\mathsf{A}\mathsf{B}$ is Hermitian only if A, B commute; *i.e.*, $\mathsf{A}\mathsf{B} = \mathsf{B}\mathsf{A}$. Furthermore, we know that all projectors (in particular O, I) are Hermitian, as also are the operators $q_\ell\cdot$ and $\frac{\hbar}{i}\frac{\partial}{\partial q_\ell}\cdot$ of the Schrödinger theory. All powers of A are Hermitian (also A^{-1} if it exists), and all polynomials with real coefficients. It is noteworthy that for Hermitian A and arbitrary X, $\mathsf{X}\mathsf{A}\mathsf{X}^*$ is also Hermitian:

$$(\mathsf{X}\mathsf{A}\mathsf{X}^*)^* = \mathsf{X}^{**}\mathsf{A}^*\mathsf{X}^* = \mathsf{X}\mathsf{A}\mathsf{X}^*$$

Therefore, for example, all $\mathsf{X}\mathsf{X}^*$ ($\mathsf{A} = \mathsf{I}$) and all $\mathsf{X}^*\mathsf{X}$ (X^* in place of X) are

---

[63] For given

$$\int_{-\infty}^{+\infty} |\phi(q)|^2\, dq$$

both

$$\int_{-\infty}^{+\infty} q^2 |\phi(q)|^2\, dq \quad \text{and} \quad \int_{-\infty}^{+\infty} |\tfrac{d}{dq}\phi(q)|^2\, dq$$

can be made arbitrarily large. Take, for example,

$$\phi(q) = ae^{-bq^2}$$

The three integrals are all finite ($b > 0$!), but are proportional respectively to

$$a^2 b^{-\frac{1}{2}}, \quad a^2 b^{-\frac{3}{2}}, \quad a^2 b^{\frac{1}{2}}$$

so that the value of any two of them can be prescribed at will.

Hermitian. For unitary U, UAU^{-1} is Hermitian because $\mathsf{U}^{-1} = \mathsf{U}^*$.

The continuity of operators, just as in the case of the numerical functions treated in analysis, is a property of basic importance. We therefore want to state several characteristic conditions for its existence in the case of linear operators.

THEOREM 18. A linear operator R is *continuous* if it is continuous at the point $f = 0$. A necessary and sufficient condition is the existence of a constant C for which, in general, $\|\mathsf{R}f\| \leqslant C \cdot \|f\|$. In turn, this condition is equivalent to the general validity of

$$|(\mathsf{R}f, g)| \leqslant C \cdot \|f\| \cdot \|g\|$$

For Hermitian R this need be required only for $f = g$:

$$|(\mathsf{R}f, f)| \leqslant C \cdot \|f\|^2$$

or, since $(\mathsf{R}f, f)$ is real (Note 61):

$$-C \cdot \|f\|^2 \leqslant (\mathsf{R}f, f) \leqslant +C \cdot \|f\|^2$$

NOTE. The concept of continuity for operators originated with Hilbert.[64] He characterized it as "boundedness," and defined it by the next to the last of the criteria given above. If only one of the $\leqslant$ in the last criterion is generally valid, then R is said to be half-bounded, above or below. For example, each definite R is half-bounded below (with $C = 0$).

PROOF: Continuity for $f = 0$ implies that for each $\epsilon > 0$ there exists a $\delta > 0$ such that $\|\mathsf{R}f\| < \epsilon$ follows from $\|f\| < \delta$. Then it follows from $\|f - f_0\| < \delta$ that

$$\|\mathsf{R}(f - f_0)\| = \|\mathsf{R}f - \mathsf{R}f_0\| < \epsilon$$

i.e., that R is also continuous for f_0, and therefore everywhere.

If $\|\mathsf{R}f\| \leqslant C \cdot \|f\|$ (of course, $C > 0$), then we have continuity: we can set $\delta = \epsilon/C$. Conversely, if continuity exists we can determine the δ for $\epsilon = 1$ and set $C = 2/\delta$. Then

$$\|\mathsf{R}f\| \leqslant C \cdot \|f\|$$

holds for $f \neq 0$. For $f \neq 0$ we have $\|f\| > 0$ so can introduce

$$g = \frac{\frac{1}{2}\delta}{\|f\|} \cdot f$$

We then have $\|g\| = \frac{1}{2}\delta$ and therefore

[64] Gött. Nachr. 1906.

$$\|\mathsf{R}g\| = \frac{\frac{1}{2}\delta}{\|f\|} \cdot \|\mathsf{R}f\| < 1, \qquad \|\mathsf{R}f\| < \frac{\|f\|}{\frac{1}{2}\delta} = C \cdot \|f\|$$

From $\|\mathsf{R}f\| \leqslant C \cdot \|f\|$ it follows that

$$|(\mathsf{R}f, g)| \leqslant \|\mathsf{R}f\| \cdot \|g\| \leqslant C \cdot \|f\| \cdot \|g\|$$

Conversely, from $|(\mathsf{R}f, g)| \leqslant C \cdot \|f\| \cdot \|g\|$ we obtain $\|\mathsf{R}f\|^2 \leqslant C \cdot \|f\| \cdot \|\mathsf{R}f\|$ if we set $g = \mathsf{R}f$, and therefore $\|\mathsf{R}f\| \leqslant C \cdot \|f\|$. It still remains to show for Hermitian R that $|(\mathsf{R}f, f)| \leqslant C \cdot \|f\|^2$ leads to $|(\mathsf{R}f, g)| \leqslant C \cdot \|f\| \cdot \|g\|$. Substitution of $\frac{1}{2}(f+g)$ and $\frac{1}{2}(f-g)$ for f gives[65]

$$\begin{aligned} |\mathrm{Re}\,(\mathsf{R}f, g)| &= |(\mathsf{R}\tfrac{f+g}{2}, \tfrac{f+g}{2}) - (\mathsf{R}\tfrac{f-g}{2}, \tfrac{f-g}{2})| \\ &\leqslant C \cdot \left(\|\tfrac{f+g}{2}\|^2 + \|\tfrac{f-g}{2}\|^2 \right) \\ &= C \cdot \frac{\|f\|^2 + \|g\|^2}{2} \end{aligned}$$

We now substitute $af, \frac{1}{a}g$ for f, g, as in the proof of THEOREM 1. Minimizing the right side gives $|\mathrm{Re}\,(\mathsf{R}f, g)| \leqslant C \cdot \|f\| \cdot \|g\|$. Then replacing f by $e^{i\alpha}f$ (α real) gives for the maximum value of the left side

$$|(\mathsf{R}f, g)| \leqslant C \cdot \|f\| \cdot \|g\|$$

Of course, this is valid only if $\mathsf{R}g$ is defined, but since these g are everywhere dense and $\mathsf{R}g$ no longer enters into the final result, it holds generally by reason of continuity.

THEOREM 19. If R is Hermitian and definite, then

$$|\overline{(\mathsf{R}f, g)}| \leqslant \sqrt{(\mathsf{R}f, f) \cdot (\mathsf{R}g, g)}$$

From $(\mathsf{R}f, f) = 0$ it then follows that $\mathsf{R}f = 0$

PROOF: The above inequality follows from the general validity of $(\mathsf{R}f, f) \geqslant 0$ (definiteness!), just as the Schwarz inequality

$$|(f, g)| \leqslant \sqrt{(f, f) \cdot (g, g)} = \|f\| \cdot \|g\|$$

was derived in THEOREM 1 from $(f, f) \geqslant 0$. If now $(\mathsf{R}f, f) = 0$ then it follows from this inequality that also $(\mathsf{R}f, g) = 0$, if $\mathsf{R}g$ is defined. Consequently, it holds for a g-set which is everywhere dense, therefore, by reason of continuity, for all g, giving $\mathsf{R}f = 0$.

[65] The Hermitian character of R is important in the reduction

$$(\mathsf{R}\tfrac{f+g}{2}, \tfrac{f+g}{2}) - (\mathsf{R}\tfrac{f-g}{2}, \tfrac{f-g}{2}) = \frac{(\mathsf{R}f, g) + (\mathsf{R}g, f)}{2} = \frac{(\mathsf{R}f, g) + \overline{(f, \mathsf{R}g)}}{2}$$

(in the third step).

Finally we shall make reference to the important concept of the *commutativity* of two operators R, S; *i.e.*, to the relation $\mathsf{RS} = \mathsf{SR}$. From $\mathsf{RS} = \mathsf{SR}$ it follows that

$$\mathsf{S}\ldots\mathsf{SSR} = \mathsf{S}\ldots\mathsf{SRS} = \mathsf{S}\ldots\mathsf{RSS} = \ldots = \mathsf{RS}\ldots\mathsf{SS}$$

i.e., R, S^n commute ($n = 1, 2, \ldots$). Since $\mathsf{RI} = \mathsf{IR} = \mathsf{R}$ and $\mathsf{S}^0 = \mathsf{I}$, this holds also for $n = 0$. If S^{-1} exists then $\mathsf{S}^{-1} \cdot \mathsf{SR} \cdot \mathsf{S}^{-1} = \mathsf{S}^{-1} \cdot \mathsf{RS} \cdot \mathsf{S}^{-1}$, therefore

$$\mathsf{S}^{-1} \cdot \mathsf{SR} \cdot \mathsf{S}^{-1} = \mathsf{S}^{-1}\mathsf{S} \cdot \mathsf{RS}^{-1} = \mathsf{RS}^{-1}$$
$$\mathsf{S}^{-1} \cdot \mathsf{RS} \cdot \mathsf{S}^{-1} = \mathsf{S}^{-1}\mathsf{R} \cdot \mathsf{SS}^{-1} = \mathsf{S}^{-1}\mathsf{R}$$

and hence $\mathsf{RS}^{-1} = \mathsf{S}^{-1}\mathsf{R}$. Consequently, $n = -1$ and therefore $n = -2, -3, \ldots$ are also admissible. That is, R commutes with all powers of S. Repeated application shows that each power of R commutes with each power of S. If R commutes with S, T then it obviously commutes with all $a\mathsf{S}$ and also with $\mathsf{S} + \mathsf{T}, \mathsf{ST}$. Together with the above results, it follows from this that if R, S commute then all polynomials of R commute with all polynomials of S. In particular, for $\mathsf{R} = \mathsf{S}$, all polynomials of R commute with each other.

6. THE EIGENVALUE PROBLEM

We have come now far enough that we can consider in abstract Hilbert space a problem which is of central importance in quantum mechanics, in its relationship to the special cases F_Z and F_Ω: the solution of (respectively) the equations $\mathbf{E}_1$ and $\mathbf{E}_2$ in section **I.3**. We call this the eigenvalue problem, and we must formulate it anew in a unified fashion.

In **I.3**, $\mathbf{E}_1$ and $\mathbf{E}_2$ both required the finding of all solutions $\phi \neq 0$ of

$$\mathbf{E} \qquad\qquad \mathsf{H}\phi = \lambda\phi$$

where H is the Hermitian operator corresponding to the Hamiltonian function (see the discussion in **I.3**), ϕ an element of the Hilbert space, and λ a real number (H given, ϕ, λ to be determined). In connection with this, however, certain requirements were made regarding the number of solutions to be found. It was required to find such a number that

1°. in matrix theory, a matrix $\mathbb{S} = \{s_{\mu\nu}\}$ could be formed from these solutions

$$\phi_1 = \{s_{11}, s_{21}, \ldots\}$$
$$\phi_2 = \{s_{12}, s_{22}, \ldots\}, \quad \text{etc.}$$

(we are in F_Z!) which possesses an inverse $\mathbb{S}^{-1}$ (see **I.3**);

2°. in the wave theory, each wave function (which need not be a solution) can be developed in a series of the solutions

$$\phi_1 = \phi_1(q_1, \ldots, q_k)$$
$$\phi_2 = \phi_2(q_1, \ldots, q_k), \quad \text{etc.}$$

($\phi_1, \phi_2, \ldots$ may belong to different λ):

$$\phi(q_1, \ldots, q_k) = \sum_{n=1}^{\infty} C_n \phi_n(q_1, \ldots, q_k)$$

(There was no mention of this latter circumstance in **I.3**, but this requirement is indispensable for the further development of the wave theory, in particular for the Schrödinger "perturbation theory."[66])

Now 1° amounts to the same thing as 2° because the matrix $\mathbb{S}$ transforms $\{1,0,0,\ldots\},\ \{0,1,0,\ldots\},\ \ldots$ respectively into

$$\{s_{11},s_{21},s_{31},\ldots\},\ \{s_{12},s_{22},s_{32},\ldots\},\ \ldots$$

and therefore the entire Hilbert space $\mathfrak{R}_\infty$ into the closed linear manifold spanned by $\phi_1,\phi_2,\ldots$. In order that $\mathbb{S}^{-1}$ exist therefore, the latter must also be equal to $\mathfrak{R}_\infty$. But 2° states the same thing directly: it also requires that each ϕ can be approximated to an arbitrary degree of accuracy by a linear combination of the $\phi_1,\phi_2,\ldots$.[67] Let us make the significance of this condition clear, and also prove once again the properties of the equation **E** with the formal apparatus now at our command.

First, since $\phi\neq 0$ is required, and since $a\phi$ is a solution if ϕ is, it is sufficient to consider solutions with $\|\phi\|=1$. Second, we do not need to require that λ be real, since this follows from $\mathsf{H}\phi=\lambda\phi$:

$$(\mathsf{H}\phi,\phi)=(\lambda\phi,\phi)=\lambda(\phi,\phi)=\lambda$$

(see **II.5**, Note 61). Third, the solutions ϕ_1,ϕ_2 which belong to different λ_1,λ_2 are mutually orthogonal:

$$(\mathsf{H}\phi_1,\phi_2)=\lambda_1(\phi_1,\phi_2)$$
$$(\mathsf{H}\phi_1,\phi_2)=(\phi_1,\mathsf{H}\phi_2)=\lambda_2(\phi_1,\phi_2)$$

Therefore, $(\phi_1,\phi_2)=0$ because $\lambda_1(\phi_1,\phi_2)=\lambda_2(\phi_1,\phi_2)$ and $\lambda_1\neq\lambda_2$.

Now let $\lambda_1,\lambda_2,\ldots$ be the λ, all different from one another, for which **E** is solvable. (If we choose a solution ϕ_λ of absolute value 1 for each λ with solvable $\mathsf{H}\phi=\lambda\phi$, then the ϕ_λ form an orthonormal set, by reason of previous comments. By **II.2**, THEOREM $3^{(\infty)}$ this set is then a finite or infinite sequence. Therefore we can also write the λ as a sequence, which may or may not terminate.) For each $\lambda=\lambda_\rho$ all solutions of $\mathsf{H}\phi=\lambda\phi$ form a linear manifold, and indeed: a closed linear manifold.[68] According to THEOREM 9, therefore, there exists an

[66] See the fifth paper in the book mentioned in Note 9 (Ann. Phys. **80** (1926)).

[67] We purposely do not go into the finer questions of convergence; these questions were not treated with exactness in the original forms of the matrix and wave theories; also, we shall settle them later (see, e.g. **II.9**).

[68] The latter is evident without further discussion only for continuous H everywhere defined; *i.e.*, for which $\mathsf{H}f_n\to f$ follows from $f_n\to f$. Moreover, the following more limited property is also a consequence, as may easily be seen: from $f_n\to f$, $\mathsf{H}f_n\to f^*$ it follows that $\mathsf{H}f=f^*$ (this is the so-called closure of H; see the work of the author in Math. Ann. **102** (1929)). This is always satisfied with the operators of quantum mechanics, even the discontinuous ones; a Hermitian operator which is not closed can be made (Hermitian and) closed by a unique extension of its domain (which is not the case for the property of continuity, for example); see **II.9**, page 92, Note 96.

orthonormal set $\phi_{\rho,1}, \ldots, \phi_{\rho,\nu_\rho}$ of such solutions which spans this closed linear manifold. The number ν_ρ is clearly the maximum number of linearly independent solutions for $\lambda = \lambda_\rho$. This is known as the *multiplicity* of the eigenvalue λ_ρ. ($\nu = 1, 2, \ldots, \infty$; $\nu = \infty$ can occur: look, for example, to the case $\mathsf{H} = \mathsf{I}$, $\lambda = 1$.) According to the preceding discussion, the $\phi_{\rho,1}, \ldots, \phi_{\rho,\nu_\rho}$ of two different ρ are also mutually orthogonal. Therefore, the totality

$$\phi_{\rho,\nu} \quad : \quad \rho = 1, 2, \ldots; \quad \nu = 1, \ldots, \nu_\rho$$

also forms an orthonormal set. By reason of its origin, we recognize that it spans the same closed linear manifold as all solutions ϕ of **E**.

We number the $\phi_{\rho,\nu}$ in any order by $\psi_1, \psi_2, \ldots$ and the corresponding λ_ρ by $\lambda^{(1)}, \lambda^{(2)}, \ldots$. The condition previously formulated that all solutions of **E** should span $\mathfrak{R}_\infty$ as a closed linear manifold then implies that $\psi_1, \psi_2, \ldots$ (a subset of solutions!) must do this by itself—therefore, by THEOREM 7, that this orthonormal set is complete.

The solution of the eigenvalue problem in the sense of quantum mechanics would therefore require the finding of a sufficient number of solutions

$$\psi = \psi_1, \psi_2, \ldots \quad \text{and} \quad \lambda = \lambda_1, \lambda_2, \ldots$$

of **E** so that a complete orthonormal set can be formed from them. But this is not possible in general. For example, in wave theory we will see that for a certain subset of solutions of **E** (*i.e.*, of $\mathbf{E}_2$ in **I.3**)—all of which are needed to develop each wave function by solutions (see above)—there exists no finite value for the integral of the square of the absolute value.[69] Therefore it does not belong to Hilbert space. Hence there is no complete orthonormal set of solutions in Hilbert space (and we consider Hilbert spaces only in **E**!).

On the other hand, the Hilbert theory of the eigenvalue problem shows that this phenomenon does not at all represent an exception to the behavior of operators (not even of the continuous ones).[70] We must therefore analyze the situations which result when it does occur. (We will soon see what this means physically. See **III.3**.) If it occurs; *i.e.*, if the orthonormal set selected from the solutions of **E** is not complete, then we may say that a "continuous spectrum of H" exists. ($\lambda_1, \lambda_2, \ldots$ form the "point" or "discrete" spectrum of H.)

Our next problem, since **E** has failed, is then to find an improved formulation of the eigenvalue problem for Hermitian operators and to apply this to quantum mechanics. We follow a pattern set by Hilbert (see above, Note 70), which must now be explained.

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[69] See, for example, Schrödinger's treatment of the hydrogen atom, in the reference cited in Note 16.

[70] See the reference cited in Note 64.

7. CONTINUATION

The equation

$$\mathsf{H}\phi = \lambda\phi$$

—as well as the requirement that a complete orthonormal set can be formed from its solutions—originates in an analogy with the case of finite dimensions, the $\mathcal{R}_n$.

In $\mathcal{R}_n$, H is a matrix

$$\mathbb{H} = \{h_{\mu\nu}\} \quad : \quad \mu\nu = 1, 2, \ldots, n \; ; \; h_{\mu\nu} = \overline{h}_{\nu\mu}$$

and it is a well-known algebraic fact that the solutions of

$$\mathbb{H}x = \lambda x \quad : \quad x = \{x_1, x_2, \ldots, x_n\}$$

i.e., form a complete orthonormal set.[71]

This property of the $\mathcal{R}_n$ cannot, as we have seen, carry over by $n \to \infty$ to the $\mathcal{R}_\infty$. So the eigenvalue problem in $\mathcal{R}_\infty$ must be formulated differently. We shall now see that the eigenvalue problem in $\mathcal{R}_n$ can be transformed in such a way that for this new formulation (which in $\mathcal{R}_n$ is equivalent to the old) a transition to $\mathcal{R}_\infty$ does become possible. That is, both express the same thing in $\mathcal{R}_n$ $(n = 1, 2, \ldots)$—namely, the possibility of the diagonalization of Hermitian matrices—but the one can be carried over into $\mathcal{R}_\infty$ while the other cannot.

Let $\{x_{11}, \ldots, x_{1n}\}, \ldots, \{x_{n1}, \ldots, x_{nn}\}$ be the complete orthonormal set of solutions of the eigenvalue equation, and let $\lambda_1, \ldots, \lambda_n$ be the corresponding λ. The vectors $\{x_{11}, \ldots, x_{1n}\}, \ldots, \{x_{n1}, \ldots, x_{nn}\}$ then form a cartesian coordinate system in $\mathcal{R}_n$. The transformation formulas of the coordinates $\mathfrak{x}_1, \ldots, \mathfrak{x}_n$ in this coordinate system to coordinates $\xi_1, \ldots, \xi_n$ that refer to the basis

$$\{1, 0, 0, \ldots, 0\}, \; \{0, 1, 0, \ldots, 0\}, \; \ldots, \; \{0, 0, 0, \ldots, 1\}$$

then run as follows:

$$\{\xi_1, \ldots, \xi_n\} = \mathfrak{x}_1\{x_{11}, \ldots, x_{1n}\} + \cdots + \mathfrak{x}_n\{x_{n1}, \ldots, x_{nn}\}$$

i.e.,

$$\xi_1 = \sum_{\mu=1}^{n} x_{\mu 1}\mathfrak{x}_\mu \, , \quad \ldots, \quad \xi_n = \sum_{\mu=1}^{n} x_{\mu n}\mathfrak{x}_\mu$$

and conversely,

$$\mathfrak{x}_1 = \sum_{\mu=1}^{n} \overline{x}_{1\mu}\xi_\mu \, , \quad \ldots, \quad \mathfrak{x}_n = \sum_{\mu=1}^{n} \overline{x}_{n\mu}\xi_\mu$$

We can write the conditions

$$\sum_{\nu=1}^{n} h_{\mu\nu}x_{\rho\nu} = \lambda_\rho x_{\rho\mu} \quad : \quad \rho = 1, \ldots, n$$

[71] See Courant-Hilbert: the reference cited in Note 30.

as follows, with the help of the variables $\mathfrak{x}_1, \ldots, \mathfrak{x}_n$ and a new set of variables $\eta_1, \ldots, \eta_n$ (in addition to corresponding variables $\mathfrak{y}_1, \ldots, \mathfrak{y}_n$) by reason of the above formula:

$$\sum_{\rho,\mu=1}^{n} \Big(\sum_{\nu=1}^{n} h_{\mu\nu} x_{\rho\nu} \Big) \mathfrak{x}_\rho \bar{\eta}_\mu = \sum_{\rho,\mu=1}^{n} \lambda_\rho x_{\rho\mu} \mathfrak{x}_\rho \bar{\eta}_\mu$$

i.e.,

D $$\sum_{\mu,\nu=1}^{n} h_{\mu\nu} \xi_\nu \bar{\eta}_\mu = \sum_{\rho=1}^{n} \lambda_\rho \Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \xi_\mu \Big) \overline{\Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \eta_\mu \Big)}$$

The cartesian character of our coordinate system may then be expressed as

O $$\sum_{\mu=1}^{n} \xi_\mu \bar{\eta}_\mu = \sum_{\rho=1}^{n} \Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \xi_\mu \Big) \overline{\Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \eta_\mu \Big)}$$

The discovery of a matrix $\{x_{\rho\mu}\}$ with the properties **D**, **O** is then equivalent in $\mathfrak{R}_n$ to solution of the eigenvalue problem. And in this form the transition to $\mathfrak{R}_\infty$ again fails. But this failure is not surprising, for the following reason: The conditions **D**, **O** do not determine the unknowns λ_ρ, $x_{\rho\mu}$ completely. Indeed, as the theory of this diagonal transformation shows (see the reference in Note 71), the λ_ρ are determined uniquely except for order, but the situation is much worse in the case of the $x_{\rho\mu}$. Each row $\{x_{\rho,1}, \ldots, x_{\rho n}\}$ can evidently be multiplied by a complex factor θ_ρ of absolute value 1. And if several of the λ_ρ coincide, even an arbitrary unitary transformation of the corresponding columns $\{x_{\rho,1}, \ldots, x_{\rho n}\}$ is possible! To attempt the difficult transition to the limit $n \to \infty$ with such quantities, which are not uniquely determined, is hopeless: for how can the process converge if the λ_ρ, $x_{\rho\mu}$ can undergo the arbitrarily large fluctuations which become possible because of the incompleteness of their determination?

But this points out the way in which the problem can be handled correctly: we must first seek to replace the conditions **D**, **O** and the unknowns λ_ρ, $x_{\rho\mu}$ by conditions and unknowns which possess the desired uniqueness property. It will be shown that the limiting process then causes less difficulty.

If ℓ is any value which one or more of the λ_ρ assume, then

$$\sum_{\lambda_\rho = \ell} \Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \xi_\mu \Big) \overline{\Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \eta_\mu \Big)}$$

is invariant under the variations (compatible with **D**, **O**) of λ_ρ, $x_{\rho\mu}$ mentioned above. If ℓ is different from all the λ_ρ then the sum vanishes, and is therefore certainly invariant. Consequently the Hermitian form (here ξ and η signify $\xi_1, \ldots, \xi_n$ and $\eta_1, \ldots, \eta_n$ respectively)

$$E(\ell; \xi, \eta) = \sum_{\lambda_\rho \leqslant \ell} \Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \xi_\mu \Big) \overline{\Big(\sum_{\mu=1}^{n} \bar{x}_{\rho\mu} \eta_\mu \Big)}$$

is also invariant (ℓ arbitrary!). If we know the $E(\ell;\xi,\eta)$ (*i.e.*, their coefficients), then it is easy to reason back from this point to the λ_ρ, $x_{\mu\nu}$. Then, if we so formulate the eigenvalue problem (*i.e.*, **D**, **O**) that only the $E(\ell;\xi,\eta)$ appear (instead of the λ_ρ, $x_{\mu\nu}$), we will have achieved the desired unique formulation.

Therefore, let $\mathbb{E}(\ell)$ be the matrix of the Hermitian form $E(\ell;\xi,\eta)$.[72] What do **D**, **O** now mean for the family of matrices $\mathbb{E}(\ell)$?

O means: if ℓ is sufficiently large (namely, larger than all λ_ρ) then $\mathbb{E}(\ell) = \mathbb{I}$ (the unit matrix). From the nature of $\mathbb{E}(\ell)$ it follows that if ℓ is sufficiently small (that is, smaller than all λ_ρ) then $\mathbb{E}(\ell) = \mathbb{O}$ and, as ℓ increases from $-\infty$ to $+\infty$, $\mathbb{E}(\ell)$ remains constant except at a finite number of points (the different values among the $\lambda_1,\ldots,\lambda_n$ which we call $\ell_1 < \ell_2 < \ldots < \ell_m$; $m \leqslant n$), at which it changes discontinuously. Furthermore, the discontinuity lies to the left of the point in question (because the

$$\sum_{\lambda_\rho \leqslant \ell}$$

is continuous to the right as a function of ℓ, while for the case

$$\sum_{\lambda_\rho < \ell}$$

it would be just the opposite). Finally, as we shall show, for $\ell' \leqslant \ell''$

$$\mathbb{E}(\ell')\mathbb{E}(\ell'') = \mathbb{E}(\ell'')\mathbb{E}(\ell') = \mathbb{E}(\ell')$$

(matrix product!).

It is more convenient to prove this for $E(\ell';\xi,\eta)$, $E(\ell'';\xi,\eta)$ in the coordinate system to which the $\mathfrak{x}_1,\ldots,\mathfrak{x}_n$ and $\mathfrak{y}_1,\ldots,\mathfrak{y}_n$ refer. After the introduction of these variables we obtain from $E(\ell';\xi,\eta)$ and $E(\ell'';\xi,\eta)$

$$\sum_{\lambda_\rho \leqslant \ell'} \mathfrak{x}_\rho \bar{\mathfrak{y}}_\rho \quad \text{and} \quad \sum_{\lambda_\rho \leqslant \ell''} \mathfrak{x}_\rho \bar{\mathfrak{y}}_\rho$$

The matrices are therefore as follows: 0 except on the diagonal; 1 on the diagonal in the ρ^{th} field if $\lambda_\rho \leqslant \ell'$ or $\leqslant \ell''$ but otherwise also 0. For such matrices the above proposition is evident.

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[72] That is,

$$\mathbb{E}(\ell) = \{e_{\mu\nu}(\ell)\}, \qquad E(\ell;\xi,\eta) = \sum_{\mu,\nu=1}^{n} e_{\mu\nu}(\ell)\xi_\mu\bar{\eta}_\nu$$

Consequently,

$$e_{\mu\nu}(\ell) = \sum_{\lambda_\rho \leqslant \ell} x_{\rho\mu}\bar{x}_{\rho\nu}$$

Now let us reformulate **D**. It clearly means

$$\sum_{\mu,\nu=1}^{n} h_{\mu\nu}\xi_\nu\bar{\eta}_\mu = \sum_{\tau=1}^{m} \ell_\tau\big\{E(\ell_\tau;\xi,\eta) - E(\ell_{\tau-1};\xi,\eta)\big\}$$

where ℓ_0 is any number $< \ell_1$. But since $E(\ell;\xi,\eta)$ is constant in each of the intervals

$$\begin{aligned} -\infty < \ell &< \ell_1 \\ \ell_1 \leqslant \ell &< \ell_2 \\ &\vdots \\ \ell_{m-1} \leqslant \ell &< \ell_m \\ \ell_m \leqslant \ell &< +\infty \end{aligned}$$

then for each set of numbers $\Lambda_0 < \Lambda_1 < \Lambda_2 < \cdots < \Lambda_k$, if $\ell_1, \ldots, \ell_m$ appear among them,

$$\sum_{\mu,\nu=1}^{n} h_{\mu\nu}\xi_\nu\bar{\eta}_\mu = \sum_{\tau=1}^{k} \Lambda_\tau\big\{E(\Lambda_\tau;\xi,\eta) - E(\Lambda_{\tau-1};\xi,\eta)\big\}$$

By application of the Stieltjes concept of integral,[73] this can also be written as

[73] For the concept of the Stieltjes integral, see Perron, *Die Lehre von den Kettenbrüchen*, Leipzig, 1913 and also, for particular consideration of the requirements of operator theory, Carleman, *Équations intégrales singulières*, Upsala, 1923. For the reader who is less interested in such things, the following definition will suffice: for a subdivision $\Lambda_0, \Lambda_1, \ldots, \Lambda_k$ of the interval a, b

$$a \leqslant \Lambda_0 < \Lambda_1 < \cdots < \Lambda_k \leqslant b$$

we form the sum

$$\sum_{\tau=1}^{k} f(\Lambda_\tau)\big\{g(\Lambda_\tau) - g(\Lambda_{\tau-1})\big\}$$

If this always converges as the subdivisions $\Lambda_0, \Lambda_1, \Lambda_2, \ldots, \Lambda_k$ are made smaller and smaller, then the integral

$$\int_a^b f(x)\, dg(x)$$

exists and is defined to be equal to this limit. (For $g(x) = x$ this goes over into the well-known Riemann integral.) In our case, therefore, the equation which has been derived means that

$$\int_{-\infty}^{+\infty} x\, dE(x;\xi,\eta)$$

exists (we have denoted the variable by λ instead of x) and is equal to

$$\sum_{\mu,\nu-=1}^{n} h_{\mu\nu}\xi_\nu\bar{\eta}_\mu$$

$$\sum_{\mu,\nu=1}^{n} h_{\mu\nu}\,\xi_\nu\bar{\eta}_\mu = \int_{-\infty}^{+\infty} \lambda\, dE(\lambda;\xi,\eta)$$

($\int_{-\infty}^{+\infty}$ can obviously be replaced by $\int_a^b$ if $a < \ell_1$, $b > \ell_m$.) Or, if we consider the coefficients, and write down instead of the matrices themselves the equation which is valid for all coefficients,

$$\mathbb{H} = \int_{-\infty}^{+\infty} \lambda\, d\mathbb{E}(\lambda)$$

where $\mathbb{H} = \{h_{\mu\nu}\}$.

Thus far, then, the problem is the following: For a given Hermitian matrix $\mathbb{H}$ a family of Hermitian matrices $\mathbb{E}(\lambda)$ $(-\infty < \lambda < +\infty)$ with the following properties is sought:

$\mathbf{S}_1$. For sufficiently $\begin{pmatrix}\text{small}\\ \text{large}\end{pmatrix}$ λ, $\mathbb{E}(\lambda) = \begin{pmatrix}\mathbb{O}\\ \mathbb{I}\end{pmatrix}$.

$\mathbb{E}(\lambda)$ is (considered as a function of λ) everywhere constant, with the exception of a finite number of points at which it changes discontinuously. Also, the discontinuity always occurs to the left of the given point.

$\mathbf{S}_2$. It is always true that $\mathbb{E}(\lambda')\mathbb{E}(\lambda'') = \mathbb{E}(\mathrm{Min}(\lambda',\lambda''))$.[74]

$\mathbf{S}_3$. We have (using the Stieltjes integral)

$$\mathbb{H} = \int_{-\infty}^{+\infty} \lambda\, d\mathbb{E}(\lambda)$$

At present we shall not stop to carry out the converse process; *i.e.*, going from $\mathbf{S}_1$, $\mathbf{S}_2$ and $\mathbf{S}_3$ back to **D**, **O** (although this would be simple) because only the present form of the eigenvalue problem will be needed in quantum mechanics. Instead, we shall proceed at once to generalize $\mathbf{S}_1$–$\mathbf{S}_3$ from a finite number to an infinite number of variables; *i.e.*, from $\mathfrak{R}_n$ to $\mathfrak{R}_\infty$.

In $\mathfrak{R}_\infty$ the roles of $\mathbb{H}$ and $\mathbb{E}(\lambda)$ will be taken over by Hermitian operators H and $\mathsf{E}(\lambda)$; we shall seek to determine, for a given H, a family $\mathsf{E}(\lambda)$ that is related to it in a certain fashion, modeled on $\mathbf{S}_1$–$\mathbf{S}_3$. Therefore, it suffices to find the $\mathfrak{R}_\infty$ analog of $\mathbf{S}_1$–$\mathbf{S}_3$.

The property $\mathbf{S}_2$ remains unchanged in the transition, since the number of dimensions of $\mathfrak{R}_n$ plays no role in it. But we want to transform it in a way that makes use of our results on projections (**II.4**). First, the property in question implies in the case $\lambda' = \lambda'' = \lambda$ that $\mathsf{E}(\lambda)^2 = \mathsf{E}(\lambda)$; *i.e.*, that the $\mathsf{E}(\lambda)$ must be projections. But then (we can limit ourselves to $\lambda' \leqslant \lambda''$ since corresponding results are obtained for $\lambda' \geqslant \lambda''$) $\mathbf{S}_2$ means this:

[74] $\mathrm{Min}(a,b,\ldots,e)$ is the smallest, $\mathrm{Max}(a,b,\ldots,e)$ is the largest of the finite set of real numbers $a,b,\ldots,e$.

$$\lambda' \leqslant \lambda'' \quad \text{implies} \quad \mathsf{E}(\lambda') \leqslant \mathsf{E}(\lambda'')$$

(see THEOREM 14 and subsequent text in **II.4**). Some caution is required, however, in the case $\mathbf{S}_3$: the expression

$$\mathsf{H} = \int_{-\infty}^{+\infty} \lambda \; d\mathsf{E}(\lambda)$$

is meaningless, since the Stieltjes integral is defined for numbers and not for operators. But it is easy to replace $\mathsf{H}, \mathsf{E}(\lambda)$ by numbers; *i.e.*, to present that equation as a relationship among numbers. We require

$$(\mathsf{H}f, g) = \int_{-\infty}^{+\infty} \lambda \; (d\mathsf{E}(\lambda)f, g)$$

for all f, g of $\mathfrak{R}_\infty$, so far as $\mathsf{H}f$ is defined. It is in that sense—as a formal abbreviation—that $\mathbf{S}_3$ is henceforth to be understood.

Lastly, the property $\mathbf{S}_1$ is essentially affected by the transition to an infinite number of dimensions. The points beyond which $\mathsf{E}(\lambda)$ assumes its terminal values 0 or 1, or where $\mathsf{E}(\lambda)$ executes its terminal jumps, are (in $\mathfrak{R}_n$) the eigenvalues of H and intervals of constancy are those free from eigenvalues. But if now $n \to \infty$, many things can happen. The smallest or largest eigenvalue can approach $-\infty$ or $+\infty$ respectively, while the others may cluster increasingly densely, since their number can increase arbitrarily, and thus the intervals of constancy may gradually contract to points. (This last circumstance is the symptom which, in the Hilbert theory, under certain circumstances indicates the appearance of a continuous spectrum.[75]) We must therefore change $\mathbf{S}_1$ considerably in the transition from $\mathfrak{R}_n$ to $\mathfrak{R}_\infty$. Allowance must be made for the possibility that the variation of $\mathsf{E}(\lambda)$ may no longer show a discrete, discontinuous character.

With this point in view, it becomes natural to abandon the assumption that $\mathsf{E}(\lambda)$ assumes terminal values 0 or 1, and to require only convergence to 0 or 1 (as $\lambda \to -\infty$ or $\lambda \to +\infty$, respectively). Then, in place of intervals of constancy and points of discontinuity, there emerges the possibility of continuous increase. On the other hand, we may try to maintain the less stringent requirement that at the possible points of discontinuity the discontinuity should appear only from the left. Consequently, we formulate $\mathbf{S}_1$ as follows: for $\lambda \to -\infty$, $\mathsf{E}(\lambda) \to \mathsf{O}$; for $\lambda \to +\infty$, $\mathsf{E}(\lambda) \to \mathsf{I}$; for $\lambda \to \lambda_0, \lambda \geqslant \lambda_0$, $\mathsf{E}(\lambda) \to \mathsf{E}(\lambda_0)$.[76]

[75] See the reference of Note 64, as well as the book of Carleman mentioned in Note 73. We shall have a great deal to do with this "continuous spectrum;" see **II.8**.

[76] By $\mathsf{A}(\lambda) \to \mathsf{B}$ (where $\mathsf{A}(\lambda), \mathsf{B}$ are operators in $\mathfrak{R}_\infty$ and λ a real parameter) we mean that for all f of $\mathfrak{R}_\infty$, $\mathsf{A}(\lambda)f \to \mathsf{B}$. It is in this sense that operator convergence statements should be understood in Hilbert space.

Something must still be said regarding $\mathbf{S}_3$. In a space with a finite number of dimensions

$$\mathbb{H} = \sum_{\tau=1}^{m} \ell_\tau \mathbb{F}_\tau \quad \text{where} \quad \mathbb{F}_\tau = \mathbb{E}(\ell_\tau) - \mathbb{E}(\ell_{\tau-1})$$

Because of $\mathbf{S}_1$ we have for $\sigma \geqslant \tau$

$$\begin{aligned} \mathbb{F}_\tau \mathbb{E}(\ell_\sigma) &= \mathbb{E}(\ell_\tau)\mathbb{E}(\ell_\sigma) - \mathbb{E}(\ell_{\tau-1})\mathbb{E}(\ell_\sigma) \\ &= \mathbb{E}(\ell_\tau) - \mathbb{E}(\ell_{\tau-1}) \\ &= \mathbb{F}_\tau \end{aligned}$$

while for $\sigma \leqslant \tau - 1$

$$\begin{aligned} \mathbb{F}_\tau \mathbb{E}(\ell_\sigma) &= \mathbb{E}(\ell_\tau)\mathbb{E}(\ell_\sigma) - \mathbb{E}(\ell_{\tau-1})\mathbb{E}(\ell_\sigma) \\ &= \mathbb{E}(\ell_\sigma) - \mathbb{E}(\ell_\sigma) \\ &= \mathbb{O} \end{aligned}$$

Therefore, because $\mathbb{F}_\sigma = \mathbb{E}(\ell_\sigma) - \mathbb{E}(\ell_{\sigma-1})$,

$$\mathbb{F}_\tau \cdot \mathbb{F}_\sigma = \begin{cases} \mathbb{F}_\tau & \text{for} \quad \tau = \sigma \\ \mathbb{O} & \text{for} \quad \tau \neq \sigma \end{cases}$$

From this

$$\mathbb{H}^2 = \Big(\sum_{\tau=1}^{m} \ell_\tau \mathbb{F}_\tau \Big)^2 = \sum_{\tau,\sigma=1}^{m} \ell_\tau \ell_\sigma \mathbb{F}_\tau \mathbb{F}_\sigma = \sum_{\tau=1}^{m} \ell_\tau^2 \mathbb{F}_\tau$$

and in the same way, $\mathbb{H}^p = \sum_{\tau=1}^{m} \ell_\tau^p \mathbb{F}_\tau$. Consequently

$$\mathbb{H}^2 = \int_{-\infty}^{+\infty} \lambda^2 \, d\mathbb{E}(\lambda)$$

which is analogous to the equation that holds for $\mathbb{H}$ itself. In $\mathfrak{R}_\infty$ we assume the analogous symbolic relation

$$\mathsf{H}^2 = \int_{-\infty}^{+\infty} \lambda^2 \, d\mathsf{E}(\lambda)$$

which acquires specific meaning from

$$(\mathsf{H}^2 f, g) = \int_{-\infty}^{+\infty} \lambda^2 \, d(\mathsf{E}(\lambda) f, g)$$

(This will actually be confirmed in our subsequent considerations.) For $f = g$ we have

$$(\mathsf{H}^2 f, f) = (\mathsf{H}f, \mathsf{H}f) = \|\mathsf{H}f\|^2, \qquad (\mathsf{E}(\lambda)f, f) = \|\mathsf{E}(\lambda)f\|^2$$

hence

$$\|\mathsf{H}f\|^2 = \int_{-\infty}^{+\infty} \lambda^2 \, d(\|\mathsf{E}(\lambda)f\|^2)$$

This formula, however, causes us to expect that $\mathsf{E}(\lambda)$ not only determines the value of $\mathsf{H}f$, whenever it is defined, but also whether it is defined for a particular f. For the integral

$$\int_{-\infty}^{+\infty} \lambda^2 \, d(\|\mathsf{E}(\lambda)f\|^2)$$

has a non-negative integrand ($\lambda^2 \geqslant 0$) and a monotonically increasing expression under the differential sign ($\mathsf{E}(\|\lambda)f\|^2$; see $\mathbf{S}_2$ and THEOREM 15 in **II.4**). Therefore it is by its nature convergent, *i.e.*, zero or positive and finite, or else is properly divergent ($= +\infty$).[77] This is true independently of the relation to H, *i.e.*, without consideration as to whether $\mathsf{H}f$ is defined or not. It is then to be expected that $\mathsf{H}f$ is defined (*i.e.*, exists in $\mathfrak{R}_\infty$) if and only if the presumed value of $\|\mathsf{H}f\|^2$ is finite; that is, the above expression is defined for all f.

Therefore our new formulation of $\mathbf{S}_1$–$\mathbf{S}_3$ runs as follows: For the given Hermitian operator H we seek a family of projections $\mathsf{E}(\lambda)$ $(-\infty < \lambda < +\infty)$ with the following properties:

$\overline{\mathbf{S}}_1$. For $\lambda \longrightarrow \begin{pmatrix} -\infty \\ +\infty \end{pmatrix}$ we have $\mathsf{E}(\lambda) \longrightarrow \begin{pmatrix} 0 \\ f \end{pmatrix}$ respectively. For $\lambda \to \lambda_0, \lambda \geqslant \lambda_0$ we have $\mathsf{E}(\lambda)f \to \mathsf{E}(\lambda_0)f$ (for each f!).

$\overline{\mathbf{S}}_2$. From $\lambda' \leqslant \lambda''$ it follows that $\mathsf{E}(\lambda') \leqslant \mathsf{E}(\lambda'')$.

$\overline{\mathbf{S}}_3$. The integral $\int_{-\infty}^{+\infty} \lambda^2 \, d(\|\mathsf{E}(\lambda)f\|^2)$, which by its nature is convergent (zero or positive and finite) or properly divergent ($+\infty$), determines the domain of H: $\mathsf{H}f$ is defined in and only in the non-divergent case, in which case

$$(\mathsf{H}f, g) = \int_{-\infty}^{+\infty} \lambda \, d(\mathsf{E}(\lambda)f, g)$$

(The latter integral is absolutely convergent whenever the expression on the left is finite.[78])

The operator H does not enter into the description of the properties $\overline{\mathbf{S}}_1$ and $\overline{\mathbf{S}}_2$. A family of projections $\mathsf{E}(\lambda)$ with these two properties is known as a "resolution of the identity." A resolution of the identity which stands in the relation $\overline{\mathbf{S}}_3$ to H is said to belong to H.

The eigenvalue problem in $\mathfrak{R}_\infty$ then runs as follows: Do there exist, for a given Hermitian operator H, resolutions of the identity belonging to H, and if so: how many? (The desired answer would be: there always exists exactly one.) Furthermore, we must establish how definition of the eigenvalue problem

[77] This follows from the definition of the Stieltjes integral given in Note 73. For proof, see the reference given there.

[78] See Math. Ann **102** (1929).

is related to the general methods used in quantum mechanics (especially in the wave theory) for the determination of the eigenvalues of Hermitian operators.

8. INITIAL CONSIDERATIONS CONCERNING THE EIGENVALUE PROBLEM

The first question which arises from our definition of the eigenvalue problem is this: $\overline{\mathbf{S}}_1$–$\overline{\mathbf{S}}_3$ sound entirely different from the problem with which we started at the beginning of the last section, and their relevance to that problem is no longer recognizable. It is true that we were led in $\mathcal{R}_n$ from that problem to formulation of the conditions $\mathbf{S}_1$–$\mathbf{S}_3$, but in $\mathcal{R}_\infty$ the conditions—though they remain equivalent in $\mathcal{R}_n$, as was previously noted—have been essentially modified. Therefore, the entire question is reopened, and we must ascertain how far the new formulation coincides with the old; *i.e.*, when and how our $\mathsf{E}(\lambda)$ determined the $\lambda_1, \lambda_2, \ldots$ and the $\phi_1, \phi_2, \ldots$.

If the resolution of the identity $\mathsf{E}(\lambda)$ belongs to the Hermitian operator A, when is the equation

$$\mathsf{A}\phi = \lambda_0\phi$$

solvable? $\mathsf{A}\phi = \lambda_0\phi$ means $(\mathsf{A}\phi, g) - \lambda_0(\phi, g) = 0$ for all g; *i.e.*,

$$\begin{aligned} 0 &= \int_{-\infty}^{+\infty} \lambda\, d(\mathsf{E}(\lambda)f, g) - \lambda_0(f, g) \\ &= \int_{-\infty}^{+\infty} \lambda\, d(\mathsf{E}(\lambda)f, g) - \lambda_0 \int_{-\infty}^{+\infty} d(\mathsf{E}(\lambda)f, g) \\ &= \int_{-\infty}^{+\infty} (\lambda - \lambda_0)\, d(\mathsf{E}(\lambda)f, g) \end{aligned}$$

We first set $g = \mathsf{E}(\lambda_0)f$; then

$$\begin{aligned} 0 &= \int_{-\infty}^{+\infty} (\lambda - \lambda_0)\, d(\mathsf{E}(\lambda)f, \mathsf{E}(\lambda_0)f) \\ &= \int_{-\infty}^{+\infty} (\lambda - \lambda_0)\, d(\mathsf{E}(\lambda_0)\mathsf{E}(\lambda)f, f) \\ &= \int_{-\infty}^{+\infty} (\lambda - \lambda_0)\, d(\mathsf{E}(\mathrm{Min}(\lambda, \lambda_0))f, f) \\ &= \int_{-\infty}^{+\infty} (\lambda - \lambda_0)\, d(\|\mathsf{E}(\mathrm{Min}(\lambda, \lambda_0))f\|^2) \end{aligned}$$

We now write $\int_{-\infty}^{+\infty} = \int_{-\infty}^{\lambda_0} + \int_{\lambda_0}^{+\infty}$. We can replace $\mathrm{Min}(\lambda, \lambda_0)$ by λ in $\int_{-\infty}^{\lambda_0}$ and by λ_0 in $\int_{\lambda_0}^{+\infty}$. In the latter integral a constant appears behind the differential sign, so that integral vanishes. But the first integral remains, and can be written

$$\int_{-\infty}^{\lambda_0} (\lambda - \lambda_0)\, d(\|\mathsf{E}(\lambda)f\|^2) = 0$$

Return now to the beginning of the preceding argument and set $g = f$; then

$$0 = \int_{-\infty}^{+\infty} (\lambda - \lambda_0)\, d(\mathsf{E}(\lambda)f, f) = \int_{-\infty}^{+\infty} (\lambda - \lambda_0)\, d(\|\mathsf{E}(\lambda)f\|^2)$$

Subtracting the preceding result from this, we get (after reversing the sign of the integrand)

$$\int_{\lambda_0}^{+\infty} (\lambda_0 - \lambda) d(\|\mathsf{E}(\lambda)f\|^2) = 0$$

Let us now examine

$$\int_{-\infty}^{\lambda_0} (\lambda_0 - \lambda)\, d(\|\mathsf{E}(\lambda)f\|^2) \quad \text{and} \quad \int_{\lambda_0}^{+\infty} (\lambda - \lambda_0) d(\|\mathsf{E}(\lambda)f\|^2)$$

somewhat more closely. The integrand in each case is $\geqslant 0$, and behind the differential sign there is a monotonically increasing function of λ. Therefore we have, for each $\epsilon > 0$,

$$\begin{aligned}
0 = \int_{-\infty}^{\lambda_0} (\lambda_0 - \lambda)\, d(\|\mathsf{E}(\lambda)f\|^2) &\geqslant \int_{-\infty}^{\lambda_0 - \epsilon} (\lambda_0 - \lambda)\, d(\|\mathsf{E}(\lambda)f\|^2) \\
&\geqslant \int_{-\infty}^{\lambda_0 - \epsilon} \epsilon \cdot d(\|\mathsf{E}(\lambda)f\|^2) \\
&= \epsilon \|\mathsf{E}(\lambda_0 - \epsilon)f\|^2 \\
0 = \int_{\lambda_0}^{+\infty} (\lambda - \lambda_0) d(\|\mathsf{E}(\lambda)f\|^2) &\geqslant \int_{\lambda_0 + \epsilon}^{+\infty} (\lambda - \lambda_0) d(\|\mathsf{E}(\lambda)f\|^2) \\
&\geqslant \int_{\lambda_0 + \epsilon}^{+\infty} \epsilon \cdot d(\|\mathsf{E}(\lambda)f\|^2) \\
&= \epsilon\big(\|f\|^2 - \|\mathsf{E}(\lambda_0 + \epsilon)f\|^2\big) \\
&= \epsilon \|f - \mathsf{E}(\lambda_0 + \epsilon)f\|^2
\end{aligned}$$

The right sides are $\leqslant 0$, but since they are also $\geqslant 0$ they must vanish. Therefore

$$\begin{aligned}
\mathsf{E}(\lambda_0 - \epsilon)f &= 0 \\
\mathsf{E}(\lambda_0 + \epsilon)f &= f
\end{aligned}$$

Because of the right hand continuity of $\mathsf{E}(\lambda)$ we may carry out $\epsilon \to 0$ in the second equation: $\mathsf{E}(\lambda_0)f = f$. For $\lambda \geqslant \lambda_0$ then, because of the second equation ($\epsilon = \lambda - \lambda_0 \geqslant 0$), $\mathsf{E}(\lambda)f = f$, while for $\lambda < \lambda_0$, because of the first equation ($\epsilon = \lambda_0 - \lambda > 0$), $\mathsf{E}(\lambda)f = 0$. Therefore

$$\mathsf{E}(\lambda)f = \begin{cases} f & \text{for} \quad \lambda \geqslant \lambda_0 \\ 0 & \text{for} \quad \lambda < \lambda_0 \end{cases}$$

But this necessary condition is also sufficient, because from it it follows that

$$(\mathsf{A}f, g) = \int_{-\infty}^{+\infty} \lambda\, d(\mathsf{E}(\lambda)f, g) = \lambda_0(f, g)$$

(the definition of the Stieltjes integral given in Note 73 should be recalled), therefore $(\mathsf{A}f - \lambda_0 f, g) = 0$ for all g; *i.e.*, $\mathsf{A}f = \lambda_0 f$.

What does this mean? First, it involves a discontinuity of $\mathsf{E}(\lambda)$ at the point $\lambda = \lambda_0$. By THEOREM 17 in **II.4**, $\mathsf{E}(\lambda)$ converges to a projection: call it $\mathsf{E}^{(1)}(\lambda)$ for $\lambda \to \lambda_0, \lambda < \lambda_0$ or $\mathsf{E}^{(2)}(\lambda)$ for $\lambda \to \lambda_0, \lambda > \lambda_0$.[79] By $\mathbf{S}_1$, $\mathsf{E}^{(2)}(\lambda_0) = \mathsf{E}(\lambda_0)$, but because of the discontinuity $\mathsf{E}^{(1)}(\lambda_0) \neq \mathsf{E}(\lambda_0)$. Further, because $\mathsf{E}(\lambda) \leqslant \mathsf{E}(\lambda_0)$ for $\lambda < \lambda_0$, we by $\mathbf{S}_2$ have $\mathsf{E}^{(1)}(\lambda_0) \leqslant \mathsf{E}(\lambda_0)$. Therefore $\mathsf{E}(\lambda_0) - \mathsf{E}^{(1)}(\lambda_0)$ is a projection, and it is characteristic for the discontinuity that it $\neq \mathsf{O}$.

$\mathsf{E}(\lambda)f = 0$ for all $\lambda < \lambda_0$ has $\mathsf{E}^{(1)}(\lambda)f = 0$ as a consequence, from which (by $\mathsf{E}(\lambda) \leqslant \mathsf{E}^{(1)}(\lambda)$) it also follows. $\mathsf{E}(\lambda)f = f$ for all $\lambda \geqslant \lambda_0$ follows from $\mathsf{E}(\lambda_0)f = f$ by the following argument: $\mathsf{E}(\lambda_0) \leqslant \mathsf{E}(\lambda)$, $\mathsf{E}(\lambda)\mathsf{E}(\lambda_0) = \mathsf{E}(\lambda_0)$, therefore $\mathsf{E}(\lambda)f = \mathsf{E}(\lambda)\mathsf{E}(\lambda_0)f = \mathsf{E}(\lambda_0)f = f$. Hence $\mathsf{E}^{(1)}(\lambda_0)f = 0, \mathsf{E}(\lambda_0)f = f$ is characteristic for $\mathsf{A}f = \lambda_0 f$, or (THEOREM 14, **II.4**) $[\mathsf{E}(\lambda_0) - \mathsf{E}^{(1)}(\lambda_0)]f = f$. That is, if we write

$$\mathsf{E}(\lambda_0) - \mathsf{E}^{(1)}(\lambda_0) = \mathsf{P}_{\mathfrak{M}_{\lambda_0}}$$

then the above implies that f belongs to $\mathfrak{M}_{\lambda_0}$.

Consequently, it has been shown that $\mathsf{A}f = \lambda f$ is solvable by an $f \neq 0$ only at the discontinuities of $\mathsf{E}(\lambda)$, and the solutions f form the closed linear manifold $\mathfrak{M}_{\lambda_0}$ defined above.

The complete orthonormal set sought in **II.6**, to be selected from these solutions (combining any λ), then exists if and only if the $\mathfrak{M}_{\lambda_0}(-\infty < \lambda_0 < +\infty)$ together span the closed linear manifold $\mathfrak{R}_\infty$. We have discussed in **II.6** how the construction of this set would then be accomplished. The mutual orthogonality of the $\mathfrak{M}_{\lambda_0}$ can be seen in another way: from $\lambda_0 < \mu_0$ it follows that

$$\mathsf{P}_{\mathfrak{M}_{\lambda_0}}\mathsf{P}_{\mathfrak{M}_{\mu_0}} = [\mathsf{E}(\lambda_0) - \mathsf{E}^{(1)}(\lambda_0)][\mathsf{E}(\mu_0) - \mathsf{E}^{(1)}(\mu_0)] = \mathsf{O}$$

because

$$\mathsf{E}(\lambda_0) = \mathsf{E}^{(1)}(\lambda_0) \leqslant \mathsf{E}(\mu_0) \leqslant \mathsf{E}^{(1)}(\mu_0)$$
$$\mathsf{E}(\mu_0) - \mathsf{E}^{(1)}(\mu_0) \leqslant \mathsf{I} - \mathsf{E}^{(1)}(\mu_0)$$

Without ascertaining the precise conditions under which this is true, we note the following: if an interval μ_1, μ_2 exists in which $\mathsf{E}(\lambda)$ increases monotonically (*i.e.*, $\mu_1 < \mu_2$, $\mathsf{E}(\lambda)$ is continuous in $\mu_1 \leqslant \lambda \leqslant \mu_2$, $\mathsf{E}(\mu_1) \leqslant \mathsf{E}(\mu_2)$) then it is certainly not the case. Because for $\lambda \leqslant \mu_1$, $\mathsf{E}(\lambda) - \mathsf{E}^{(1)}(\lambda) \leqslant \mathsf{E}(\lambda) \leqslant \mathsf{E}(\mu_1)$ while for $\mu_1 \leqslant \lambda \leqslant \mu_2$, $\mathsf{E}(\lambda) - \mathsf{E}^{(1)}(\lambda) = 0$ because of continuity, and for $\mu_2 < \lambda$, $\mathsf{E}(\lambda) - \mathsf{E}^{(1)}(\lambda) \leqslant \mathsf{I} - \mathsf{E}^{(1)}(\lambda) \leqslant \mathsf{I} - \mathsf{E}(\mu_2)$. Therefore $\mathsf{E}(\lambda) - \mathsf{E}^{(1)}(\lambda)$ is always orthogonal to $\mathsf{E}(\mu_2) - \mathsf{E}(\mu_1)$. Let $\mathsf{E}(\mu_2) - \mathsf{E}(\mu_1) = \mathsf{P}_{\mathfrak{N}}$. Then all $\mathfrak{M}_\lambda$ are orthogonal to $\mathfrak{N}$. If a complete orthonormal set were to be chosen from

[79] This was shown only for λ sequences. However, the limit for all such λ sequences ($\lambda \to \lambda_0$ and $\lambda < \lambda_0$ or $\lambda > \lambda_0$) must be the same because two such sequences can be combined to form one, and since this has a limit, both constituents must have the same limit. From this it follows that the convergence (to the common limit of all sequences) also occurs in the case of continuous variation of λ.

this, then $\mathfrak{N}$ would contain only the zero; *i.e.*, $\mathsf{E}(\mu_2) - \mathsf{E}(\mu_1) = \mathsf{O}$, contrary to assumption.

The discontinuities of $\mathsf{E}(\lambda)$ are known as the *discrete spectrum* of A. They are the same λ for which $\mathsf{A}f = \lambda f, f \neq 0$ is solvable. If we choose from each $\mathfrak{M}_\lambda \neq 0$ an f with $\|f\| = 1$ then, because of the orthogonality of the $\mathfrak{M}_\lambda$, an orthonormal set is obtained. By THEOREM 3 in **II.3** this is finite, or is a sequence. Therefore the λ of the discrete spectrum form at most a sequence.

All points in whose neighborhood $\mathsf{E}(\lambda)$ is not constant form the spectrum of A. We have seen that if there are intervals into which the spectrum—but not the point spectrum—of A penetrates (*i.e.*, intervals of continuity of $\mathsf{E}(\lambda)$ in which it is not constant), then the eigenvalue problem is certainly not solvable in the same sense as that in which it was formulated at the beginning of **II.6**. The precise conditions for this insolvability we do not investigate further, because insolvability may also arise under certain other circumstances, when the discrete spectrum does penetrate into all intervals in which points of the spectrum lie. The separation of the discrete spectrum from the rest of the spectrum is then considerably more laborious, and is beyond the scope of this work. (The reader will find these investigations in Hilbert's papers, which have been referred to previously).

On the other hand, we do want to show how in cases where there does exist a complete orthonormal set $\phi_1, \phi_2, \ldots$ of solutions of $\mathsf{A}\phi = \lambda\phi$ (with $\lambda = \lambda_1, \lambda_2, \ldots$ corresponding to $\phi = \phi_1, \phi_2, \ldots$)—cases with a pure discrete spectrum, as we shall say—the $\mathsf{E}(\lambda)$ are to be constructed. We have[80]

$$\mathsf{E}(\lambda) = \sum_{\lambda_\rho \leqslant \lambda} \mathsf{P}_{[\phi_\rho]}$$

(The sum $\sum$ can have 0 summands, giving $\mathsf{E}(\lambda) = \mathsf{O}$. Or a finite positive number, when its meaning is clear. Or indefinitely many, in which case it converges according to the final considerations of **II.4**.)

$\overline{\mathbf{S}}_2$ is evident, because for $\lambda' \leqslant \lambda''$

$$\mathsf{E}(\lambda'') - \mathsf{E}(\lambda') = \sum_{\lambda' < \lambda_\rho \leqslant \lambda''} \mathsf{P}_{[\phi_\rho]}$$

is a projection, therefore $\mathsf{E}(\lambda') \leqslant \mathsf{E}(\lambda'')$ (THEOREM 14).

We prove $\overline{\mathbf{S}}_1$ as follows: For each f we by THEOREM 7 have[81]

$$\sum_\rho \|\mathsf{P}_{[\phi_\rho]} f\|^2 = \sum_\rho |(f, \phi_\rho)|^2 = \|f\|^2$$

i.e., $\sum_\rho \|\mathsf{P}_{[\phi_\rho]} f\|^2$ is convergent. Therefore for each $\epsilon > 0$ we can give a finite

[80] This is the precise restatement of the definition of $\mathsf{E}(\lambda; \xi, \eta)$ given in **II.7**.

[81] Recall in this connection that, as the construction carried out in the proof of THEOREM 10 shows, if $\|\phi\| = 1$ then $\mathsf{P}_{[\phi]} f = (f, \phi) \cdot \phi$ gives

$$\|\mathsf{P}_{[\phi]} f\| = |(f, \phi)| = |(\phi, f)|$$

number of ρ so that the sum $\sum_\rho$ taken over these alone is $> \|f\|^2 - \epsilon$, and therefore each $\sum'_\rho$ from which they are missing is $< \epsilon$. Then also

$$\|\sum_\rho{}' \mathsf{P}_{[\phi_\rho]} f\|^2 = \sum_\rho{}' \|\mathsf{P}_{[\phi_\rho]} f\|^2 < \epsilon$$

From this it follows in particular that

$$\|\sum_{\lambda_\rho \leqslant \lambda} \mathsf{P}_{[\phi_\rho]} f\|^2 < \epsilon \quad : \quad \lambda \text{ sufficiently small}$$

$$\|\sum_{\lambda_\rho > \lambda} \mathsf{P}_{[\phi_\rho]} f\|^2 < \epsilon \quad : \quad \lambda \text{ sufficiently large}$$

$$\|\sum_{\lambda_0 < \lambda_\rho \leqslant \lambda} \mathsf{P}_{[\phi_\rho]} f\|^2 < \epsilon \quad : \quad \lambda \geqslant \lambda_0 \text{ near enough to } \lambda_0$$

Then[82]

$$\mathsf{E}(\lambda) f = \sum_{\lambda_\rho \leqslant \lambda} \mathsf{P}_{[\phi_\rho]} f \longrightarrow 0 \text{ for } \lambda \to -\infty$$

$$f - \mathsf{E}(\lambda) f = \sum_{\lambda_\rho > \lambda} \mathsf{P}_{[\phi_\rho]} f \longrightarrow 0 \text{ for } \lambda \to +\infty$$

$$\mathsf{E}(\lambda) f - \mathsf{E}(\lambda_0) f = \sum_{\lambda_0 < \lambda_\rho \leqslant \lambda} \mathsf{P}_{[\phi_\rho]} f \longrightarrow 0 \text{ for } \lambda (\geqslant \lambda_0) \to \lambda_0$$

i.e., $\overline{\mathbf{S}}_1$ is satisfied.

In order to convince ourselves of the validity of $\overline{\mathbf{S}}_3$, we set

$$f = x_1\phi_1 + x_2\phi_2 + \cdots \quad : \quad \text{then} \quad \mathsf{A} = \lambda_1 x_1 \phi_1 + \lambda_2 x_2 \phi_2 + \cdots$$

In order that $\mathsf{A}f$ be defined, $\sum_{\rho=1}^\infty \lambda_\rho^2 |x_\rho|^2$ must be finite. But[83]

$$\int_\infty^{+\infty} \lambda^2 d\|\mathsf{E}(\lambda) f\|^2 = \int_\infty^{+\infty} \lambda^2 d\Big(\sum_{\lambda_\rho \leqslant \lambda} |x_\rho|^2\Big) = \sum_{\rho=1}^\infty \lambda_\rho^2 |x_\rho|^2$$

$$\int_\infty^{+\infty} \lambda\, d(\mathsf{E}(\lambda) f, g) = \int_\infty^{+\infty} \lambda\, d\Big(\sum_{\lambda_\rho \leqslant \lambda} x_\rho \overline{y}_\rho\Big) = \sum_{\rho=1}^\infty \lambda_\rho x_\rho \overline{y}_\rho = (\mathsf{A}f, g)$$

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[82] We have (by THEOREM 7)

$$f = \sum_\rho (f, \phi_\rho) \cdot \phi_\rho = \sum_\rho \mathsf{P}_{[\phi_\rho]} f$$

This also follows from the final considerations of **II.4**, and pertains to the second of the following equations.

[83] By Note 73,

$$\int_\infty^{+\infty} \lambda^2 d\Big(\sum_{\lambda_\rho \leqslant \lambda} |x_\rho|^2\Big) = \lim \sum_{\tau=1}^k \Lambda_\tau^2 \cdot \sum_{\Lambda_{\tau-1} < \lambda_\rho \leqslant \Lambda_\tau} |x_\rho|^2$$

If, throughout, $\Lambda_\tau^2 - \Lambda_{\tau-1}^2 < \epsilon$ (*i.e.*, if the $\Lambda_0, \Lambda_1, \ldots, \Lambda_k$ mesh is sufficiently fine) the expression on the right changes by less than $\epsilon \sum_{\rho=1}^\infty |x_\rho|^2 = \epsilon \|f\|^2$ if

Consequently, $\overline{\mathbf{S}}_3$ is satisfied.

Let us consider two cases of a pure continuous spectrum; *i.e.*, two cases in which there exists no discrete spectrum. We take as our **first example** the case in which $\mathfrak{R}_\infty$ is the space of all functions $f(q_1, \ldots, q_\ell)$ with finite

$$\int \cdots \int_{-\infty}^{+\infty} |f(q_1, \ldots, q_\ell)|^2 dq_1 \cdots dq_\ell$$

and A is the operator $q_j \cdot$, the Hermitian character of which is evident.

Evidently $\mathsf{A}f = \lambda f$ implies that

$$(q_j - \lambda) f(q_1, \ldots, q_\ell) = 0$$

i.e., $f(q_1, \ldots, q_\ell) = 0$ everywhere, with the possible exception of the $\ell - 1$ dimensional plane $q_j = \lambda$. However, this plane is (according to the discussion in **II.3** relative to condition **B**) unimportant, because its Lebesgue measure (*i.e.*, volume) is zero. Then $f \equiv 0$.[84] Consequently there exists no non-zero solution of $\mathsf{A}f = \lambda f$. But we also see (inexactly) where the solution is to be

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we replace it by

$$\sum_{\tau=1}^{k} \sum_{\Lambda_{\tau-1} < \lambda_\rho \leqslant \Lambda_\tau} \lambda_\rho^2 |x_\rho|^2 = \sum_{\Lambda_0 < \lambda_\rho \leqslant \Lambda_k} \lambda_\rho^2 |x_\rho|^2$$

and if Λ_0 is small enough, and Λ_k large enough, this is arbitrarily close to

$$\sum_{\tau=1}^{\infty} \lambda_\rho^2 |x_\rho|^2$$

This sum is then the desired limit; *i.e.*, the value of the integral. The next integral formula is proved in exactly the same way.

[84] At this point the correct mathematical method followed by us deviates from the symbolic method of Dirac (see, e.g., his book mentioned in Note 1). The latter method in essence is to consider the f with $(q - \lambda) f(q) \equiv 0$ as solutions (for simplicity we set $\ell = j = 1$, $q_j = q$). But since each $(f, g) = \int f(q)\overline{g(q)} dq = 0$ and $f(q) \neq 0$, $f(q)$ is infinite at the point $q = \lambda$ (the only point where it differs from zero!), and indeed, so strongly infinite that $(f, g) \neq 0$. Since for $q \neq \lambda$, $f(q) = 0$ the integral $\int f(q)\overline{g(q)} dq$ can depend only on $\overline{g(\lambda)}$, and indeed it is clear that the integral, because of its additive property, must be proportional to $\overline{g(\lambda)}$. It suffices, of course, to consider the case $\lambda = 0$. We write $f(q) = \delta(q)$, which is defined by

$$\mathbf{\Delta} \qquad q\delta(q) = 0 \quad \text{and} \quad \int \delta(q) f(q) = f(0)$$

For arbitrary λ, $\delta(q - \lambda)$ is a solution; although a function δ with the property $\mathbf{\Delta}$ does not exist, there are function sequences which converge toward such

expected. $(q_j - \lambda)f(q_1, \ldots, q_\ell) = 0$ implies that only for $q_j = \lambda$ may $f \neq 0$. A linear combination of the solutions for several λ, say $\lambda = \lambda', \lambda'', \ldots, \lambda^{(s)}$, would then be non-zero for

$$q_j = \lambda', \lambda'', \ldots, \lambda^{(s)}$$

We can then consider an f as a linear combination of all solutions with $\lambda \leqslant \lambda_0$ if it is non-zero only for $\lambda \leqslant \lambda_0$. But in the case of the pure discrete spectrum we had

$$\mathsf{E}(\lambda_0) = \sum_{\lambda_\rho \leqslant \lambda_0} \mathsf{P}_{[\phi_\rho]} = \mathsf{P}_{\mathfrak{N}_{\lambda_0}}, \qquad \mathfrak{N}_{\lambda_0} = [\phi_{\rho:\lambda_\rho \leqslant \lambda_0}]$$

i.e., $\mathfrak{N}_\lambda$ consisted of the linear combinations of all ϕ_ρ with $\lambda_\rho \leqslant \lambda_0$; *i.e.*, of all solutions of $\mathsf{A}f = \lambda f$ with $\lambda \leqslant \lambda_0$. Consequently—to be sure, inexactly and heuristically—it is to be expected that

$$\mathsf{E}(\lambda_0) = \mathsf{P}_{\mathfrak{N}_{\lambda_0}}$$

where $\mathfrak{N}_{\lambda_0}$ consists of those f which $\neq 0$ only for $q_j \leqslant \lambda_0$. $\mathfrak{R}_\infty - \mathfrak{N}_\infty$ then clearly consists of those f which always vanish for $q_j > 0$; consequently

$$\mathsf{E}(\lambda_0)f(q_1, \ldots, q_\ell) = \begin{cases} f(q_1, \ldots, q_\ell) & \text{for} \quad q_j \leqslant \lambda_0 \\ 0 & \text{for} \quad q_j > \lambda_0 \end{cases}$$

In a rather inexact way, then, we have found a family of projections $\mathsf{E}(\lambda)$ of which it is to be supposed that they satisfy $\overline{\mathbf{S}}_1$–$\overline{\mathbf{S}}_3$ for our A. In fact, $\overline{\mathbf{S}}_1$ and $\overline{\mathbf{S}}_2$ are satisfied in a trivial fashion; indeed, for $\overline{\mathbf{S}}_1$ the $\lambda \to \lambda_0$ case holds even without the condition $\lambda \geqslant \lambda_0$; *i.e.*, $\mathsf{E}(\lambda)$ is continuous everywhere. In order to see that $\overline{\mathbf{S}}_3$ also is satisfied, it suffices to prove the validity of the following equations (in which all unstated upper/lower limits are $\pm\infty$):

$$\begin{aligned} \int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{E}(\lambda)f\|^2 &= \int \lambda^2 d\Big(\int \cdots \int_{-\infty}^{\lambda} \cdots \int |f(q_1, \ldots, q_j, \ldots, q_\ell)|^2 dq_1 \ldots dq_j \ldots dq_\ell \Big) \\ &= \int \lambda^2 \Big(\int \cdots \int |f(q_1, \ldots, q_{j-1}, \lambda, q_{j+1}, \ldots, q_\ell)|^2 dq_1 \ldots dq_{j-1} dq_{j+1} \ldots dq_\ell \Big) d\lambda \\ &= \int \cdots \int q_j^2 |f(q_1, \ldots, q_{j-1}, q_j, q_{j+1}, \ldots, q_\ell)|^2 dq_1 \ldots dq_{j-1} dq_j dq_{j+1} \ldots dq_\ell \\ &= \|\mathsf{A}f\|^2 \end{aligned}$$

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behavior (even though the limiting function does not exist). For example,

$$f_\epsilon(q) = \begin{cases} \frac{1}{2\epsilon} & \text{for} \quad |x| < \epsilon \\ 0 & \text{for} \quad |x| \geqslant \epsilon \end{cases} \qquad \text{as} \quad \epsilon \to +0$$

and

$$f_a(q) = \sqrt{\tfrac{a}{\pi}} e^{-ax^2} \qquad \text{as} \quad a \to +\infty$$

provide instances of such sequences (see also **I.3**, particularly Note 32).

$$\begin{aligned}\int_{-\infty}^{+\infty}\lambda\, d(\mathsf{E}(\lambda)f,g) &= \int \lambda\, d\Big(\int\cdots\int_{-\infty}^{\lambda}\cdots\int f(q_1,\ldots,q_j,\ldots,q_\ell)\overline{g(q_1,\ldots,q_j,\ldots,q_\ell)}dq_1\ldots dq_j\ldots dq_\ell\\ &= \int\lambda\Big(\int\cdots\int f(q_1,\ldots,q_{j-1},\lambda,q_{j+1},\ldots,q_\ell)\overline{g(q_1,\ldots,q_{j-1},\lambda,q_{j+1},\ldots,q_\ell)}dq_1\ldots dq_{j-1}dq_{j+1}\ldots dq_\ell\Big)d\lambda\\ &= \int\cdots\int q_j f(q_1,\ldots,q_{j-1},q_j,q_{j+1},\ldots,q_\ell)\overline{g(q_1,\ldots,q_{j-1},q_j,q_{j+1},\ldots,q_\ell)}dq_1\ldots dq_{j-1}dq_j dq_{j+1}\ldots dq_\ell\\ &= (\mathsf{A}f,g)\end{aligned}$$

We again recognize that the discrete spectrum and the old formulation of the eigenvalue problem both must fail, since $\mathsf{E}(\lambda)$ increases continuously everywhere.

This example also indicates, more generally, a possible way to find $\mathsf{E}(\lambda)$ when the spectrum is continuous: one may determine (incorrectly!) the solutions of $\mathsf{A}f = \lambda f$ (since λ lies in the continuous spectrum, these f do not belong to $\mathfrak{R}_\infty$!), and form their linear combinations for all $\lambda \leqslant \lambda_0$. These belong in part to $\mathfrak{R}_\infty$ again, and perhaps form a closed linear manifold $\mathfrak{N}_{\lambda_0}$. Then we set

$$\mathsf{E}(\lambda_0) = \mathsf{P}_{\mathfrak{N}_{\lambda_0}}$$

If we have handled everything properly, it becomes possible on this basis to verify $\overline{\mathbf{S}}_1$–$\overline{\mathbf{S}}_3$ (for A and these $\mathsf{E}(\lambda)$), and so to transform the heuristic argument into an exact one.[85]

The **second example** which we wish to consider is the other important operator of wave mechanics, $\frac{\hbar}{i}\frac{\partial}{\partial q_j}$. In order to avoid unnecessary complications, let $\ell = j = 1$ (the treatment is the same for other values). We must then investigate the operator

$$\mathsf{A}'f(q) = \tfrac{\hbar}{i}\tfrac{\partial}{\partial q}f(q)$$

If the domain of q is $-\infty < q < +\infty$ then this is a Hermitian operator, as we saw in **II.5**. On the other hand, for a finite domain $a \leqslant q \leqslant b$ this is not the case:

$$\begin{aligned}(\mathsf{A}'f,g) - (f,\mathsf{A}'g) &= \int_a^b \tfrac{\hbar}{i}f'(q)\overline{g(q)}\,dq - \int_a^b f(q)\overline{\tfrac{\hbar}{i}g'(q)}\,dq\\ &= \tfrac{\hbar}{i}\int_a^b\Big\{f'(q)\overline{g(q)} + f(q)\overline{g'(q)}\Big\}dq\\ &= \tfrac{\hbar}{i}\Big[f(q)\overline{g(q)}\Big]_a^b\\ &= \tfrac{\hbar}{i}\Big[f(b)\overline{g(b)} - f(a)\overline{g(a)}\Big]\end{aligned}$$

In order for this to vanish the domain of $\frac{\hbar}{i}\frac{\partial}{\partial q}$ must be limited in such a way that for two f, g picked arbitrarily from it, $f(a)\overline{g(a)} = f(b)\overline{g(b)}$. That is,

$$f(a) : f(b) = \overline{g(b)} : \overline{g(a)}$$

If we vary f for fixed g then we see that $f(a) : f(b)$ must be the same number

[85] The exact formulation of this idea (to be considered here only as an heuristic statement) is found in papers of Hellinger (J. f. Math. **136** (1909)) and Weyl (Math. Ann. **68** (1910)).

θ throughout the entire domain (θ may even be 0 or ∞). Substitutions $f \leftrightarrow g$ give $\theta = 1/\bar{\theta}$; *i.e.*, $|\theta| = 1$. So in order for $\frac{\hbar}{i}\frac{\partial}{\partial q}$ to be Hermitian we must postulate a "boundary condition" of the form

$$f(a) : f(b) = \theta \quad : \quad \theta \text{ a fixed number of unit absolute value}$$

First we take the interval $-\infty < q < +\infty$. The solutions of $\mathsf{A}f = \lambda f$; *i.e.*, of $\frac{\hbar}{i}\phi'(q) = \lambda\phi(q)$, are the functions

$$\phi(q) = ce^{(i/\hbar)\lambda q}$$

But these cannot be used for our purposes without further discussion, since

$$\int_{-\infty}^{+\infty} |\phi(q)|^2 dq = \int_{-\infty}^{+\infty} |c|^2 dq = \infty$$

(unless $c = 0$, $\phi \equiv 0$). We observe that in the first example we found the solution $\delta(q-\lambda)$; *i.e.*, a fictitious, non-existent function (see Note 84). Now we find

$$e^{(i/\hbar)\lambda q}$$

which is an entirely well-behaved function, but which does not belong to $\mathfrak{R}_\infty$ because of the unboundedness of the integral of the square of its absolute value. For our point of view, these two facts have the same meaning, because for us what does not belong to $\mathfrak{R}_\infty$ does not exist.[86]

As in the first case, we now form the linear combinations of the solutions with $\lambda \leqslant \lambda_0$; *i.e.*, the functions

$$f(q) = \int_{-\infty}^{\lambda_0} c(\lambda) e^{(i/\hbar)\lambda q} dq$$

It is to be hoped that among these, functions in $\mathfrak{R}_\infty$ will be present, and furthermore that these will form a closed linear manifold $\mathfrak{N}'_{\lambda_0}$, and finally that the projections

$$\mathsf{E}(\lambda_0) = \mathsf{P}_{\mathfrak{N}'_{\lambda_0}}$$

will form the resolution of the identity belonging to A'.

We obtain an example confirming the first surmise if we set

$$f(q) = \int_{\lambda_1}^{\lambda_0} e^{(i/\hbar)\lambda q} dq = \frac{e^{(i/\hbar)\lambda_0 q} - e^{(i/\hbar)\lambda_1 q}}{(i/\hbar)q}$$

$$c(\lambda) = \begin{cases} 1 & \text{for} \quad \lambda \geqslant \lambda_1 \\ 0 & \text{for} \quad \lambda < \lambda_1 \end{cases} \quad : \quad \lambda_1 < \lambda_0$$

[86] Of course, only success in the physical application can justify this point of view or its use in quantum mechanics.

because this $f(q)$ is everywhere regular for finite values, while for $q \to \pm\infty$ it behaves like $1/q$, so that $\int_{-\infty}^{+\infty} |f(q)|^2 dq$ is finite. But the other surmises also prove to be correct, and actually follow from the theory of the Fourier integral. Indeed, this theory asserts the following:[87]

Let $f(x)$ be any function with finite

$$\int_{-\infty}^{+\infty} |f(x)|^2 dx$$

Then the function

$$\mathtt{L}f(x) = F(y) = \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ixy} f(x)\, dx$$

can be formed, and for this

$$\int_{-\infty}^{+\infty} |F(y)|^2 dy$$

is also finite, and is actually equal to $\int_{-\infty}^{+\infty} |f(x)|^2 dx$. Moreover, $\mathtt{LL}f(x) = f(-x)$. (This is the so-called Fourier transform which plays an important role elsewhere in the theory of differential equations.)

If we replace x, y by $\frac{1}{\sqrt{\hbar}}q, \frac{1}{\sqrt{\hbar}}p$ then we obtain the transform

$$\mathtt{M}f(q) = F(p) = \tfrac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} e^{\frac{i}{\hbar}pq} f(q)\, dq$$

which has the same properties. Consequently, it maps $\mathfrak{R}_\infty$ on itself [$\mathtt{M}f(q) = g(p)$ is solvable for each $g(p)$ of $\mathfrak{R}_\infty$: $f(q) = \mathtt{M}g(-p)$], leaves $\|f\|$ invariant, and is linear. By **II.5** this $\mathtt{M}$ is unitary. Therefore $\mathtt{M}^2 f(q) = f(-q)$: $\mathtt{M}^{-1} f(q) = \mathtt{M}^* f(q) = \mathtt{M}f(-q)$ so $\mathtt{M}$ commutes with $\mathtt{M}^2$; *i.e.*, with the operation $f(q) \to f(-q)$.

What we then had in mind for $\mathfrak{N}'_{\lambda_0}$ was the following: $f(q)$ belongs to $\mathfrak{N}'_{\lambda_0}$ if $F(p) = \mathtt{M}^{-1} f(p)$ is equal to zero for all $p < \lambda_0$. (Here

$$F(p) = \sqrt{h}\, c(p)$$

where $c(\lambda)$ was defined above.) But these $F(p)$, as we know, form a closed linear manifold $\mathfrak{N}_{\lambda_0}$. Therefore the image $\mathfrak{N}'_{\lambda_0}$ of this $\mathfrak{N}_{\lambda_0}$ obtained by $\mathtt{M}$ is also a closed linear manifold. $\mathsf{E}'(\lambda_0)$ is formed from $\mathsf{E}(\lambda_0)$ just as was $\mathfrak{N}'_{\lambda_0}$ from $\mathfrak{N}_{\lambda_0}$, by transformation of the entire $\mathfrak{R}_\infty$ with $\mathtt{M}$. Therefore $\mathsf{E}'(\lambda_0) = \mathtt{M}\mathsf{E}(\lambda_0)\mathtt{M}^{-1}$. Then $\mathsf{E}'(\lambda)$, as well as $\mathsf{E}(\lambda)$, has the properties $\overline{\mathbf{S}}_1$ and $\overline{\mathbf{S}}_2$. It still remains to prove $\overline{\mathbf{S}}_3$; *i.e.*, that the resolution of the identity $\mathsf{E}(\lambda)$ belongs to A'.

In this, we limit ourselves to the demonstration of the following: If $f(q)$ is differentiable without special convergence difficulties, and if

$$\int_{-\infty}^{+\infty} |\tfrac{\hbar}{i} f'(q)|^2 dq$$

[87] Plancherel, Circ. Math. di. Pal. **30** (1910); Titchmarsh, Lond. Math. Soc. Proc. **22** (1924).

is finite, then

$$\int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{E}'(\lambda)f\|^2$$

is finite, and[88]

$$(\mathsf{A}'f, g) = \int_{-\infty}^{+\infty} \lambda\, d(\mathsf{E}'(\lambda)f, g)$$

Indeed (recall that $\mathtt{M}^{-1}f(p) = F(p)$)

$$\begin{aligned}\mathsf{A}'f(q) &= \tfrac{\hbar}{i}f'(q)\\ &= \tfrac{\hbar}{i}\tfrac{\partial}{\partial q}(\mathtt{M}F(p))\\ &= \tfrac{\hbar}{i}\tfrac{\partial}{\partial q}\Big(\tfrac{1}{\sqrt{h}}\int F(p)e^{\frac{i}{\hbar}pq}dp\Big)\\ &= \tfrac{1}{\sqrt{h}}\int F(p)\cdot p\cdot e^{\frac{i}{\hbar}pq}dp\\ &= \mathtt{M}(pF(p))\end{aligned}$$

Therefore, for the f mentioned, $\mathsf{A}' = \mathtt{M}\mathsf{A}\mathtt{M}^{-1}$ (here A is the operator $q\cdot$, or—since we use the variable p here—$p\cdot$). Since the above propositions hold for $\mathsf{A}, \mathsf{E}(\lambda)$ they also are valid after the transformation of $\mathcal{R}_\infty$ with $\mathtt{M}$. Therefore they also hold for $\mathsf{A} = \mathtt{M}\mathsf{A}\mathtt{M}^{-1}$ and $\mathsf{E}'(\lambda) = \mathtt{M}\mathsf{E}(\lambda)\mathtt{M}^{-1}$.

The situation for $\frac{\hbar}{i}\frac{\partial}{\partial q}$ in the interval $a \leqslant q \leqslant b$ ($a < b$; a, b finite) is essentially different. In this case, as we know, a boundary condition

$$f(a) : f(b) = \theta \quad : \quad |\theta| = 1$$

is forced by the Hermiticity requirement. Again, $\frac{\hbar}{i}\frac{\partial}{\partial q}f(q) = \lambda f(q)$ is solved by

$$f(q) = ce^{(i/\hbar)\lambda q}$$

but now

$$\int_a^b |f(q)|^2 dq = \int_a^b |c|^2 dq = (b-a)|c|^2$$

is finite, so that $f(q)$ always belongs to $\mathcal{R}_\infty$. On the other hand, there is the boundary condition

$$f(a) : f(b) = e^{(i/\hbar)\lambda(b-a)} = \theta$$

to be satisfied, which, if we set $\theta = e^{-i\alpha}$ ($0 \leqslant \alpha < 2\pi$), becomes

$$\tfrac{2\pi i}{h}\lambda(a-b) = -i(\alpha + 2\pi k) \quad : \quad k = 0, \pm 1, \pm 2, \ldots$$

$$\lambda = \frac{h}{b-a}\Big(\frac{\alpha}{2\pi} + k\Big)$$

[88] Regarding the following equation: $\mathsf{E}'(\lambda)$ does not belong to $\mathsf{A}' = \frac{\hbar}{i}\frac{\partial}{\partial q}$ itself, but to an operator whose domain includes that of A' and which coincides in this domain with A'. See the developments regarding this in **II.9**.

Therefore we have a discrete spectrum, and the normalized solutions are then determined by $(b-a)|c|^2 = 1$ whence $c = 1/\sqrt{b-a}$:

$$\begin{aligned}\phi_k(q) &= \frac{1}{\sqrt{b-a}}\, e^{(i/\hbar)\lambda q} \\ &= \frac{1}{\sqrt{b-a}}\, e^{i\frac{2\pi}{a-b}\left(\frac{\alpha}{2\pi}+k\right)q} \quad : \quad k = 0, \pm 1, \pm 2, \ldots\end{aligned}$$

This is then an orthonormal set, but it is also complete. For if $f(q)$ is orthogonal to $\phi_k(q)$ then

$$e^{i\frac{\alpha}{b-a}q} f(q)$$

is orthogonal to all

$$e^{i\frac{2\pi}{b-a}kq}$$

and therefore

$$e^{i\frac{\alpha}{2\pi}x} f\left(\tfrac{b-a}{2\pi}x\right)$$

is orthogonal to all e^{ikx}; *i.e.*, to $1, \cos x, \sin x, \cos 2x, \sin 2x, \ldots$. Moreover, it is defined in the interval

$$a \leqslant \frac{b-a}{2\pi}x \leqslant b$$

whose length is 2π, so it must vanish according to well-known theorems.[89] Therefore $f(q) \equiv 0$.

Consequently, we have a pure discrete spectrum, a case which we treated in general at the beginning of this section. One should observe how the "boundary condition"—*i.e.*, θ or α—affects the eigenvalues and eigenfunctions.

In conclusion, we can also consider the case of a one-way infinite interval (domain); say $0 \leqslant q < +\infty$. First of all, we must again prove the Hermitian nature of the operator. We have

$$\begin{aligned}(\mathsf{A}'f, g) - (f, \mathsf{A}'g) &= \tfrac{\hbar}{i}\int_a^b \left\{f'(q)\overline{g(q)} + f(q)\overline{g'(q)}\right\}dq \\ &= \tfrac{\hbar}{i}\left[f(q)\overline{g(q)}\right]_0^\infty\end{aligned}$$

We argue that $f(q)\overline{g(q)}$ approaches zero as $q \to \infty$ just as we did in **II.5** in the case of the (both ways) infinite interval (domain). Therefore the requirement has to be $f(0)\overline{g(0)} = 0$. If we set $f = g$ it can be seen that the "boundary condition" is $f(0) = 0$.

In this case, serious difficulties present themselves. The solutions of $\mathsf{A}'\phi = \lambda\phi$ are the same as in the interval $-\infty < q < +\infty$, namely the functions

$$\phi(q) = ce^{(i/\hbar)\lambda q}$$

[89] All Fourier coefficients disappear, therefore the function itself vanishes (see, for example, Courant-Hilbert in the reference given in Note 30).

but they do not belong to $\mathcal{R}_\infty$ and they do not satisfy the boundary condition. The latter is suspicious. Nevertheless, it is rather surprising that we must by the method sketched earlier necessarily obtain the same $\mathsf{E}(\lambda)$ as in the interval $-\infty < q < +\infty$ since the (improper; *i.e.*, not belonging to $\mathcal{R}_\infty$) solutions are the same. How is this to be reconciled with the fact that the operator is a different one? Also, they are not what we need. For if we again define $\mathtt{M}$, $\mathtt{M}^{-1}$ in the Hilbert space F_Ω functions $f(q)$ $(0 \leqslant q < +\infty$, $\int_0^\infty |f(q)|^2 dq$ finite):

$$\mathtt{M}f(q) = F(p) = \tfrac{1}{\sqrt{h}} \int_0^{+\infty} e^{\frac{i}{h}pq} f(q)\, dq$$

$$\mathtt{M}^{-1}F(p) = f(q) = \tfrac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} e^{-\frac{i}{h}pq} F(p)\, dp = \mathtt{M}F(-p)$$

then $\mathtt{M}$ maps the Hilbert space $F_{\Omega'}$ of all $f(q)$ with

$$0 \leqslant q < +\infty, \qquad \int_0^{+\infty} |f(q)|^2 dq \ \text{ finite}$$

onto another Hilbert space $F_{\Omega''}$ of all $F(p)$ with

$$-\infty \leqslant q < +\infty, \qquad \int_0^{+\infty} |F(p)|^2 dp \ \text{ finite}$$

While $\|\mathtt{M}f(q)\| = \|f(q)\|$ always holds (this follows from the theorems previously mentioned if we set $f(q) = 0$ for $-\infty < q < 0$), $\|\mathtt{M}^{-1}F(p)\| = \|F(p)\|$ is not the case in general because, by reason of the theorems previously discussed, if we define $f(q)$ for $q < 0$ by

$$f(q) = \tfrac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} e^{-\frac{i}{h}pq} F(p)\, dp$$

then

$$\|F\|^2 = \int_{-\infty}^{+\infty} |F(p)|^2 dp = \int_{-\infty}^{+\infty} |f(q)|^2 dq$$

$$\|\mathtt{M}^{-1}F\|^2 = \|f\|^2 = \int_0^{+\infty} |f(q)|^2 dq$$

So $\|\mathtt{M}^{-1}F\| < \|F\|$ unless, by chance, $f(q)$—defined as above—vanishes for all $q < 0$. Therefore $\mathsf{E}'(\lambda) = \mathtt{M}\mathsf{E}(\lambda)\mathtt{M}^{-1}$ is not a resolution of the identity:[90] the method has failed.

[90] It is indeed true that $\mathtt{M}^{-1}\mathtt{M}f(q) = f(q)$ (it suffices to define $f(q) = 0$ for $q < 0$ and to make use of earlier theorems) but it is not always true that $\mathtt{M}^{-1}\mathtt{M}F(p) = F(p)$ because in general $\|\mathtt{M}^{-1}F\| < \|F\|$, therefore $\|\mathtt{M}^{-1}\mathtt{M}F\| < \|F\|$. Consequently $\mathtt{M}^{-1}\mathtt{M} = \mathtt{I}$, $\mathtt{M}\mathtt{M}^{-1} \neq \mathtt{I}$; *i.e.*, $\mathtt{M}^{-1}$ is not a true reciprocal of $\mathtt{M}$. (Also, no other can exist because if there were one, then, since $\mathtt{M}^{-1}\mathtt{M} = \mathtt{I}$, it would have to be still equal to our $\mathtt{M}^{-1}$.) As a consequence of this, from $\mathsf{E}'(\lambda) = \mathtt{M}\mathsf{E}(\lambda)\mathtt{M}^{-1}$ for example the conclusion $\mathsf{E}'^2(\lambda) = \mathsf{E}'(\lambda)$ can still be made (since only $\mathtt{M}^{-1}\mathtt{M}$ is involved), but $\mathsf{E}'(\lambda \to +\infty) \longrightarrow \mathtt{M}\mathtt{M}^{-1} \neq \mathtt{I}$.

We shall soon see (in Note 105) that this lies in the nature of the case, because no resolution of the identity belongs to this operator.

Before we conclude these introductory discussions we shall give a few formal rules of calculation for operators, which are put in the symbolic form

$$\mathsf{A} = \int_{-\infty}^{+\infty} \lambda d\mathsf{E}(\lambda)$$

by use of the resolution of the identity.

First, let F be a projection that commutes with $\mathsf{E}(\lambda)$. Then for all $\lambda' < \lambda''$

$$\begin{aligned} \|\mathsf{E}(\lambda'')\mathsf{F}f - \mathsf{E}(\lambda')\mathsf{F}f\|^2 &= \|\{\mathsf{E}(\lambda'') - \mathsf{E}(\lambda')\}\mathsf{F}f\|^2 \\ &= \|\mathsf{F}\{\mathsf{E}(\lambda'') - \mathsf{E}(\lambda')\}f\|^2 \\ &\leqslant \|\{\mathsf{E}(\lambda'') - \mathsf{E}(\lambda')\}f\|^2 \end{aligned}$$

Since

$$\mathsf{E}(\lambda'') \ , \quad \mathsf{E}(\lambda') \quad \text{and} \quad \mathsf{E}(\lambda'') - \mathsf{E}(\lambda')$$

as well as

$$\mathsf{E}(\lambda'')\mathsf{F}, \quad \mathsf{E}(\lambda')\mathsf{F} \quad \text{and} \quad \{\mathsf{E}(\lambda'') - \mathsf{E}(\lambda')\}\mathsf{F}$$

are projections, we have

$$\|\mathsf{E}(\lambda'')\mathsf{F}f\|^2 - \|\mathsf{E}(\lambda')\mathsf{F}f\|^2 \leqslant \|\mathsf{E}(\lambda'')f\|^2 - \|\mathsf{E}(\lambda')f\|^2$$

Therefore

$$\int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{E}(\lambda)f\|^2 \geqslant \int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{E}(\lambda)\mathsf{F}f\|^2$$

Then, by $\overline{\mathbf{S}}_3$, $\mathsf{AF}f$ is defined if $\mathsf{A}f$ is. Furthermore,[91]

$$\mathsf{AF} = \int_{-\infty}^{+\infty} \lambda d(\mathsf{E}(\lambda)\mathsf{F}) = \int_{-\infty}^{+\infty} \lambda d(\mathsf{F}\mathsf{E}(\lambda)) = \mathsf{FA}$$

i.e., A and F also commute. In particular, we can take any of the projectors

[91] Actually, this must be proved non-symbolically with the help of the rigorous equation

$$(\mathsf{A}f, g) = \int \lambda d(\mathsf{E}(\lambda)f, g)$$

The calculation runs as follows:

$$\begin{aligned} (\mathsf{AF}f, g) = \int \lambda d(\mathsf{E}(\lambda)\mathsf{F}f, g) = \int \lambda d(\mathsf{F}\mathsf{E}(\lambda)f, g) &= \int \lambda d(\mathsf{E}(\lambda)f, \mathsf{F}g) \\ &= (\mathsf{A}f, \mathsf{F}g) \\ &= (\mathsf{FA}f, g) \end{aligned}$$

From this it follows that $\mathsf{AF} \equiv \mathsf{FA}$.

$\mathsf{E}(\lambda)$ for F (because of $\overline{\mathbf{S}}_3$). Then

$$\mathsf{AE}(\lambda) = \int_{-\infty}^{+\infty} \lambda' \, d(\mathsf{E}(\lambda')\mathsf{E}(\lambda)) = \int_{-\infty}^{+\infty} \lambda' \, d\mathsf{E}(\mathrm{Min}(\lambda, \lambda'))$$

Splitting the integral ($\int_{-\infty}^{+\infty} = \int_{-\infty}^{\lambda} + \int_{\lambda}^{+\infty}$), we have

$$\begin{aligned} \mathsf{AE}(\lambda) &= \int_{-\infty}^{\lambda} \lambda' \, d\mathsf{E}(\lambda') + \int_{\lambda}^{+\infty} \lambda' \, d\mathsf{E}(\lambda) \\ &= \int_{-\infty}^{\lambda} \lambda' \, d\mathsf{E}(\lambda') + 0 \\ &= \mathsf{E}(\lambda)\mathsf{A} \end{aligned}$$

because the function following the second differential is constant. In addition, it follows from this that[92]

$$\mathsf{A}^2 = \int_{-\infty}^{+\infty} \lambda \, d(\mathsf{E}(\lambda)\mathsf{A}) = \int_{-\infty}^{+\infty} \lambda \, d\Big(\int_{-\infty}^{\lambda} \lambda' \, d\mathsf{E}(\lambda') \Big) = \int_{-\infty}^{+\infty} \lambda^2 d\mathsf{E}(\lambda)$$

In general we have

$$\mathsf{A}^n = \int_{-\infty}^{+\infty} \lambda^n d\mathsf{E}(\lambda)$$

because we can reason inductively from $n-1$ to n:[92]

$$\begin{aligned} \mathsf{A}^n = \mathsf{A}^{n-1}\mathsf{A} = \int_{-\infty}^{+\infty} \lambda^{n-1} \, d(\mathsf{E}(\lambda)\mathsf{A}) &= \int_{-\infty}^{+\infty} \lambda^{n-1} \, d\Big(\int_{-\infty}^{\lambda} \lambda' \, d\mathsf{E}(\lambda') \Big) \\ &= \int_{-\infty}^{+\infty} \lambda^{n-1} \cdot \lambda \, d\mathsf{E}(\lambda) \\ &= \int_{-\infty}^{+\infty} \lambda^n \, d\mathsf{E}(\lambda) \end{aligned}$$

It now follows that if $p(x) = a_0 + a_1 x + \cdots + a_n x^n$ is any polynomial, then

$$p(\mathsf{A}) = \int_{-\infty}^{+\infty} p(\lambda) \, d\mathsf{E}(\lambda)$$

(By $p(\mathsf{A})$ we mean, of course, $p(x) = a_0\mathsf{I} + a_1\mathsf{A} + \cdots + a_n\mathsf{A}^n$. $\int_{-\infty}^{+\infty} d\mathsf{E}(\lambda) = \mathsf{I}$ follows from $\overline{\mathbf{S}}_1$.)

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[92] The third equality follows from the equation

$$\int f(\lambda) d\Big(\int^{\lambda} g(\lambda') dh(\lambda') \Big) = \int f(\lambda) g(\lambda) dh(\lambda)$$

which is generally valid for the Stieltjes integral. This equation is clear without further discussion, by reason of the reciprocal relation between d and $\int^{\lambda}$. A rigorous proof has been given by the author: Annals of Mathematics **32** (1931).

Furthermore, we have the following: If $r(\lambda)$ and $s(\lambda)$ are any two functions, and if we define two operators B, C (symbolically) by[93]

$$\mathsf{B} = \int_{-\infty}^{+\infty} r(\lambda)\, d\mathsf{E}(\lambda), \qquad \mathsf{C} = \int_{-\infty}^{+\infty} s(\lambda)\, d\mathsf{E}(\lambda)$$

then it follows that

$$\mathsf{BC} = \int_{-\infty}^{+\infty} r(\lambda)s(\lambda)\, d\mathsf{E}(\lambda)$$

For proof we proceed exactly as in the special case $\mathsf{B} = \mathsf{C} = \mathsf{A}$:

$$\begin{aligned}\mathsf{BE}(\lambda) &= \int_{-\infty}^{+\infty} r(\lambda')d(\mathsf{E}(\lambda')\mathsf{E}(\lambda)) = \int_{-\infty}^{+\infty} r(\lambda')d(\mathsf{E}(\mathrm{Min}(\lambda,\lambda')))\\ &= \int_{-\infty}^{\lambda} r(\lambda')d\mathsf{E}(\lambda') + \int_{\lambda}^{+\infty} r(\lambda')d\mathsf{E}(\lambda)\\ &= \int_{-\infty}^{\lambda} r(\lambda')d\mathsf{E}(\lambda')\end{aligned}$$

$$\begin{aligned}\mathsf{CB} = \int_{-\infty}^{+\infty} s(\lambda)d(\mathsf{BE}(\lambda)) &= \int_{-\infty}^{+\infty} s(\lambda)d\Big(\int_{-\infty}^{\lambda} r(\lambda')d\mathsf{E}(\lambda')\Big)\\ &= \int_{-\infty}^{+\infty} s(\lambda)\cdot r(\lambda)d\mathsf{E}(\lambda)\\ &= \int_{-\infty}^{+\infty} s(\lambda)r(\lambda)d\mathsf{E}(\lambda)\end{aligned}$$

The following relations may easily be verified:

$$\begin{aligned}\mathsf{B}^* &= \int_{-\infty}^{+\infty} \overline{r(\lambda)}d\mathsf{E}(\lambda)\\ a\mathsf{B} &= \int_{-\infty}^{+\infty} ar(\lambda)d\mathsf{E}(\lambda)\\ \mathsf{B}\pm\mathsf{C} &= \int_{-\infty}^{+\infty} \{r(\lambda)\pm s(\lambda)\}d\mathsf{E}(\lambda)\end{aligned}$$

There then exists no formal obstacle to writing $\mathsf{B} = r(\mathsf{A})$ for such functions $r(\lambda)$.[94] Particularly noteworthy are the (discontinuous!) functions

[93] That is,

$$(\mathsf{B}f, g) = \int_{-\infty}^{+\infty} r(\lambda)d(\mathsf{E}(\lambda), g), \quad (\mathsf{C}f, g) = \int_{-\infty}^{+\infty} s(\lambda)d(\mathsf{E}(\lambda), g)$$

[94] The precise foundation of this function concept was given by the author in Annals of Math. **32** (1931). F. Riesz was the first one to define general operator functions by limiting processes applied to polynomials.

$$e_\lambda(\lambda') = \begin{cases} 1 & \text{for} \quad \lambda' \leqslant \lambda \\ 0 & \text{for} \quad \lambda' > \lambda \end{cases}$$

For these we have (by $\overline{\mathbf{S}}_1$)

$$e_\lambda(\mathsf{A}) = \int_{-\infty}^{+\infty} e_\lambda(\lambda') d\mathsf{E}(\lambda) = \int_{-\infty}^{\lambda} d\mathsf{E}(\lambda') = \mathsf{E}(\lambda)$$

(At the beginning of this section we discussed the operator $\mathsf{A} = q_j \cdot$. Its $\mathsf{E}(\lambda)$ was multiplication by 1 or 0 according as $q_j \leqslant \lambda$ or $q_j > \lambda$; *i.e.*, multiplication by $e_\lambda(q_j)$. This example is well suited to furnish an intuitive picture of the above concepts.)

9. DIGRESSION ON THE EXISTENCE AND UNIQUENESS OF THE SOLUTIONS OF THE EIGENVALUE PROBLEM

The last section gave only a qualitative survey, emphasizing special cases, of the problem as to which resolutions of the identity $\mathsf{E}(\lambda)$ correspond to a given Hermitian operator A. A systematic investigation of the question still remains to be effected. To do this in mathematical completeness goes beyond the scope of this book. We limit ourselves to the proof of a few points, and the statement of the rest—particularly since precise knowledge of these circumstances is not absolutely necessary for understanding of quantum mechanics.[95]

In THEOREM 18 it was shown that the continuity of linear operators is expressed by

Co $\qquad \|\mathsf{A}f\| \leqslant C \cdot \|f\| \quad : \quad C$ arbitrary, but fixed

but by THEOREM 18 there are several equivalent forms of the condition **Co**:

Co$_1$ $\qquad |(\mathsf{A}f, g)| \leqslant C \cdot \|f\| \|g\|$

Co$_2$ $\qquad |(\mathsf{A}f, f)| \leqslant C \cdot \|f\|^2$ but only if A is Hermitian

The condition **Co**$_1$, equivalent to continuity, is the Hilbert concept of boundedness. Hilbert has formulated and solved the eigenvalue problem for bounded (*i.e.*, continuous) Hermitian operators (see Note 70). But before we discuss this case we must introduce an additional concept.

A Hermitian operator A is said to be *closed* if it has the following property: Given a point sequence $f_1, f_2, \ldots$, assume that all $\mathsf{A}f_n$ are defined, and that $f_n \to f$, $\mathsf{A}f_n \to f^*$. Then A is closed if and only if $\mathsf{A}f$ is also defined, and is

[95] The theory of unbounded Hermitian operators, to which reference will be made in the following (in addition to the Hilbert theory of bounded operators), was developed by the author (see reference in Note 78). M. Stone (PNAS 1929 and 1930) arrived at similar results independently.

equal to f^*. It should be observed that continuity could be defined in a way which is closely related to the above definition, namely the following: If all $\mathsf{A}f_n$, $\mathsf{A}f$ are defined and if $f_m \to f$, then $\mathsf{A}f_n \to \mathsf{A}f$. The difference between the two definitions is that for closure one is required to have $\mathsf{A}f_n \to f^* = \mathsf{A}f$, while for continuity it is required only that $\mathsf{A}f_n \to f^*$ (*i.e.*, that f^* exists).

A few examples: Let $\mathfrak{R}_\infty$ again be the space of all $f(q)$ with finite

$$\int_{-\infty}^{+\infty} |f(q)|^2 dq \quad : \quad -\infty < q < +\infty$$

Let A be the operator $q\cdot$, defined for all $f(q)$ with finite

$$\int_{-\infty}^{+\infty} |f(q)|^2 dq \quad \text{and} \quad \int_{-\infty}^{+\infty} q^2 |f(q)|^2 dq$$

And let A' be the operator $\frac{\hbar}{i}\frac{\partial}{\partial q}$ defined for all everywhere-differentiable functions $f(q)$ with finite

$$\int_{-\infty}^{+\infty} |f(q)|^2 dq \quad \text{and} \quad \int_{-\infty}^{+\infty} |\tfrac{\hbar}{i} f'(q)|^2 dq$$

As we know, both of these operators are Hermitian.

A is shown to be closed by the following argument: Let $f_n \to f$, $\mathsf{A}f_n \to f^*$; *i.e.*,

$$\int_{-\infty}^{+\infty} |f_n(q) - f(q)|^2 dq \to 0, \qquad \int_{-\infty}^{+\infty} |q f_n(q) - f^*(q)|^2 dq \to 0$$

By reason of the discussion in **II.3** of the proof of **D**, there exists a subsequence $f_{n_1}, f_{n_2}, \ldots$ of the $f_1, f_2, \ldots$ which converges to a limit everywhere with the exception of a q-set of measure 0: $f_{n_\nu}(q) \to g(q)$. Therefore

$$\int_{-\infty}^{+\infty} |g(q) - f(q)|^2 dq \to 0, \qquad \int_{-\infty}^{+\infty} |q\, g(q) - f^*(q)|^2 dq \to 0$$

i.e., except for a set of measure 0, $g(q) = f(q)$ and also $q\,g(q) = f^*(q)$; *i.e.*, $f^*(q)$ and $q f(q)$ are not essentially different. But, since $f^*(q)$ belongs to $\mathfrak{R}_\infty$ by assumption, $q\,g(q)$ does also. Consequently $\mathsf{A}f(q)$ is defined and is equal to $q f(q) = f^*(q)$.

On the other hand, A' is not closed: Set

$$f_n(q) = e^{-\sqrt{q^2 + \frac{1}{n}}}, \qquad f(q) = e^{-|q|}$$

Clearly, all $\mathsf{A}'f_n$ are defined, but not $\mathsf{A}'f$ (f has no derivative at $q = 0$). Nevertheless, $f_n \to f$, $\mathsf{A}'f_n \to f^*$, as can easily be calculated if we set

$$f^*(q) = -\mathrm{sgn}(q) e^{-|q|} \quad \text{where} \quad \mathrm{sgn}(q) = \begin{cases} -1 & \text{for} \quad q < 0 \\ 0 & \text{for} \quad q = 0 \\ +1 & \text{for} \quad q > 0 \end{cases}$$

We now show that—in contrast to continuity—closure is a property which can always be achieved with little difficulty for Hermitian operators. This is done by the process of *extension*; *i.e.*, we leave the operator unchanged at all points of $\mathfrak{R}_\infty$ where it is defined, but in addition define it for some of those points where it was not previously defined.

Indeed, let A be an arbitrary Hermitian operator. We define an operator $\widetilde{\mathsf{A}}$ as follows: $\widetilde{\mathsf{A}}f$ is defined if a sequence $f_1, f_2, \ldots$ with defined $\mathsf{A}f_n$ exists in such a way that f is the limit of the f_n and the $\mathsf{A}f_n$ also possess a limit f^*. Then $\widetilde{\mathsf{A}}f = f^*$. This definition is admissible only if it is unique; *i.e.*, it follows from $f_n \to f$, $g_n \to f$, $\mathsf{A}f_n \to f^*$, $\mathsf{A}g_n \to g^*$ that $f^* = g^*$. But if $\mathsf{A}g$ is defined

$$(f^*, g) = \lim(\mathsf{A}f_n, g) = \lim(f_n, \mathsf{A}g) = (f, \mathsf{A}g)$$
$$(g^*, g) = \lim(\mathsf{A}g_n, g) = \lim(g_n, \mathsf{A}g) = (f, \mathsf{A}g)$$

therefore $(f^*, g) = (g^*, g)$. But these g are everywhere dense, so $f^* = g^*$. Therefore we have defined $\widetilde{\mathsf{A}}$ correctly. This $\widetilde{\mathsf{A}}$ is an extension of A; *i.e.*, whenever A is defined then $\widetilde{\mathsf{A}}$ is also defined, and $\widetilde{\mathsf{A}} = \mathsf{A}$. From the fact that A is linear and Hermitian the same follows for $\widetilde{\mathsf{A}}$ (by continuity). Finally, $\widetilde{\mathsf{A}}$ is closed, by the following argument: Let all $\widetilde{\mathsf{A}}f$ be defined; $f_n \to f$, $\widetilde{\mathsf{A}}f_n \to f^*$. Then there are sequences $f_{n,1}, f_{n,2}, \ldots$ with defined $\mathsf{A}f_{n,m}$ such that $f_{n,m} \to f_n$, $\mathsf{A}f_{n,m} \to f_n^*$ and $\widetilde{\mathsf{A}}f_n = f_n^*$. For each such n there is an N_n such that for $m \geqslant N_n$

$$\|f_{n,m} - f_n\| \leqslant \tfrac{1}{n}, \qquad \|\mathsf{A}f_{n,m} - f_n^*\| \leqslant \tfrac{1}{n}$$

Therefore $f_{n,N_n} - f_n \to 0$, $\mathsf{A}f_{n,N_n} - \widetilde{\mathsf{A}}f \to 0$ whence $f_{n,N_n} - f \to 0$, $\mathsf{A}f_{n,N_n} - f^* \to 0$. From this it follows by definition that $\widetilde{\mathsf{A}}f = f^*$.

(It should be noted that a discontinuous operator can never be made continuous by extension.)

If an operator B extends an operator A—*i.e.*, if, whenever $\mathsf{A}f$ is defined, $\mathsf{B}f$ is also defined and $\mathsf{B}f = \mathsf{A}f$—we write $\mathsf{B} \succ \mathsf{A}$ or $\mathsf{A} \prec \mathsf{B}$. We have just proved that $\mathsf{A} \prec \widetilde{\mathsf{A}}$, and that $\widetilde{\mathsf{A}}$ is Hermitian and closed. It is evident without further discussion that for each closed B with $\mathsf{A} \prec \mathsf{B}$, $\widetilde{\mathsf{A}} \prec \mathsf{B}$ must also hold. Consequently, $\widetilde{\mathsf{A}}$ is the smallest closed extension of A. (Therefore $\widetilde{\widetilde{\mathsf{A}}} = \widetilde{\mathsf{A}}$.)

The close relation between A and $\widetilde{\mathsf{A}}$ makes it plain that A may be replaced by $\widetilde{\mathsf{A}}$ in all considerations, since $\widetilde{\mathsf{A}}$ extends the domain of A in a natural way or, looking at it from the opposite point of view, A restricts the domain of $\widetilde{\mathsf{A}}$ in an unnecessary manner. Let this replacement of A by $\widetilde{\mathsf{A}}$ take place. Then, as a consequence, we may assume that all Hermitian operators with which we have to deal are closed.

Let us again consider a continuous Hermitian operator A. In this case, closure is equivalent to closure of the domain. Now the condition $\|\mathsf{A}f\| \leqslant C \cdot \|f\|$, characteristic for continuity, clearly holds for $\widetilde{\mathsf{A}}$ also. Therefore $\widetilde{\mathsf{A}}$ is also continuous. Since the domain of $\widetilde{\mathsf{A}}$ is then closed, but is on the other hand

everywhere dense, it is equal to $\mathfrak{R}_\infty$. That is: $\widetilde{\mathsf{A}}$ is defined everywhere, and consequently each closed and continuous operator is also. The converse holds too: if a closed operator is defined everywhere, then it is continuous (this is the theorem of Toeplitz,[96] into the proof of which we do not enter here.)

Hilbert's result runs as follows: To each continuous operator there corresponds one and only one resolution of the identity (see the reference in Note 70). Since a continuous operator is always defined, and

$$\int \lambda^2 d\|\mathsf{E}(\lambda)f\|^2$$

and must always be finite; since, in addition, this equals $\|\mathsf{A}f\|^2$ and consequently, by **Co**, is $\leqslant C^2\|f\|^2$, we have

$$\begin{aligned} 0 \geqslant \|\mathsf{A}f\|^2 - C^2\|f\|^2 &= \int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{E}(\lambda)f\|^2 - C^2 \int_{-\infty}^{+\infty} d\|\mathsf{E}(\lambda)f\|^2 \\ &= \int_{-\infty}^{+\infty} (\lambda^2 - C^2) d\|\mathsf{E}(\lambda)f\|^2 \end{aligned}$$

Now let $f = \mathsf{E}(-C-\epsilon)g$. Then $\mathsf{E}(\lambda)f = \mathsf{E}(\mathrm{Min}(\lambda, -C-\epsilon))g$, and therefore for $\lambda \geqslant -C-\epsilon$ it is constant, so that we need only consider $\int_{-\infty}^{-C-\epsilon}$. In this case, $\mathsf{E}(\lambda)f = \mathsf{E}(\lambda)g$ and

$$\lambda^2 - C^2 \geqslant (C+\epsilon)^2 - C^2 > 2C\epsilon$$

so that

$$0 \geqslant 2C\epsilon \int_{-\infty}^{-C-\epsilon} d\|\mathsf{E}(\lambda)g\|^2 = 2C\epsilon\|\mathsf{E}(-C-\epsilon)g\|^2$$

$$\|\mathsf{E}(-C-\epsilon)g\|^2 \leqslant 0, \quad E(-C-\epsilon)g = 0$$

In the same way, it may be shown for $f = g - \mathsf{E}(C+\epsilon)g$ that

$$g - \mathsf{E}(C+\epsilon)g = 0$$

Consequently, for all $\epsilon > 0$, $\mathsf{E}(-C-\epsilon) = \mathsf{O}$, $\mathsf{E}(C+\epsilon) = \mathsf{I}$; *i.e.*,

$$\mathsf{E}(\lambda) = \begin{cases} \mathsf{O} & \text{for} \quad \lambda < -C \\ \mathsf{I} & \text{for} \quad \lambda < +C \end{cases}$$

(Because of $\overline{\mathbf{S}}_2$ the latter holds also for $\lambda = 0$.) That is, $\mathsf{E}(\lambda)$ is variable only on the range $-C \leqslant \lambda \leqslant +C$.

Conversely, this has the continuity of A as a consequence: we have

$$\begin{aligned} \|\mathsf{A}f\|^2 &= \int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{E}(\lambda)f\|^2 = \int_{-C}^{+C} \lambda^2 d\|\mathsf{E}(\lambda)f\|^2 \\ &\leqslant C^2 \int_{-C}^{+C} d\|\mathsf{E}(\lambda)f\|^2 = C^2 \int_{-\infty}^{+\infty} d\|\mathsf{E}(\lambda)f\|^2 = C^2\|f\|^2 \end{aligned}$$

which gives $\|\mathsf{A}f\| \leqslant C\|f\|$. We see therefore that the continuous A are entirely

[96] Math. Ann. **69** (1911).

exhausted by resolutions of the identity variable only in a finite λ-interval. But what is the situation with the other, discontinuous Hermitian operators? There are still available all resolutions of the identity for which the λ-interval is not finite. Do these exhaust the Hermitian operators just mentioned?

The circumstances under which these operators cannot be defined everywhere must first be assessed correctly.

It is perfectly possible that a Hermitian operator may not be defined at points in Hilbert space at which definition might actually be feasible. For example, our operator $\mathsf{A}' = \frac{\hbar}{i}\frac{\partial}{\partial q}$ was undefined for $f(q) = e^{-|q|}$ but could have been limited to analytic functions (in $-\infty < q < +\infty$, q real),[97] etc. The domain was protected from entirely arbitrary contractions by the fact that we required it to be everywhere dense. Furthermore, we can restrict ourselves to closed operators. Still, even this is not sufficiently effective. Indeed, let us take, for example, the operator $\mathsf{A}' = \frac{\hbar}{i}\frac{\partial}{\partial q}$ in the interval $0 \leqslant q \leqslant 1$. Then let $f(q)$ be assumed differentiable everywhere, with $\int_{-\infty}^{+\infty} |f(q)|^2 dq$, $\int_{-\infty}^{+\infty} |f'(q)|^2 dq$ finite. In order that A' be Hermitian a boundary condition $f(0) : f(1) = e^{-i\alpha}$ $(0 \leqslant \alpha < 2\pi)$ must be imposed; let the set of these $f(q)$ be $\mathcal{A}_\alpha$, with A' itself —thus restricted—becoming A'_α. Furthermore, let us consider the boundary condition $f(0) = f(1) = 0$. We call this $f(q)$-set $\mathcal{A}^0$ and the A', restricted accordingly, A'^0. All $\widetilde{\mathsf{A}}'_\alpha$ are extensions of $\widetilde{\mathsf{A}}'^0$, which is then Hermitian, and its domain is everywhere dense,[98] and therefore the closed $\widetilde{\mathsf{A}}'_\alpha$ are also extensions of $\widetilde{\mathsf{A}}'^0$. All are different from one another, and from $\widetilde{\mathsf{A}}'^0$. Indeed, the clearly

[97] Even the functions $f(q)$ which are analytic in $-\infty < q < +\infty$ (with finite $\int_{-\infty}^{+\infty} |f(q)|^2 dq$, $\int_{-\infty}^{+\infty} |f'(q)|^2 dq, \ldots$) are everywhere dense in $\mathfrak{R}_\infty$. Indeed, by **II.3 D**, the linear combinations of

$$f_{a,b}(q) = \begin{cases} 1 & \text{for} \quad a < q < b \\ 0 & \text{elsewhere} \end{cases}$$

are everywhere dense. Therefore it suffices to approximate these arbitrarily well by analytic functions $f(q)$. Such, for example, as

$$f^{(\epsilon)}_{a,b}(q) = \tfrac{1}{2} - \tfrac{1}{2}\tanh\left[\frac{(q-a)(q-b)}{\epsilon}\right] = \left(1 + \exp\left[2\frac{(q-a)(q-b)}{\epsilon}\right]\right)^{-1}$$

which is of the desired type, and converges to $f_{a,b}(q)$ as $\epsilon \to 0$.

[98] It is again sufficient to approximate the $f_{a,b}(q)$, $0 \leqslant a < b \leqslant 1$ with functions from $\mathcal{A}^0$. For example, the functions

$$f^{(\epsilon)}_{a,b}(q) = \tfrac{1}{2} - \tfrac{1}{2}\tanh\left[\epsilon^{-1}\frac{(q-a-\epsilon)(q-b+\epsilon)}{q(1-q)}\right]$$

with $\epsilon \to 0$ can be used for this purpose.

unitary operation $f(q) \to e^{i\beta q} f(q)$ transforms A' into $\mathsf{A}' + \hbar\beta \mathsf{I}$ and

$$\begin{array}{rlll} & \mathcal{A}_\alpha & \text{into} & \mathcal{A}_{\alpha+\beta} \\ & \mathcal{A}^0 & \text{into} & \mathcal{A}^0 \\ \therefore & \mathsf{A}'_\alpha & \text{into} & \mathsf{A}'_{\alpha-\beta} + \hbar\beta \mathsf{I} \\ & \mathsf{A}'^0 & \text{into} & \mathsf{A}'^0 + \hbar\beta \mathsf{I} \\ \therefore & \widetilde{\mathsf{A}}'_\alpha & \text{into} & \widetilde{\mathsf{A}}'_{\alpha+\beta} + \hbar\beta \mathsf{I} \\ & \widetilde{\mathsf{A}}'^0 & \text{into} & \widetilde{\mathsf{A}}'^0 + \hbar\beta \mathsf{I} \end{array}$$

Hence it would follow from $\widetilde{\mathsf{A}}'_\alpha = \widetilde{\mathsf{A}}'^0$ that $\widetilde{\mathsf{A}}'_{\alpha-\beta} = \widetilde{\mathsf{A}}'^0$; *i.e.*, all $\widetilde{\mathsf{A}}'_\gamma$ would be equal to one another. Consequently it suffices to show that $\widetilde{\mathsf{A}}'_\alpha \neq \widetilde{\mathsf{A}}'_\gamma$ if $\alpha \neq \gamma$, and this is certainly the case if $\widetilde{\mathsf{A}}'_\alpha, \widetilde{\mathsf{A}}'_\gamma$ possess no common Hermitian extension; *i.e.*, if A' is not Hermitian in the union of $\mathcal{A}_\alpha$, $\mathcal{A}_\gamma$. Since $e^{i\alpha q}$ belongs to $\mathcal{A}_\alpha$, $e^{i\gamma q}$ to $\mathcal{A}_\gamma$, and

$$\begin{aligned} (\mathsf{A}' e^{i\alpha q}, e^{i\gamma q}) - (e^{i\alpha q}, \mathsf{A}' e^{i\gamma q}) &= i\alpha \int_0^1 e^{i(\alpha-\gamma)q}\, dq - i\gamma \int_0^1 e^{i(\alpha-\gamma)q}\, dq \\ &= i(\alpha-\gamma) \int_0^1 e^{i(\alpha-\gamma)q}\, dq \\ &= e^{i(\alpha-\gamma)} - 1 \\ &\neq 0 \end{aligned}$$

this is indeed the case. Consequently the closed Hermitian operator $\widetilde{\mathsf{A}}'^0$ is defined in too restricted a region, because there exist proper (*i.e.*, different from $\widetilde{\mathsf{A}}'^0$) closed Hermitian extensions of it: $\widetilde{\mathsf{A}}'_\alpha$—and therefore the extension process—is infinitely many valued, since each $\widetilde{\mathsf{A}}'_\alpha$ can be used and each produces another solution of the eigenvalue problem. (It is always a pure discrete spectrum, but depends upon α: $\lambda_k = h\left(\frac{\alpha}{2\pi} + k\right)$, $k = 0, \pm 1, \pm 2, \ldots$) On the other hand, with the operator $\widetilde{\mathsf{A}}'^0$ itself we in general expect no reasonable solutions of the eigenvalue problem. In fact we shall show in the course of this section that a Hermitian operator which belongs to a resolution of the identity (*i.e.*, has a solvable eigenvalue problem) possesses no proper extensions. An operator which possesses no proper extensions—which is already defined at all points where it could be defined in a reasonable fashion (*i.e.*, without violation of its Hermitian nature)—we call a *maximal* operator. Then, by the above, resolutions of the identity can belong only to maximal operators.

On the other hand, the following theorem holds: Each Hermitian operator can be extended to a maximal Hermitian operator. (In fact, a non-maximal but closed operator may always be extended in an infinite number of different ways. The only unique step of the extension process is the closure $\mathsf{A} \to \widetilde{\mathsf{A}}$. See Note 95.) Therefore the most generally valid solution of the problem which we can expect is this: to each maximal Hermitian operator belongs one and

only one resolution of the identity (each closed continuous operator is defined everywhere in $\mathfrak{R}_\infty$ and is therefore maximal).

Therefore it is necessary to answer these questions: Does a resolution of the identity belong to a maximal Hermitian operator? Can it ever happen that several belong to the same operator?

We begin by stating the answers: to a given maximal Hermitian operator there belongs none or exactly one resolution of the identity, and the former situation does sometimes occur; *i.e.*, the eigenvalue problem is certainly unique, but under certain conditions it is insolvable. Nevertheless, the latter case is to be regarded in a certain sense as an exception. The argument which leads to this conclusion will now be sketched in broad outline.

If we consider a rational function $f(\lambda)$ of a matrix $\mathbb{A}$ (of finite dimensions, and capable of transformation to diagonal form by a unitary transformation), then the eigenvectors are preserved, and the eigenvalues $\lambda_1, \ldots, \lambda_n$ go over into $f(\lambda_1), \ldots, f(\lambda_n)$.[99] If now the $f(\lambda)$ maps the real axis (in the complex plane) onto the circumference of the unit circle, then the matrices with exclusively real eigenvalues go over into those with eigenvalues of absolute value 1; *i.e.*, the Hermitian go over into the unitary.[100] For example, $f(\lambda) = \frac{\lambda-1}{\lambda+1}$ has this property. The corresponding transformation

$$\mathbb{U} = \frac{\mathbb{A} - i\,\mathbb{I}}{\mathbb{A} + i\,\mathbb{I}}, \qquad \mathbb{A} = -i\,\frac{\mathbb{U} + \mathbb{I}}{\mathbb{U} - \mathbb{I}}$$

is known as the *Cayley transformation*. We shall now look to the effect of this transformation for the Hermitian operators of $\mathfrak{R}_\infty$; *i.e.*, we define an operator U as follows: $\mathsf{U}f$ is defined if and only if $f = (\mathsf{A} + i\,\mathsf{I})\phi = \mathsf{A}\phi + i\,\phi$, and then $\mathsf{U}f = (\mathsf{A} - i\mathsf{I})\phi = \mathsf{A}\phi - i\,\phi$. We hope that this definition will yield a single-valued $\mathsf{U}f$ for all f, and that U will be unitary. The proof in $\mathfrak{R}_n$ is not relevant now, since it presumes the transformability to diagonal form; *i.e.*, the solvability of the eigenvalue problem, in fact with a pure discrete spectrum. But if the statements about U prove to be correct, then we can solve the eigenvalue problem in the following way:

[99] Since the function $f(\lambda)$ can be approximated by polynomials, it suffices to consider polynomials, and therefore their components, simple powers: $f(\lambda) = \lambda^s$ $(s = 0, 1, 2, \ldots)$. Since a unitary transformation does not matter here, we may assume $\mathbb{A}$ to be a diagonal matrix. Since the diagonal elements are the eigenvalues, they are $\lambda_1, \lambda_2, \ldots, \lambda_n$. We must then show only that $\mathbb{A}^s$ is also diagonal, and that it has the diagonal elements $\lambda_1^s, \lambda_2^s, \ldots, \lambda_n^s$. But this is obvious.

[100] To demonstrate that these properties are characteristic of Hermitian and unitary matrices respectively, we again need only to verify them for diagonal matrices. For the diagonal matrix $\mathbb{A}$ with elements $\lambda_1, \ldots, \lambda_n$, the diagonal matrix $\mathbb{A}^*$ with elements $\bar{\lambda}_1, \ldots, \bar{\lambda}_n$ is the transposed conjugate; therefore $\mathbb{A} = \mathbb{A}^*$ implies that $\lambda_1 = \bar{\lambda}_1, \ldots, \lambda_n = \bar{\lambda}_1$; *i.e.*, that $\lambda_1, \ldots, \lambda_n$ are real. Moreover, $\mathbb{A}\,\mathbb{A}^* = \mathbb{A}^*\mathbb{A} = \mathbb{I}$ implies that $\lambda_1\bar{\lambda}_1 = 1, \ldots, \lambda_n\bar{\lambda}_n = 1$; that is, that $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_n| = 1$.

For U, the eigenvalue problem is solvable in the following form: There is a unique family of projectors $\mathsf{E}(\sigma)$ $(0 \leqslant \sigma \leqslant 1)$ which satisfies the following conditions:

$\overline{\overline{\mathbf{S}}}_1$: $\mathsf{E}(0) = \mathsf{O}$, $\mathsf{E}(1) = \mathsf{I}$ and for $\sigma \to \sigma_0$, $\sigma \geqslant \sigma_0$, $\mathsf{E}(\sigma)f \to \mathsf{E}(\sigma_0)f$.

$\overline{\overline{\mathbf{S}}}_2$: From $\sigma' \leqslant \sigma''$ it follows that $\mathsf{E}(\sigma') \leqslant \mathsf{E}(\sigma'')$.

$\overline{\overline{\mathbf{S}}}_3$: It is always true that

$$(\mathsf{U}f, g) = \int_0^1 e^{2\pi i\sigma} d(\mathsf{E}(\sigma)f, g)$$

(U is defined everywhere, and the integral on the right is always absolutely convergent.[101])

This is proved in the framework and with the methods of the Hilbert theory. This is made possible by the fact that the unitary operator U is always continuous (see references in Notes 70, 101). The analogy to the conditions $\overline{\mathbf{S}}_1$–$\overline{\mathbf{S}}_3$ for Hermitian operators comes to mind. The only differences are: instead of the real integrands λ $(-\infty < \lambda < +\infty)$ the complex integrand $e^{2\pi i\sigma}$ here is taken around the circumference of the unit circle (even in $\mathcal{R}_n$ the Hermitian-unitary relation possesses a far-reaching analogy to the real axis-unit circle relation: see Note 100), and the description of the operator domain in $\overline{\mathbf{S}}_3$ is superfluous because unitary operators are defined everywhere.

Because of $\overline{\overline{\mathbf{S}}}_1$, $\mathsf{E}(\sigma)f \to \mathsf{E}(0)f = 0$ for $\sigma \to 0$ (since $\sigma \geqslant 0$ by its nature), while for $\sigma \to 1$ (since $\sigma \leqslant 1$) there need not be $\mathsf{E}(\sigma)f \to \mathsf{E}(1)f = f$. If this is actually not the case, then $\mathsf{E}(\sigma)$ is discontinuous at $\sigma = 1$. But since a projection E' exists, such that for $\sigma \to 1$, $\sigma < 1$, $\mathsf{E}(\sigma)f \to \mathsf{E}'f$ (see THEOREM 17 in **II.4**, as well as Note 79), this means that $\mathsf{E}' \neq \mathsf{E}(1) = \mathsf{I}$; *i.e.*, that $\mathsf{E}'f = 0$ also possesses solutions $f \neq 0$. Because of $\mathsf{E}(\sigma) \leqslant \mathsf{E}'$ it follows from $\mathsf{E}'f = 0$

[101] For the proof of this fact, see the work of the author cited in Note 78; also A. Wintner: Math. Z. **30** (1929). The absolute convergence of all integrals

$$\int_0^1 f(\sigma)\, d(\mathsf{E}(\sigma)f, g)$$

with bounded $f(\sigma)$ is shown as follows. It is sufficient to consider $\mathrm{Re}(\mathsf{E}(\sigma)f, g)$ since substitution of if, g for f, g changes this into $\mathrm{Im}(\mathsf{E}(\sigma)f, g)$. Because

$$\mathrm{Re}(\mathsf{E}(\sigma)f, g) = \left(\mathsf{E}(\sigma)\tfrac{f+g}{2}, \tfrac{f+g}{2}\right) - \left(\mathsf{E}(\sigma)\tfrac{f-g}{2}, \tfrac{f-g}{2}\right)$$

only the $(\mathsf{E}(\sigma)f, g)$ need be investigated. In $\int_0^1 f(\sigma)\, d(\mathsf{E}(\sigma)f, g)$ the integrand is bounded and the σ-function behind the differential sign is monotonic; therefore the proposition is demonstrated.

that $\mathsf{E}(\sigma)f = 0$ for all $\sigma < 1$. Conversely, by the definition of E', the former is also a consequence of the latter. If all $\mathsf{E}(\sigma)f = 0$ $(\sigma < 1)$, then we see—just as at the beginning of **II.8**—that $(\mathsf{U}f, g) = (f, g)$ for all g, therefore $\mathsf{U}f = f$. Conversely, if $\mathsf{U}f = f$ then

$$\int_0^1 e^{2\pi i\sigma} d(\mathsf{E}(\sigma)f, f) = (\mathsf{U}f, f) = (f, f)$$

$$\operatorname{Re}\int_0^1 e^{2\pi i\sigma} d(\mathsf{E}(\sigma)f, f) = (f, f)$$

$$\int_0^1 (1 - \cos 2\pi\sigma) d(\mathsf{E}(\sigma)f, f) = 0$$

$$\int_0^1 (1 - \cos 2\pi\sigma) d(\|\mathsf{E}(\sigma)f\|^2) = 0$$

From this we get—exactly as at the beginning of **II.8**—$\mathsf{E}(\sigma)f = 0$ for all $\sigma < 1$ (and $\sigma \geqslant 0$). Consequently, the discontinuity of $\mathsf{E}(\sigma)$ at $\sigma = 1$ means that $\mathsf{U}f = f$ is solvable with $f \neq 0$.

With our Cayley transforms U we now have $\phi = \mathsf{A}f + if$, $\mathsf{U}\phi = \mathsf{A}f - if$ and from $\mathsf{U}\phi = 0$ it then follows that $f = 0$, $\phi = 0$. Here $\mathsf{E}(\sigma) \to f$ must also hold for $\sigma \to 1$. Consequently, by the mapping

$$\lambda = -i\,\frac{e^{2\pi i\sigma} + 1}{e^{2\pi i\sigma} - 1} = -\cot \pi\sigma, \qquad \sigma = -\tfrac{1}{\pi}\cot^{-1}\lambda$$

(which maps the intervals $0 < \sigma < 1$ and $-\infty < \lambda < +\infty$ one-to-one and monotonically onto each other) we can produce a resolution of the identity $\mathsf{F}(\lambda)$ from $\mathsf{E}(\sigma)$ in the sense of $\overline{\mathbf{S}}_1$–$\overline{\mathbf{S}}_2$:

C $$\mathsf{F}(\lambda) = \mathsf{E}(-\tfrac{1}{\pi}\cot^{-1}\lambda), \qquad \mathsf{E}(\sigma) = \mathsf{F}(-\cot \pi\sigma)$$

We now want to show that $\mathsf{F}(\lambda)$ satisfies $\overline{\mathbf{S}}_3$ for A if and only if $\mathsf{E}(\sigma)$ satisfies $\overline{\overline{\mathbf{S}}}_3$ for U. In this way, the questions of the existence and uniqueness for the solutions of the eigenvalue problem for the (possibly discontinuous) Hermitian operator A are reduced to the corresponding questions for the unitary operator U. These, however, as has been described, are answered in the most favorable way.

Therefore, let A be Hermitian and U be its Cayley transform. We look first to the case in which U is unitary. Its $\mathsf{E}(\sigma)$ must then conform to $\overline{\overline{\mathbf{S}}}_1$, $\overline{\overline{\mathbf{S}}}_2$ as well as to $\overline{\overline{\mathbf{S}}}_3$. We form the $\mathsf{F}(\lambda)$ according to **C**, and then $\overline{\mathbf{S}}_1$, $\overline{\mathbf{S}}_2$ are fulfilled. If $\mathsf{A}f$ is defined, then

$$\mathsf{A}f + if = \phi, \qquad \mathsf{A}f - if = \mathsf{U}\phi$$

and therefore

$$f = \frac{\phi - \mathsf{U}\phi}{2i}, \qquad \mathsf{A}f = \frac{\phi + \mathsf{U}\phi}{2}$$

We calculate, in part symbolically:[102]

$$f = \frac{\phi - \mathsf{U}\phi}{2i} = \frac{1}{2i}\Big(\phi - \int_0^1 e^{2\pi i\sigma} d\mathsf{E}(\sigma)\,\phi\Big) = \int_0^1 \frac{1 - e^{2\pi i\sigma}}{2i}\, d\mathsf{E}(\sigma)\,\phi$$

$$\begin{aligned}
\mathsf{E}(\sigma)f &= \int_0^1 \frac{1 - e^{2\pi i\sigma'}}{2i}\, d(\mathsf{E}(\sigma)\mathsf{E}(\sigma')\,\phi) \\
&= \int_0^1 \frac{1 - e^{2\pi i\sigma'}}{2i}\, d(\mathsf{E}(\mathrm{Min}(\sigma,\sigma'))\,\phi) = \int_0^\sigma \frac{1 - e^{2\pi i\sigma'}}{2i}\, d\mathsf{E}(\sigma')\,\phi \\
\|\mathsf{E}(\sigma)f\|^2 = (\mathsf{E}(\sigma)f, f) &= \int_0^\sigma \frac{1 - e^{2\pi i\sigma'}}{2i}\, d(\mathsf{E}(\sigma')\,\phi, f) \\
&= \int_0^\sigma \frac{1 - e^{2\pi i\sigma'}}{2i}\, d\overline{(\mathsf{E}(\sigma')\,f, \phi)} \\
&= \int_0^\sigma \frac{1 - e^{2\pi i\sigma'}}{2i}\, d\Big(\int_0^{\sigma'} \frac{1 - e^{-2\pi i\sigma''}}{-2i}\, d\overline{(\mathsf{E}(\sigma'')\,\phi, \phi)}\Big) \\
&= \int_0^\sigma \frac{1 - e^{2\pi i\sigma'}}{2i}\frac{1 - e^{-2\pi i\sigma'}}{-2i}\, d\overline{(\mathsf{E}(\sigma')\,\phi, \phi)} \\
&= \int_0^\sigma \frac{(1 - e^{2\pi i\sigma'})(1 - e^{-2\pi i\sigma'})}{4}\, d\|\mathsf{E}(\sigma')\phi\|^2 \\
&= \int_0^\sigma \sin^2(\pi\sigma')\, d\|\mathsf{E}(\sigma')\phi\|^2
\end{aligned}$$

Therefore the integral given in $\overline{\mathbf{S}}_3$ is

$$\begin{aligned}
\int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{F}(\lambda)f\|^2 &= \int_0^1 \cot^2(\pi\sigma)\, d\|\mathsf{E}(\sigma)f\|^2 \\
&= \int_0^1 \cot^2(\pi\sigma)\, d\Big(\int_0^\sigma \sin^2(\pi\sigma')\, d\|\mathsf{E}(\sigma')\phi\|^2\Big) \\
&= \int_0^1 \cot^2(\pi\sigma)\sin^2(\pi\sigma')\, d\|\mathsf{E}(\sigma')\phi\|^2 \\
&= \int_0^1 \cos^2(\pi\sigma)\, d\|\mathsf{E}(\sigma)\phi\|^2
\end{aligned}$$

But since this is dominated absolutely by

$$\int_0^1 d\|\mathsf{E}(\sigma)\phi\|^2 = \|\phi\|^2$$

[102] We apply the Stieltjes integral to the elements of $\mathfrak{R}_\infty$ instead of to numbers. All our relations are to be understood to hold if we choose any fixed g from $\mathfrak{R}_\infty$ and form $(\bullet f, g)$, where f can be any element of $\mathfrak{R}_\infty$ and $\bullet$ represents an operator. In contrast to the operator-Stieltjes integrals in **II.7**, this is a half-symbolic process; instead of one g from $\mathfrak{R}_\infty$, there two elements f, g were to be chosen arbitrarily from $\mathfrak{R}_\infty$, and instead of $(\bullet, g)$, there $(\bullet f, g)$ was to be formed.

the result is finite. Furthermore,

$$\begin{aligned}\mathsf{A}f = \frac{\phi + \mathsf{U}\phi}{2} &= \frac{1}{2}\Big(\phi + \int_0^1 e^{2\pi i\sigma} d\mathsf{E}(\sigma)\,\phi\Big) = \int_0^1 \frac{1+e^{2\pi i\sigma}}{2}\, d\mathsf{E}(\sigma)\,\phi \\ &= \int_0^1 i\,\frac{1+e^{2\pi i\sigma}}{1-e^{2\pi i\sigma}}\cdot\frac{1-e^{2\pi i\sigma}}{2i}\, d\mathsf{E}(\sigma)\,\phi \\ &= -\int_0^1 \cot(\pi\sigma)\, d\Big(\int_0^1 \frac{1-e^{2\pi i\sigma'}}{2i}\, d\mathsf{E}(\sigma')\,\phi\Big) \\ &= -\int_0^1 \cot(\pi\sigma)\, d(\mathsf{E}(\sigma)f) \\ &= \int_{-\infty}^{+\infty} \lambda\, d(\mathsf{E}(\sigma)f)\end{aligned}$$

i.e., the final relation $\overline{\mathbf{S}}_3$ also holds. Consequently, A is in any case an extension of that operator which, by $\overline{\mathbf{S}}_3$, belongs to $\mathsf{F}(\lambda)$. But since this is maximal (as we shall show), A must be equal to it.[103]

We now discuss the converse. Let $\mathsf{F}(\lambda)$ belong to A by $\overline{\mathbf{S}}_1$–$\overline{\mathbf{S}}_3$. What about U? We first define $\mathsf{E}(\sigma)$ by $\mathbf{C}$. It therefore satisfies $\overline{\overline{\mathbf{S}}}_1$, $\overline{\overline{\mathbf{S}}}_2$. Let ϕ be arbitrary. We write (again symbolically)

$$\begin{aligned}f = \int_{-\infty}^{+\infty} \frac{1}{\lambda+i}\, d\mathsf{F}(\lambda)\phi &= \int_0^1 \frac{1}{-\cot(\pi\sigma)+i}\, d\mathsf{E}(\sigma)\phi \\ &= \int_0^1 \frac{1-e^{2\pi i\sigma}}{2i}\, d\mathsf{E}(\sigma)\phi\end{aligned}$$

where, since $\frac{1}{\lambda+i}$ or $\frac{1-e^{2\pi i\sigma}}{2i}$ is bounded, all integrals converge. Then

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[103] There is an implied assumption here that there actually exists such an operator for each given resolution of the identity $\mathsf{F}(\lambda)$. That is, for finite

$$\int_{-\infty}^{+\infty} \lambda^2 d\|\mathsf{F}(\lambda)f\|^2$$

it is assumed than an f^* can be found such that for all g

$$(f^*, g) = \int_{-\infty}^{+\infty} \lambda\, d(\mathsf{F}(\lambda)f, g)$$

and also that the f^* with this property is everywhere dense. (The Hermitian character of the operator thus defined follows from $\overline{\mathbf{S}}_3$: We exchange f, g in the final equation and take the complex conjugate.) Both of these propositions are proved in the reference given in Note 78.

$$\begin{aligned}\mathsf{F}(\lambda)f = \mathsf{E}(\sigma)f &= \int_0^1 \frac{1-e^{2\pi i\sigma'}}{2i}\, d(\mathsf{E}(\sigma)\mathsf{E}(\sigma')\phi)\\ &= \int_0^1 \frac{1-e^{2\pi i\sigma'}}{2i}\, d(\mathsf{E}(\mathrm{Min}(\sigma,\sigma'))\phi)\\ &= \int_0^\sigma \frac{1-e^{2\pi i\sigma'}}{2i}\, d\mathsf{E}(\sigma')\phi\end{aligned}$$

$$\begin{aligned}\mathsf{A}f &= \int_{-\infty}^{+\infty} \lambda\, d\mathsf{F}(\lambda)f\\ &= -\int_0^1 \cot(\pi\sigma)\, d\mathsf{E}(\sigma)f\\ &= \int_0^1 i\,\frac{1+e^{2\pi i\sigma}}{1-e^{2\pi i\sigma}}\, d\Big(\int_0^\sigma \frac{1-e^{2\pi i\sigma'}}{2i}\, d\mathsf{E}(\sigma')\phi\Big)\\ &= \int_0^1 i\,\frac{1+e^{2\pi i\sigma}}{1-e^{2\pi i\sigma}}\,\frac{1-e^{2\pi i\sigma}}{2i}\, d\mathsf{E}(\sigma)\phi\\ &= \int_0^1 \frac{1+e^{2\pi i\sigma}}{2}\, d\mathsf{E}(\sigma)\phi\end{aligned}$$

Therefore

$$\mathsf{A}f + if = \int_0^1 d\mathsf{E}(\sigma)\phi = \phi$$

$$\mathsf{A}f - if = \int_0^1 e^{2\pi i\sigma} d\mathsf{E}(\sigma)\phi$$

So $\mathsf{U}\phi$ is defined and is equal to $\int_0^1 e^{2\pi i\sigma} d\mathsf{E}(\sigma)\phi$. Since ϕ was arbitrary, U is defined everywhere. When we form the inner product with any ψ and take the complex conjugate, we see that $\mathsf{U}^*\psi = \int_0^1 e^{-2\pi i\sigma} d\mathsf{E}(\sigma)\psi$. The final calculation of **II.8** then shows that $\mathsf{U}\mathsf{U}^* = \mathsf{U}^*\mathsf{U} = \mathsf{I}$; *i.e.*, U is unitary and belongs to $\mathsf{E}(\sigma)$.

The solvability of the eigenvalue problem of A is then equivalent to the unitary nature of its Cayley transform U, and its uniqueness is established. The only questions remaining are: Can we always form U, and if so, is it unitary? To decide these questions, we begin again with a closed Hermitian operator A.

U was defined as follows: If $\phi = \mathsf{A}f + if$, and only then, $\mathsf{U}\phi$ is defined and is equal to $\mathsf{A}f - if$. But first it must be shown that this definition is admissible in general; *i.e.*, that several f cannot exist for one ϕ. That is, that it follows from $\mathsf{A}f + if = \mathsf{A}g + ig$ that $f = g$ or—because of the linearity of A—that $f = 0$ follows from $\mathsf{A}f + if = 0$.

We have

$$\begin{aligned}\|\mathsf{A}f \pm if\|^2 &= (\mathsf{A}f \pm if, \mathsf{A}f \pm if)\\ &= (\mathsf{A}f, \mathsf{A}f) \pm (if, \mathsf{A}f) \pm (\mathsf{A}f, if) + (if, if)\\ &= \|\mathsf{A}f\|^2 \pm i\,(\mathsf{A}f, f) \mp i\,(\mathsf{A}f, f) + \|f\|^2\\ &= \|\mathsf{A}f\|^2 + \|f\|^2\end{aligned}$$

Hence $\mathsf{A}f + if = 0$ has $\|f\|^2 \leqslant \|\mathsf{A}f + if\|^2 = 0$, $f = 0$ as a consequence, and therefore our mode of definition is justified. Second, $\|\mathsf{A}f - if\| = \|\mathsf{A}f + if\|$; *i.e.*, $\|\mathsf{U}f\| = \|\phi\|$. Therefore U is continuous insofar as it is defined. Furthermore, let $\mathcal{E}$ be the domain of U (the set of all $\mathsf{A}f + if$) and $\mathcal{F}$ the range of U (the set of all $\mathsf{U}\phi$, therefore the set of all $\mathsf{A}f - if$). Since A and U are linear, $\mathcal{E}$ and $\mathcal{F}$ are linear manifolds, but they are also closed. Indeed, let ϕ be a limit point of $\mathcal{E}$ or $\mathcal{F}$ respectively. Then there is a sequence $\phi_1, \phi_2, \ldots$ from $\mathcal{E}$ or $\mathcal{F}$ respectively, with $\phi_n \to \phi$. Hence $\phi_n = \mathsf{A}f_n \pm if_n$. Since the ϕ_n converge they satisfy the Cauchy convergence criterion (see **D** in **II.1**), and because

$$\|f_m - f_n\|^2 \leqslant \|\mathsf{A}(f_m - f_n) \pm i(f_m - f_n)\|^2 = \|\phi_m - \phi_n\|^2$$

the f_n certainly satisfy this condition, and since

$$\begin{aligned}\|\mathsf{A}f_m - \mathsf{A}f_n\|^2 &= \|\mathsf{A}(f_m - f_n)\|^2 \\ &\leqslant \|\mathsf{A}(f_m - f_n) \pm i(f_m - f_n)\|^2 = \|\phi_m - \phi_n\|^2\end{aligned}$$

the $\mathsf{A}f_n$ do also. Therefore the $f_1, f_2, \ldots$ and the $\mathsf{A}f_1, \mathsf{A}f_2, \ldots$ (by **D** in **II.1**) converge: $f_n \to f$, $\mathsf{A}f_n \to f^*$. Since A is closed, $\mathsf{A}f$ is defined and is equal to f^*. Consequently we have

$$\phi_n = \mathsf{A}f_n \pm if_n \to f^* \pm if = \mathsf{A}f \pm if, \qquad \phi_n \to \phi$$

Therefore $\phi = \mathsf{A}f \pm if$; *i.e.*, ϕ also belongs to $\mathcal{E}$ or $\mathcal{F}$, respectively.

Therefore U is defined in the closed linear manifold $\mathcal{E}$, and maps this onto the closed linear manifold $\mathcal{F}$. U is linear, and because

$$\|\mathsf{U}f - \mathsf{U}g\| = \|\mathsf{U}(f - g)\| = \|f - g\|$$

it leaves all distances invariant. We then say that it is isometric. Consequently $\mathsf{U}f \neq \mathsf{U}g$ follows from $f \neq g$; *i.e.*, the mapping is one-to-one. It is also true that $(f, g) = (\mathsf{U}f, \mathsf{U}g)$, which we prove just as the analogous relation was proved in **II.5**. Therefore U leaves all inner products invariant. But U is clearly unitary if and only if $\mathcal{E} = \mathcal{F} = \mathcal{R}_\infty$.

If A, B are two closed Hermitian operators; U, V their Cayley transforms; and $\mathcal{E}$, $\mathcal{F}$ and $\mathcal{G}$, $\mathcal{H}$ their respective domains and ranges, then we see immediately that if B is a proper extension of A then V is also a proper extension of U. Therefore $\mathcal{E}$ is a proper subset of $\mathcal{G}$ and $\mathcal{F}$ a proper subset of $\mathcal{H}$. Consequently, $\mathcal{E} \neq \mathcal{R}_\infty$ and $\mathcal{F} \neq \mathcal{R}_\infty$. Then U is not unitary, and the eigenvalue problem of A is unsolvable. Thus have we proved the theorem repeatedly cited before: If the eigenvalue problem of A is solvable, then there are no proper extensions of A; *i.e.*, A is maximal.

Let us now look again to the closed Hermitian operator A and its $\mathcal{E}$, $\mathcal{F}$, U. If $\mathsf{A}f$ is defined then, for $\mathsf{A}f + if = \phi$, $\mathsf{U}f$ is defined and $\mathsf{A}f - if = \mathsf{U}\phi$; therefore $f = \frac{1}{2i}(\phi - \mathsf{U}\phi)$, $\mathsf{A}f = \frac{1}{2}(\phi + \mathsf{U}\phi)$ and if we set $\psi = \frac{1}{2i}\phi$ we have $f = \psi - \mathsf{U}\psi$, $\mathsf{A}f = i(\psi + \mathsf{U}\psi)$. Conversely, for $f = \psi - \mathsf{U}\psi$, $\mathsf{A}f$ is certainly defined; because,

since $\mathsf{U}\psi$ is defined, $\psi = \mathsf{A}f' + if'$ ($\mathsf{A}f'$ defined!) and $\mathsf{U}\psi = \mathsf{A}f' - if'$ give $f = \psi - \mathsf{U}\psi = 2if'$. The domain of A is then the set of all $\psi - \mathsf{U}\psi$, and for $f = \psi - \mathsf{U}\psi$ we have $\mathsf{A}f = i(\psi + \mathsf{U}\psi)$. Consequently, A is also uniquely determined by U (as also are $\mathcal{E}$, $\mathcal{F}$). Simultaneously we see that the $\psi - \mathsf{U}\psi$ must be everywhere dense (as the domain of A).

Conversely, we start out now from two closed linear manifolds $\mathcal{E}$, $\mathcal{F}$ and a linear isometric mapping U of $\mathcal{E}$ onto $\mathcal{F}$. Is there a Hermitian operator A whose Cayley transform is this U? Since it is necessary that the $\psi - \mathsf{U}\psi$ be everywhere dense, this also will be assumed. The A in question is then uniquely determined by the foregoing, except that the question again presents itself as to whether this definition is possible; whether this A is really Hermitian, and whether U actually is its Cayley transform. The first is quite certainly correct if f determines the ϕ (whenever this in general exists) in $f = \phi - \mathsf{U}\phi$ uniquely; *i.e.*, if $\phi = \psi$ follows from $\phi - \mathsf{U}\phi = \psi - \mathsf{U}\psi$, or $\phi = 0$ from $\phi - \mathsf{U}\phi = 0$. But let us suppose that $\phi - \mathsf{U}\phi = 0$. Then it follows from $g = \psi - \mathsf{U}\psi$ that

$$\begin{aligned}(\phi, g) = &\quad (\phi, \psi) \quad - (\phi, \mathsf{U}\psi) \\ &= (\mathsf{U}\phi, \mathsf{U}\psi) - (\phi, \mathsf{U}\psi) = (\mathsf{U}\phi - \phi, \mathsf{U}\psi) = 0\end{aligned}$$

and since these g are everywhere dense, $\phi = 0$.

Second, we must prove $(\mathsf{A}f, g) = (f, \mathsf{A}g)$; *i.e.*, that $(\mathsf{A}f, g)$ goes over into its complex conjugate upon the exchange of f and g. Let $f = \phi - \mathsf{U}\phi$, $g = \psi - \mathsf{U}\psi$. Then $\mathsf{A}f = i(\phi + \mathsf{U}\phi)$ and

$$\begin{aligned}(\mathsf{A}f, g) &= (i(\phi + \mathsf{U}\phi), \psi - \mathsf{U}\psi) \\ &= i(\phi, \psi) + i(\mathsf{U}\phi, \psi) - i(\phi, \mathsf{U}\psi) - i(\mathsf{U}\phi.\mathsf{U}\psi) \\ &= i\big[(\mathsf{U}\phi, \psi) - \overline{(\mathsf{U}\phi, \psi)}\,\big] \\ &= i(\mathsf{U}\phi, \psi) + \overline{i(\mathsf{U}\phi, \psi)}\end{aligned}$$

which accomplishes what is desired of the exchange $f \leftrightarrow g$ (*i.e.*, of $\phi \leftrightarrow \psi$). The answer to the third question is seen in the following way: Let the Cayley transform of A be called V. Its domain is the set of all

$$\mathsf{A}f + if = i(\phi + \mathsf{U}\phi) + i(\phi - \mathsf{U}\phi) = 2i\phi$$

i.e., the domain of U, and in this domain

$$\mathsf{V}(2i\phi) = \mathsf{V}(\mathsf{A}f + if) = \mathsf{A}f - if = i(\phi + \mathsf{U}\phi) - i(\phi - \mathsf{U}\phi) = 2i\mathsf{U}\phi$$

i.e., $\mathsf{V}\phi = \mathsf{U}\phi$. Therefore $\mathsf{V} = \mathsf{U}$.

The (closed) Hermitian operators therefore correspond to our linear isometric U, with everywhere dense $\phi - \mathsf{U}\phi$, in a one-to-one correspondence, if we associate with each A its Cayley transform U.[104] We can now characterize

[104] In order that the eigenvalue problem of A always be solvable, the unitary character of U (*i.e.*, $\mathcal{E} = \mathcal{F} = \mathfrak{R}_n$ or $\mathfrak{R}_\infty$) must follow from this. This is not

all Hermitian extensions B of A, since all isometric extensions V of U can be found without difficulty (the $\phi - \mathsf{V}\phi$ are automatically everywhere dense since the $\phi - \mathsf{U}\phi$, which are a subset of the former, are everywhere dense). In order that A be maximal, U must be also, and conversely. If U is not maximal. then $\mathcal{E} \neq \mathcal{R}_\infty$, $\mathcal{F} \neq \mathcal{R}_\infty$. These inequalities in turn imply that U is not maximal; indeed, then $\mathcal{R}_\infty - \mathcal{E} \neq 0$, $\mathcal{R}_\infty - \mathcal{F} \neq 0$. We can therefore select a ϕ_0 from $\mathcal{R}_\infty - \mathcal{E}$ and a ψ_0 from $\mathcal{R}_\infty - \mathcal{F}$ with $\phi_0 \neq 0$, $\psi_0 \neq 0$, and if we replace these with

$$\frac{\phi_0}{\|\phi_0\|}, \quad \frac{\psi_0}{\|\psi_0\|}$$

we even have $\|\phi_0\| = \|\psi_0\| = 1$. We now define an operator V in $[\mathcal{E}, \phi_0]$ such that for $f = \phi + a\phi_0$ (ϕ from $\mathcal{E}$, a a complex number) $\mathsf{V}f = \mathsf{U}\phi + a\psi_0$. V is clearly linear. And since ϕ is orthogonal to ϕ_0 and $\mathsf{U}\phi$ to ψ_0 we have

$$\|f\|^2 = \|\phi\|^2 + |a|^2, \qquad \|\mathsf{V}f\|^2 = \|\mathsf{U}\phi\|^2 + |a|^2$$

Therefore $\|\mathsf{V}f\| = \|f\|$ and V is isometric. Finally, V is a proper extension of U. Consequently it is characteristic for the maximal nature of A that $\mathcal{E} = \mathcal{R}_\infty$ or $\mathcal{F} = \mathcal{R}_\infty$.

If, on the other hand, A is not maximal, then the closed linear manifolds $\mathcal{R}_\infty - \mathcal{E}$ and $\mathcal{R}_\infty - \mathcal{F}$ are both non-empty. Let the orthonormal sets spanning them be $\phi_1, \phi_2, \ldots, \phi_p$ and $\psi_1, \psi_2 \ldots, \psi_q$ respectively (see THEOREM 9, **II.2**; here $p = 1, 2, \ldots, \infty$; $q = 1, 2, \ldots, \infty$; the ϕ series does not terminate if $p = \infty$; similarly for the ψ series). Letting $r = \mathrm{Min}(p, q)$, we use the first of the following equations to construct f and the second to define a V in $[\mathcal{E}, \phi_1, \ldots, \phi_r]$:

$$f = \quad \phi + \sum_{\nu=1}^{r} a_\nu \phi_\nu \quad : \quad \phi \text{ from } \mathcal{E}; \;\; a_1, \ldots, a_r \text{ numbers}$$

$$\mathsf{V}f = \mathsf{U}\phi + \sum_{\nu=1}^{r} a_\nu \psi_\nu$$

It can easily be seen that V is linear and isometric, and is moreover a proper extension of U. Its domain is $[\mathcal{E}, \phi_1, \ldots, \phi_r]$, therefore for $r = p$ it is equal to $[\mathcal{E}, \mathcal{R}_\infty - \mathcal{E}] = \mathcal{R}_\infty$; its range is $[\mathcal{F}, \psi_1, \ldots, \psi_r]$, therefore for $r = q$ it is equal to $[\mathcal{F}, \mathcal{R}_\infty - \mathcal{F}] = \mathcal{R}_\infty$. One of the two is certainly equal to $\mathcal{R}_\infty$. Let V be the Cayley transform of the Hermitian operator B. According to the discussion, B is the maximal extension of A. We may observe that the ϕ and ψ can be chosen in an infinite number of ways (for example, we can replace ψ_1 by any $\theta\psi_1$, $|\theta| = 1$), and so also, therefore, can V and B be.

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the case in $\mathcal{R}_\infty$ as we deduced from the existence of non-maximal A. In $\mathcal{R}_n$, on the other hand, this must be the case. This can also be seen directly: since each linear manifold of $\mathcal{R}_n$ is closed, that of the $\phi - \mathsf{U}\phi$ is also, and since it is everywhere dense, it is just $\mathcal{R}_n$ itself. $\mathcal{F}$, the set of the ϕ, has no fewer dimensions than its linear image, the set of the $\phi - \mathsf{U}\phi$; *i.e.*, the maximal dimension number n. This latter must hold also for $\mathcal{F}$ as a linear one-to-one image of $\mathcal{E}$. But for finite n it follows from this that $\mathcal{E} = \mathcal{F} = \mathcal{R}_n$.

Thus has our examination been brought to its conclusion, with the following result: If it is solvable, then it has only one solution, but for non-maximal operators it is certainly not solvable. Non-maximal operators can always be extended in an infinite number of ways to maximal ones (we are discussing Hermitian operators throughout). But the maximality condition is not exactly the same as the solvability condition for the eigenvalue problem. The former is equivalent to $\mathcal{E} = \mathcal{R}_\infty$ *or* $\mathcal{F} = \mathcal{R}_\infty$, the latter to $\mathcal{E} = \mathcal{R}_\infty$ *and* $\mathcal{F} = \mathcal{R}_\infty$.

We do not wish to investigate in any greater detail those operators for which the former but not the latter is the case. These are the operators for which the eigenvalue problem is unsolvable, and since no proper extensions exist (because of maximality) this state of affairs is the final one. These operators are characterized by $\mathcal{E} = \mathcal{R}_\infty$, $\mathcal{F} \neq \mathcal{R}_\infty$ or $\mathcal{E} \neq \mathcal{R}_\infty$, $\mathcal{F} = \mathcal{R}_\infty$. Such operators in fact exist, and they can all be generated from two simple normal forms, so they can be regarded as exceptional cases when compared with the maximal operators with a solvable eigenvalue problem. The reader will find more on this subject in the paper of the author mentioned in Note 95. In any case, such operators must be eliminated for the present from quantum mechanical considerations. The reason for this is that the resolution of the identity belonging to a Hermitian operator enters (as we shall see later) so essentially into all quantum mechanical concepts that we cannot dispense with its existence; *i.e.*, with the solvability of the eigenvalue problem.[105] We shall accordingly admit only such Hermitian operators in general whose eigenvalue problem is solvable. Since this requires a sharpening of maximality, these will be called *hypermaximal* operators.[106]

In conclusion, mention should be made of two classes of (closed) Hermitian operators which are certainly hypermaximal too. First the continuous operators: these are defined everywhere, and are therefore maximal, and since their

[105] Nevertheless, as the author has pointed out (see the reference in Note 78), the following operator is maximal, but not hypermaximal: let $\mathcal{R}_\infty$ be the closed space of all $f(q)$ defined on $0 \leqslant q < +\infty$ with $f(0) = 0$ and finite

$$\int_0^\infty |f(q)|^2 dq$$

and let R be the operator $i\frac{d}{dq}$ which is defined for all continuously differentiable $f(q)$ with finite

$$\int_{-\infty}^{+\infty} |f'(q)|^2 dq$$

and $f(0) = 0$, and which is closed. It is then equal to $-\frac{1}{\hbar}\mathsf{A}'$ if we take the A' in **II.8** for the interval $0, \infty$. This R is now maximal but not hypermaximal. This can be verified by effective calculation of $\mathcal{E}$, $\mathcal{F}$. This is noteworthy because $\mathsf{A}' = \hbar\mathsf{R}$ can be interpreted physically as the momentum operator in the half space bounded on one side by the plane $q = 0$.

[106] This concept originated with Erhard Schmidt. See the reference in Note 78.

eigenvalue problem is solvable according to Hilbert (see the reference in Note 70) they are even hypermaximal. Second, the real operators in any realization of $\mathfrak{R}_\infty$, if they are maximal. The only difference between $\mathcal{E}$ and $\mathcal{F}$ in their definitions was the sign of i which—if everything else is real—can make no difference. Therefore $\mathcal{F} = \mathfrak{R}_\infty$ follows from $\mathcal{E} = \mathfrak{R}_\infty$, and conversely; *i.e.*, the hypermaximality from the maximality. Without assumption of the maximal property, we can in any event say that $\mathfrak{R}_\infty - \mathcal{E}$ and $\mathfrak{R}_\infty - \mathcal{F}$ have equally many dimensions. Therefore (in the terminology employed above in the investigation of the extension relations) $p = q$, therefore $r = p = q$ and

$$[\mathcal{E}, \phi_1, \ldots, \phi_r] = [\mathcal{E}, \mathfrak{R}_\infty - \mathcal{E}\,] = \mathfrak{R}_\infty$$
$$[\mathcal{F}, \phi_1, \ldots, \phi_r] = [\mathcal{F}, \mathfrak{R}_\infty - \mathcal{F}] = \mathfrak{R}_\infty$$

i.e., the extensions obtained at that time were hypermaximal. In any case, real operators possess hypermaximal extensions. In the reference given in Note 95 it is shown that the same holds true for all definite operators.

10. COMMUTATIVE OPERATORS

Two operators R, S commute, by reason of the definition given in **II.4**, if $\mathsf{RS} = \mathsf{SR}$; if the two are not defined everywhere, the domains on either side must coincide. To begin, we restrict ourselves to Hermitian operators, and in order to avoid difficulties with regard to the domains we limit ourselves to those operators which are defined everywhere, hence to continuous operators. Along with R, S we also consider the resolutions of the identity belonging to them: $\mathsf{E}(\lambda)$, $\mathsf{F}(\lambda)$.

The commutativity of R, S means that $(\mathsf{RS}f, g) = (\mathsf{SR}f, g)$ for all f, g; *i.e.*, $(\mathsf{S}f, \mathsf{R}g) = (\mathsf{R}f, \mathsf{S}g)$. Furthermore, the commutativity of R^n, S $(n = 0, 1, 2, \ldots)$ follows from that of R, S, from which the commutativity of $p(\mathsf{R})$, S also follows, where $p(x) = a_0 + a_1 x + \cdots + a_n x^n$.

Now symbolically,

$$\mathsf{R} = \int_{-C}^{+C} \lambda \, d\mathsf{E}(\lambda), \qquad s(\mathsf{R}) = \int_{-C}^{+C} s(\lambda)\, d\mathsf{E}(\lambda)$$

(C is the constant introduced in **II.9** for the continuous operator R, which was called A at that time; $s(x)$ is any function, see Note 94 in **II.8**). For polynomials $s(x)$ we have $(s(\mathsf{R})f, \mathsf{S}g) = (\mathsf{S}f, s(\mathsf{R})g)$, therefore

$$* \qquad \int_{-C}^{+C} s(\lambda) d(\mathsf{E}(\lambda)f, \mathsf{S}g) = \int_{-C}^{+C} s(\lambda) d(\mathsf{S}f, \mathsf{E}(\lambda)\, g)$$

Since we can approximate every continuous function $s(x)$ arbitrarily well by polynomials (uniformly in $-C \leqslant x \leqslant +C$), $*$ also holds for continuous $s(\lambda)$. Now let

$$s(x) = \begin{cases} \lambda_0 - x & \text{for} \quad x \leqslant \lambda_0 \\ 0 & \text{for} \quad x \geqslant \lambda_0 \end{cases}$$

Then ✱ gives

$$\int_{-C}^{\lambda_0}(\lambda_0-\lambda)d(\mathsf{E}(\lambda)f,\mathsf{S}g)=\int_{-C}^{\lambda_0}(\lambda_0-\lambda)d(\mathsf{S}f,\mathsf{E}(\lambda)\,g)$$

If we replace λ_0 by $\lambda_0+\epsilon$ ($\epsilon>0$), then subtraction and division by ϵ gives

$$\int_{-C}^{\lambda_0}d(\mathsf{E}(\lambda)f,\mathsf{S}g)+\int_{\lambda_0}^{\lambda_0+\epsilon}\frac{\lambda-\lambda_0}{\epsilon}\,d(\mathsf{E}(\lambda)f,\mathsf{S}g)$$
$$=\int_{-C}^{\lambda_0}d(\mathsf{S}f,\mathsf{E}(\lambda)\,g)+\int_{\lambda_0}^{\lambda_0+\epsilon}\frac{\lambda-\lambda_0}{\epsilon}\,d(\mathsf{S}f,\mathsf{E}(\lambda)\,g)$$

and as $\epsilon\to 0$ (recall $\overline{\mathbf{S}}_1$!):

$$\int_{-C}^{\lambda_0}d(\mathsf{E}(\lambda)f,\mathsf{S}g)=\int_{-C}^{\lambda_0}d(\mathsf{S}f,\mathsf{E}(\lambda)\,g)$$
$$(\mathsf{E}(\lambda_0)f,\mathsf{S}g)=(\mathsf{S}f,\mathsf{E}(\lambda_0)\,g)$$

Consequently, all $\mathsf{E}(\lambda_0)$, $-C\leqslant\lambda_0\leqslant+C$ commute with S. But this is all the more true for the remaining $\mathsf{E}(\lambda_0)$, since for $\lambda_0<-C$ and $\lambda_0>+C$ we have, respectively, $\mathsf{E}(\lambda_0)=\mathsf{O}$ and $\mathsf{E}(\lambda_0)=\mathsf{I}$.

Therefore, if R commutes with S then all $\mathsf{E}(\lambda_0)$ do likewise. Conversely, if all $\mathsf{E}(\lambda_0)$ commute with S then ✱ holds for each $s(x)$. Consequently all $s(\mathsf{R})$ commute with S. From this we may conclude: first, that R commutes with S if and only if all $\mathsf{E}(\lambda)$ do; and second, that in this case all functions of R [the $s(\mathsf{R})$] also commute with S.

But an $\mathsf{E}(\lambda)$ commutes with S if and only if this holds for $\mathsf{E}(\lambda)$ and all $\mathsf{F}(\mu)$ (we apply our theorem to $\mathsf{S},\mathsf{E}(\lambda)$ instead of R,S). Therefore this is also characteristic for the commutativity of R,S: all $\mathsf{E}(\lambda)$ commute with all $\mathsf{F}(\mu)$. Furthermore, the commutativity of R,S has, from the above, the commutativity of $r(\mathsf{R}),\mathsf{S}$ as a consequence. If we replace R,S by $\mathsf{S},r(\mathsf{R})$ we then obtain the commutativity of $r(\mathsf{R}),s(\mathsf{S})$.

If the Hermitian operators R,S are not subject to a continuity requirement then the situation is more complicated, for the relationship between the domains of RS and SR may then become quite involved. For example, $\mathsf{R}\cdot\mathsf{O}$ is always defined ($\mathsf{O}f=0$, $\mathsf{R}\cdot\mathsf{O}f=\mathsf{R}(\mathsf{O}f)=\mathsf{R}(0)=0$) while, on the other hand, $\mathsf{O}\cdot\mathsf{R}$ is defined only if R is defined (see the comments on this in **II.5**). Therefore for R not defined everywhere, $\mathsf{R}\cdot\mathsf{O}\neq\mathsf{O}\cdot\mathsf{R}$ because of the difference in the domains. That is—taking it literally—R,O do not commute. Such a state of affairs is unsatisfactory for our later purposes: O should commute not only with all continuous Hermitian operators but also even with Hermitian operators that are not continuous.[107] We therefore want to define commutativity for

[107] Since (see **II.5**) $\mathsf{R}\cdot\mathsf{I},\mathsf{I}\cdot\mathsf{R}$ are defined if and only if R is defined, the same holds for $\mathsf{R}\cdot a\mathsf{I}$, $a\mathsf{I}\cdot\mathsf{R}$ ($a\neq 0$). Then these two products are equal; *i.e.*, R and $a\mathsf{I}$ commute. Consequently, the commutativity of R and $a\mathsf{I}$ holds with a single exception: $a=0$, R not defined everywhere. This is unfortunate, and strengthens our motivation to adjust the definition of continuity.

discontinuous R, S in a different way. We limit ourselves to hypermaximal R, S which, by **II.9**, are the only operators of interest to us. Operators R, S will be called commutative in the new sense if all $\mathsf{E}(\lambda)$ commute with all $\mathsf{F}(\mu)$ (where these are again the respective resolutions of the identity) in the old sense. For continuous R and S the new definition is identical to the old, while if either (or both) of R and S is discontinuous it differs. An example of the latter case is provided by R and O: in the old sense they did not commute, but in the new sense they do, since for O each $\mathsf{F}(\mu)$ is either O or I;[108] therefore each $\mathsf{F}(\mu)$ commutes with each of the $\mathsf{E}(\lambda)$.

We have proved above that if R, S are two commutative (continuous) Hermitian operators then each function $r(\mathsf{R})$ of R commutes with each function $s(\mathsf{S})$ of S. Since the hypothesis is always satisfied for $\mathsf{R} = \mathsf{S}$, two functions $r(\mathsf{R}), s(\mathsf{R})$ of the same operator always commute (this also follows from the multiplication formula at the end of **II.8**: $r(\mathsf{R})s(\mathsf{R}) = t(\mathsf{R})$ with $r(x)s(x) = t(x)$). If $r(x), s(x)$ are real, by the way, then $r(\mathsf{R}), s(\mathsf{R})$ are Hermitian (by **II.8**: if $r(x)$ is real then $(r(\mathsf{R}))^* = \bar{r}(\mathsf{R}) = r(\mathsf{R})$).

The converse is also valid. If A, B are two commuting Hermitian operators, then there exists a Hermitian operator R of which both are functions; *i.e.*, $\mathsf{A} = r(\mathsf{R}), \mathsf{B} = s(\mathsf{R})$. Indeed, even more is true: if an arbitrary (finite or infinite) set $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ of commuting Hermitian operators is given, then there exists a Hermitian operator R of which all $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ are functions. We give no proof of this theorem here, and can only refer to the literature on the subject.[109] For our purposes this theorem is of importance only for a finite number of operators $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ with pure discrete spectra. It will be proved for this case in following paragraphs; regarding the general case we can give only a few orienting remarks.

Therefore, let $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ be a finite number of Hermitian operators with pure discrete spectra. If λ is any number, let the closed linear manifold spanned by all the solutions of $\mathsf{A}f = \lambda f$ be called $\mathfrak{L}_\lambda$, and its projection E_λ. Then λ is a discrete eigenvalue of A if and only if solutions $f \neq 0$ exist, hence $\mathfrak{L}_\lambda \neq \mathfrak{O}$; *i.e.*, $\mathsf{E}_\lambda \neq \mathsf{O}$. Correspondingly, we have $\mathfrak{M}_\lambda, \mathsf{F}_\lambda$ for B; $\mathfrak{N}_\lambda, \mathsf{G}_\lambda$ for C; etc. From $\mathsf{A}f = \lambda f$ is follows that $\mathsf{AB}f = \mathsf{BA}f = \mathsf{B}(\lambda f) = \lambda(\mathsf{B}f)$; *i.e.*, along with f, $\mathsf{B}f$ also belongs to $\mathfrak{L}_\lambda$. Since E_λ always belongs to $\mathfrak{L}_\lambda$, $\mathsf{BE}_\lambda f$ does also, therefore

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[108] This resolution of the identity belongs to $a \cdot \mathsf{I}$:

$$\mathsf{F}(\mu) = \begin{cases} \mathsf{I} & \text{for} \quad \mu \geqslant a \\ \mathsf{O} & \text{for} \quad \mu < a \end{cases}$$

This can easily be verified.

[109] For two Hermitian operators A, B which belong to a special class (the so-called totally continuous class; see the reference in Note 70) Toeplitz proved (see the reference in Note 33) a theorem from which the above follows; namely, the existence of a complete orthonormal set from the common eigenfunctions of A, B. The general theorem for arbitrary A, B or $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ has been proved by the author (see Note 94).

$\mathsf{E}_\lambda \mathsf{B}\mathsf{E}_\lambda f = \mathsf{B}\mathsf{E}_\lambda f$. This holds identically: $\mathsf{E}_\lambda \mathsf{B}\mathsf{E}_\lambda = \mathsf{B}\mathsf{E}_\lambda$. Application of $*$ results in $\mathsf{E}_\lambda \mathsf{B}\mathsf{E}_\lambda = \mathsf{E}_\lambda \mathsf{B}$, therefore $\mathsf{E}_\lambda \mathsf{B} = \mathsf{B}\mathsf{E}_\lambda$. In the same way that we just now deduced the commutativity of $\mathsf{B}, \mathsf{E}_\lambda$ from that of A, B, that of $\mathsf{E}_\lambda, \mathsf{F}_\mu$ follows from that of $\mathsf{B}, \mathsf{E}_\lambda$. Since A, B are in no way distinguished from the other $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ we can say that all $\mathsf{E}_\lambda, \mathsf{F}_\mu, \mathsf{G}_\nu, \ldots$ commute with each other. Consequently $\mathsf{K}(\lambda\mu\nu \ldots) = \mathsf{E}_\lambda \mathsf{F}_\mu \mathsf{G}_\nu \cdots$ is a projection. Let its closed linear manifold be called $\mathcal{K}(\lambda\mu\nu \cdots)$. By THEOREM 14 (**II.4**), $\mathcal{K}(\lambda\mu\nu \cdots)$ is the intersection of $\mathfrak{L}_\lambda$, $\mathfrak{M}_\mu$, $\mathfrak{N}_\nu, \ldots$; *i.e.*, the totality of common solutions of

$$\mathsf{A}f = \lambda f, \quad \mathsf{B}f = \mu f, \quad \mathsf{C}f = \nu f, \quad \ldots$$

Let $\lambda, \mu, \nu, \ldots$ and $\lambda', \mu', \nu', \ldots$ be two different sets of numbers; *i.e.*, $\lambda \neq \lambda'$ or $\mu \neq \mu'$ or $\nu \neq \nu'$ or.... If f belongs to $\mathcal{K}(\lambda\mu\nu \ldots)$ and f' to $\mathcal{K}(\lambda'\mu'\nu' \ldots)$ then f, f' are orthogonal. For $\lambda \neq \lambda'$ this is so because $\mathsf{A}f = \lambda f, \mathsf{A}f' = \lambda' f'$; for $\mu \neq \mu'$ because $\mathsf{B}f = \mu f, \mathsf{B}f' = \mu' f'$; .... Consequently the entire $\mathcal{K}(\lambda\mu\nu \ldots)$ is orthogonal to the entire $\mathcal{K}(\lambda'\mu'\nu' \ldots)$.

Since A has a pure discrete spectrum, $\mathfrak{L}_\lambda$ spans the entire $\mathfrak{R}_\infty$ (as a closed linear manifold). An $f \neq 0$ therefore cannot be orthogonal to all $\mathfrak{L}_\lambda$; *i.e.*, for at least one $\mathfrak{L}_\lambda$ the projection of f in $\mathfrak{L}_\lambda$ must be non-zero; *i.e.*, $\mathsf{E}_\lambda f \neq 0$. In the same way, a μ must exist with $\mathsf{F}_\mu f \neq 0$, and moreover a ν with $\mathsf{G}_\nu f \neq 0$, etc. Consequently, for each $f \neq 0$ we can find a λ with $\mathsf{E}_\lambda f \neq 0$, hence a μ with $\mathsf{F}_\mu(\mathsf{E}_\lambda f) \neq 0$, then a ν with $\mathsf{G}_\nu(\mathsf{F}\mu(\mathsf{E}_\lambda f))) \neq 0$, etc. Thus are we led finally to $\cdots \mathsf{G}_\nu \mathsf{F}_\mu \mathsf{E}_\lambda f \neq 0$, $\mathsf{E}_\lambda \mathsf{F}_\mu \mathsf{G}_\nu \cdots f \neq 0$, $\mathsf{K}(\lambda\mu\nu \ldots) f \neq 0$; *i.e.*, f is not orthogonal to $\mathcal{K}(\lambda\mu\nu \ldots)$. Therefore an f orthogonal to all $\mathcal{K}(\lambda\mu\nu \ldots)$ is $= 0$. Consequently, the $\mathcal{K}(\lambda\mu\nu \ldots)$ together span all $\mathfrak{R}_\infty$ as a closed linear manifold.

Now let $\phi^{(1)}_{\lambda\mu\nu\ldots}, \phi^{(2)}_{\lambda\mu\nu\ldots}, \ldots$ be an orthonormal set which spans the linear manifold $\mathcal{K}(\lambda\mu\nu \ldots)$. (This sequence may or may not terminate, depending on whether $\mathcal{K}(\lambda\mu\nu \ldots)$ has a finite or infinite number of dimensions. On the other hand, if $\mathcal{K}(\lambda\mu\nu \ldots) = 0$ then it consists of 0 terms.) Each $\phi^{(n)}_{\lambda\mu\nu\ldots}$ belongs to a $\mathcal{K}(\lambda\mu\nu \ldots)$ and is therefore an eigenfunction of all $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$. Two different such functions are always mutually orthogonal: if they have the same $_{\lambda\mu\nu\ldots}$ indices they are so by reason of their definition, while if they have different $_{\lambda\mu\nu\ldots}$ indices they are so because they belong to different $\mathcal{K}(\lambda\mu\nu \ldots)$. The set of all $\phi^{(n)}_{\lambda\mu\nu\ldots}$ span the same linear manifold as the set of all $\mathcal{K}(\lambda\mu\nu \ldots)$, namely $\mathfrak{R}_\infty$. Consequently the $\phi^{(n)}_{\lambda\mu\nu\ldots}$ form a complete orthonormal set.

We have now produced a complete orthonormal set from the common eigenfunctions of $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$. We now call these $\psi_1, \psi_2, \ldots$ and we write the corresponding eigenvalue equations

$$\mathsf{A}\psi_m = \lambda_m \psi_m, \quad \mathsf{B}\psi_m = \mu_m \psi_m, \quad \mathsf{C}\psi_m = \nu_m \psi_m, \quad \ldots$$

We now take any set of pairwise different numbers $\kappa_1, \kappa_2, \kappa_3, \ldots$ and form a Hermitian operator R with the pure discrete spectrum $\kappa_1, \kappa_2, \kappa_3, \ldots$ and with

the corresponding eigenfunctions $\psi_1, \psi_2, \psi_3, \ldots$:[110]

$$\mathsf{R}\Big(\sum_{m=1}^{\infty} x_m \psi_m\Big) = \sum_{m=1}^{\infty} x_m \kappa_m \psi_m$$

Now let $F(\kappa)$ be a function defined in $-\infty < \kappa < +\infty$ for which $F(\kappa_m) = \lambda_m$ $(m = 1, 2, 3, \ldots)$ (at all other points κ the value of $F(\kappa)$ may be arbitrary). Similarly, let $G(\kappa)$ have the property $G(\kappa_m) = \mu_m$, $H(\kappa)$ have the property $H(\kappa_m) = \nu_m$, etc. We wish to show that

$$\mathsf{A} = F(\mathsf{R}), \quad \mathsf{B} = G(\mathsf{R}), \quad \mathsf{C} = H(\mathsf{R}), \quad \ldots$$

To that end, we must show that if R has a pure discrete spectrum $\kappa_1, \kappa_2, \ldots$ with eigenfunctions $\psi_1, \psi_2, \ldots$ then $F(\mathsf{R})$ has the pure discrete spectrum $F(\kappa_1), F(\kappa_2), \ldots$ with the same eigenfunctions $\psi_1, \psi_2, \ldots$. But since these also form a complete orthonormal set, it suffices to show that $F(\mathsf{R})\psi_m = F(\kappa_m) \cdot \psi_m$.

Let (by **II.8**)

$$\mathsf{E}(\lambda) = \sum_{\kappa_m \leqslant \lambda} \mathsf{P}_{[\psi_m]}$$

be the resolution of the identity belonging to R. Then symbolically

$$\mathsf{R} = \int \lambda \, d\mathsf{E}(\lambda)$$

and by definition

$$F(\mathsf{R}) = \int F(\lambda) \, d\mathsf{E}(\lambda)$$

Furthermore,

$$\mathsf{E}(\lambda)\psi_m = \begin{cases} \psi_m & \text{for} \quad \kappa_m \leqslant \lambda \\ 0 & \text{for} \quad \kappa_m > \lambda \end{cases}$$

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[110] The chosen $\kappa_1, \kappa_2, \kappa_3, \ldots$ are to be bounded (for example, $\kappa_m = \frac{1}{m}$) in order that R be continuous. In fact,

$$\|\mathsf{R}\psi_m\| = \|\kappa_m \psi_m\| = |\kappa_m| \leqslant C \cdot \|\psi_m\|, \qquad |\kappa_m| < C$$

follows immediately from the continuity of R; *i.e.*, from $\|\mathsf{R}f\| \leqslant C \cdot \|f\|$. Conversely, from $|\kappa_m| \leqslant C$ $(m = 1, 2, \ldots)$ it follows that

$$\|\mathsf{R}f\|^2 = \|\mathsf{R}\Big(\sum_{m=1}^{\infty} x_m \psi_m\Big)\|^2 = \|\sum_{m=1}^{\infty} x_m \kappa_m \psi_m\|^2 = \sum_{m=1}^{\infty} |x_m|^2 |\kappa_m|^2$$

$$\|f\|^2 = \|\sum_{m=1}^{\infty} x_m \psi_m\|^2 = \sum_{m=1}^{\infty} |x_m|^2$$

Therefore $\|\mathsf{R}f\|^2 \leqslant C^2 \cdot \|f\|^2$, $\|\mathsf{R}f\| \leqslant C \cdot \|f\|$; *i.e.*, R is continuous.

From this it follows that

$$(F(\mathsf{R})\psi_m, g) = \int F(\lambda)\, d(\mathsf{E}(\lambda)\psi_m, g) = F(\kappa_m)\cdot(\psi_m, g)$$

for all g. Therefore it is actually true that $F(\mathsf{R})\psi_m = F(\kappa_m)\cdot\psi_m$.

With this, the problem is settled for the case of pure discrete spectra, as we asserted previously. In the case of continuous spectra we must be content with the reference of Note 109, and shall discuss here only an especially characteristic case.

Let $\mathfrak{R}_\infty$ be the space of all $f(q_1, q_2)$ with finite $\iint |f(q_1, q_2)|^2 dq_1 dq_2$, and let the unit square $0 \leqslant q_1, q_2 \leqslant 1$ be their domain of variation. We form the operators $\mathsf{A} = q_1\cdot$ and $\mathsf{B} = q_2\cdot$. They are Hermitian for this $\{q_1, q_2\}$-region (but not for $-\infty \leqslant q_1, q_2 \leqslant +\infty$!) and they commute. Therefore both must be functions of an R. Consequently, this R commutes with A, B, from which it follows (although we will not prove this here) that R has the form $s(q_1, q_2)\cdot$ ($s(q_1, q_2)$ a bounded function). Consequently R^n is equal to $s(q_1, q_2)^n\cdot$, and $F(\mathsf{R})$ is equal to $F(s(q_1, q_2))\cdot$ if $F(\kappa)$ is a polynomial. But this formula can be extended to all $F(\kappa)$, which we will again not discuss in detail. It also follows from $F(\mathsf{R}) = \mathsf{A}$, $G(\mathsf{R}) = \mathsf{B}$ that[111]

$$F(s(q_1, q_2)) = q_1, \qquad G(s(q_1, q_2)) = q_2$$

That is, the mappings $s(q_1, q_2) = \kappa$ and $F(\kappa) = q_1$, $G(\kappa) = q_2$ (which are reciprocal to each other) must map the square surface $0 \leqslant q_1, q_2 \leqslant 1$ to the linear number set of the κ uniquely—something which conflicts with ordinary geometric intuition.

But on the basis or our previously discussed proof we know that this must nevertheless be possible—and indeed: a mapping of the desired type is accomplished by means of the so-called Peano curve.[112] The more rigorous treatment of the proof given in Note 109 actually shows that this leads in the present case to the Peano curve or to constructs that are closely related to it.

11. THE TRACE

Several important invariants of operators shall be defined here.

For a matrix $\{a_{\mu\nu}\}$ that acts on $\mathfrak{R}_n$, the *trace* $\sum_{\mu=1}^{n} a_{\mu\mu}$ is one such invariant. It is unitary-invariant; that is, it does not change if we transform the $\{a_{\mu\nu}\}$ to another (cartesian) coordinate system.[113] But if we replace $\{a_{\mu\nu}\}$ by the corresponding operator

$$\mathsf{A}\{x_1, \ldots, x_n\} = \{y_1, \ldots, y_n\} \quad : \quad y_\mu = \sum_{\nu=1}^{n} a_{\mu\nu} x_\nu$$

[111] Exceptions may occur in a $\{q_1, q_2\}$-set of Lebesgue measure 0.

[112] See, for example, the reference in Note 45.

[113] $\{a_{\mu\nu}\}$ refers to the transformation (*i.e.*, to the operator that accomplishes the transformation)

continued on the next page

then the $a_{\mu\nu}$ are expressed as follows, with the help of A:

$$\begin{aligned}\phi_1 &= \{1, 0, \ldots, 0\}\\ \phi_2 &= \{0, 1, \ldots, 0\}\\ &\vdots\\ \phi_n &= \{0, 0, \ldots, 1\}\end{aligned}$$

form a complete orthonormal set, and obviously $a_{\mu\nu} = (\mathsf{A}\phi_\nu, \phi_\mu)$ (see **II.5**, in particular Note 60). The trace is therefore $\sum_{\mu=1}^{n}(\mathsf{A}\phi_\mu, \phi_\mu)$ and its unitary invariance means that its value is the same for each complete orthonormal set.

We can immediately consider the analogy of this concept in $\mathfrak{R}_\infty$. Let A be a linear operator. We take a complete orthonormal set $\phi_1, \phi_2, \ldots$ for which all $\mathsf{A}\phi_n$ are defined (this is certainly possible if the domain of A is everywhere dense; it suffices to orthogonalize a dense sequence $f_1, f_2, \ldots$ in it, by **II.2**, THEOREM 8), and set

$$\operatorname{Tr}\mathsf{A} = \sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\mu)$$

where $\operatorname{Tr}\mathsf{A}$ signifies the trace of A. We must now show that this actually depends on A (and not on the ϕ_μ!).

For this purpose we introduce two complete orthonormal sets, $\phi_1, \phi_2, \ldots$ and $\psi_1, \psi_2, \ldots$, and set

$$\operatorname{Tr}(\mathsf{A}; \phi, \psi) = \sum_{\mu,\nu=1}^{\infty}(\mathsf{A}\phi_\mu, \psi_\nu)(\psi_\nu, \phi_\mu)$$

$$\eta_\mu = \sum_{\nu=1}^{n} a_{\mu\nu}\xi_\nu \quad : \quad \mu = 1, \ldots, n$$

(see the developments in **II.7**). If we transform by

$$\xi_\mu = \sum_{\nu=1}^{n} x_{\nu\mu}\mathfrak{x}_\nu, \quad \eta_\mu = \sum_{\nu=1}^{n} x_{\nu\mu}\mathfrak{y}_\nu \quad : \quad \mu = 1, \ldots, n$$

then we obtain

$$\mathfrak{y}_\nu = \sum_{\nu=1}^{n} \mathfrak{a}_{\mu\nu}\mathfrak{x}_\nu \quad : \quad \mu = 1, \ldots, n$$

with

$$\mathfrak{a}_{\mu\nu} = \sum_{\rho,\sigma=1}^{n} a_{\rho\sigma}\bar{x}_{\mu\rho}x_{\nu\sigma} \quad : \quad \mu, \nu = 1, \ldots, n$$

$\{\mathfrak{a}_{\mu\nu}\}$ is the transformed matrix. Clearly

$$\sum_{\mu=1}^{n}\mathfrak{a}_{\mu\mu} = \sum_{\mu,\rho,\sigma=1}^{n} a_{\rho\sigma}\bar{x}_{\mu\rho}x_{\mu\sigma} = \sum_{\rho,\sigma=1}^{n} a_{\rho\sigma}\Big(\sum_{\mu=1}^{n}\bar{x}_{\mu\rho}x_{\mu\sigma}\Big) = \sum_{\rho=1}^{n} a_{\rho\rho}$$

i.e., the trace is invariant.

From **II.2**, THEOREM 7$\boldsymbol{\gamma}$ it follows that this is equal to $\sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\mu)$, and so depends only apparently on the ψ_ν. Furthermore,

$$\sum_{\mu,\nu=1}^{\infty}(\mathsf{A}\phi_\mu, \psi_\nu)(\psi_\nu, \phi_\mu) = \sum_{\mu,\nu=1}^{\infty}(\phi_\mu, \mathsf{A}^*\psi_\nu)(\psi_\nu, \phi_\mu)$$
$$= \sum_{\mu,\nu=1}^{\infty}\overline{(\mathsf{A}^*\psi_\nu, \phi_\mu)(\phi_\mu, \psi_\nu)}$$

i.e., $\mathrm{Tr}(\mathsf{A}; \phi, \psi) = \overline{\mathrm{Tr}(\mathsf{A}^*; \psi, \phi)}$. Since the right side, according to the above, depends only apparently on the ϕ_μ, the same holds on the left; the dependence of these expressions on ϕ_μ and ψ_ν is therefore only apparent. In reality, therefore, the trace depends only on A. Consequently, we may designate $\mathrm{Tr}(\mathsf{A}; \phi, \psi)$ with $\mathrm{Tr}\,\mathsf{A}$. Since this is equal to $\sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\mu)$, the desired invariance proof has been achieved. But from the last equation it also follows that

$$\mathrm{Tr}\,\mathsf{A} = \overline{\mathrm{Tr}\,\mathsf{A}^*}$$

The relations

$$\mathrm{Tr}\,(a\mathsf{A}) = a\,\mathrm{Tr}\,\mathsf{A}, \qquad \mathrm{Tr}\,(\mathsf{A} \pm \mathsf{B}) = \mathrm{Tr}\,\mathsf{A} \pm \mathrm{Tr}\,\mathsf{B}$$

are obvious. Furthermore

$$\mathrm{Tr}\,(\mathsf{AB}) = \mathrm{Tr}\,(\mathsf{BA})$$

holds, even for non-commuting A, B. This may be shown as follows:

$$\mathrm{Tr}\,(\mathsf{AB}) = \sum_{\mu-1}^{\infty}(\mathsf{AB}\phi_\mu, \phi_\mu) = \sum_{\mu-1}^{\infty}(\mathsf{B}\phi_\mu, \mathsf{A}^*\phi_\mu)$$
$$= \sum_{\mu,\nu=1}^{\infty}(\mathsf{B}\phi_\mu, \psi_\nu)(\psi_\nu, \mathsf{A}^*\phi_\mu) = \sum_{\mu,\nu=1}^{\infty}(\mathsf{B}\phi_\mu, \psi_\nu)(\mathsf{A}\psi_\nu, \phi_\mu)$$

in which $\phi_1, \phi_2, \ldots$ and $\psi_1, \psi_2, \ldots$ can be two arbitrary complete orthonormal sets. The symmetry of this expression under simultaneous interchange of A, B and ϕ, ψ is evident. It follows, moreover, that for Hermitian operators A, B

$$\mathrm{Tr}\,(\mathsf{AB}) = \overline{\mathrm{Tr}\,[(\mathsf{AB})^*]} = \overline{\mathrm{Tr}\,(\mathsf{B}^*\mathsf{A}^*)}$$
$$= \overline{\mathrm{Tr}\,(\mathsf{B\ A}\ )} = \overline{\mathrm{Tr}\,(\mathsf{AB})}$$

Therefore $\mathrm{Tr}\,(\mathsf{AB})$ is real (and $\mathrm{Tr}\,\mathsf{A}$, $\mathrm{Tr}\,\mathsf{B}$ are, of course, real too).

If $\mathcal{M}$ is a closed linear manifold, and E its projection, then $\mathrm{Tr}\,\mathsf{E}$ is determined as follows: Let $\psi_1, \ldots, \psi_k$ be an orthonormal set which spans the closed linear manifold $\mathcal{M}$ and $\chi_1, \ldots, \chi_\ell$ one which spans $\mathcal{R}_\infty - \mathcal{M}$ (of course, one of k or ℓ

—or both—must be infinite). Then $\psi_1, \ldots, \psi_k, \chi_1, \ldots, \chi_\ell$ together span $\mathfrak{R}_\infty$; *i.e.*, they form a complete orthonormal set (THEOREM 7$\boldsymbol{\alpha}$ in **II.2**). Therefore

$$\begin{aligned}\operatorname{Tr}\mathsf{E} &= \sum_{\mu=1}^{k}(\mathsf{E}\psi_\mu, \psi_\mu) + \sum_{\mu=1}^{\ell}(\mathsf{E}\chi_\mu, \chi_\mu) \\ &= \sum_{\mu=1}^{k}(\psi_\mu, \psi_\mu) + \sum_{\mu=1}^{\ell}(0, \chi_\mu) = \sum_{\mu=1}^{k} 1 = k\end{aligned}$$

i.e., $\operatorname{Tr}\mathsf{E}$ is the dimension of $\mathfrak{M}$.

If A is definite then all $(\mathsf{A}\phi_\mu, \phi_\mu) \geqslant 0$, therefore $\operatorname{Tr}\mathsf{A} \geqslant 0$. If in this case $\operatorname{Tr}\mathsf{A} = 0$ then all the $(\mathsf{A}\phi_\mu, \phi_\mu)$ must vanish, therefore $\mathsf{A}\phi_\mu = 0$ (THEOREM 19 in **II.5**). If $\|\phi\| = 1$ then we can find a complete orthonormal set $\phi_1, \phi_2, \ldots$ with $\phi_1 = \phi$. (Indeed, let $f_1, f_2, \ldots$ be everywhere dense. We can then orthogonalize $\phi, f_1, f_2, \ldots$—see the proof of THEOREM 7 in **II.2**—by which means we obtain a complete orthonormal set beginning with ϕ.) Therefore $\mathsf{A}\phi = 0$. If now f is arbitrary, then $\mathsf{A}f = 0$ holds for $f = 0$, while for $f \neq 0$ we recover $\mathsf{A}f = 0$ from the above by writing

$$\phi = \frac{1}{\|f\|} f$$

So $\operatorname{Tr}\mathsf{A} = 0$ would entail $\mathsf{A} = \mathsf{O}$. We conclude that if A is definite, then $\operatorname{Tr}\mathsf{A} > 0$.

In the brevity and simplicity of our observations concerning the trace our treatment has not been mathematically rigorous. For example, we have considered the series

$$\sum_{\mu,\nu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\nu)(\psi_\nu, \phi_\mu) \quad \text{and} \quad \sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\mu)$$

without examining their convergence, and we have transformed one into the other. In short, everything has been done which one should not do when working in correct mathematical fashion. As a matter of fact, this kind of negligence is present elsewhere in theoretical physics, and the present treatment actually will produce no disastrous consequences in our quantum mechanical applications. Nevertheless it must be understood that we have been careless.

It is therefore the more important to point out that in the fundamental statistical assertions of quantum mechanics the trace is employed only for operators of the form AB, where A, B are both definite—and that this concept can be established with complete rigor. In the remainder of this section we shall therefore assemble those facts concerning the trace which are capable of proof with absolute mathematical rigor.

We first consider the trace of $\mathsf{A}^*\mathsf{A}$ (A arbitrary: $\mathsf{A}^*\mathsf{A}$ is Hermitian by **II.4** and, since $(\mathsf{A}^*\mathsf{A}f, f) = (\mathsf{A}f, \mathsf{A}f) \geqslant 0$, it is definite). Then

$$\operatorname{Tr}(\mathsf{A}^*\mathsf{A}) = \sum_{\mu=1}^{\infty}(\mathsf{A}^*\mathsf{A}\phi_\mu, \phi_\mu) = \sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \mathsf{A}\phi_\mu) = \sum_{\mu=1}^{\infty}\|\mathsf{A}\phi_\mu\|^2$$

Since all terms in this series are $\geqslant 0$ it is either convergent or diverges to $+\infty$, and therefore it is in any case defined. We now want to show—independently of the previous discussion—that its sum is independent of the choice of the $\phi_1, \phi_2, \ldots$. In this case, only series with terms $\geqslant 0$ will appear, therefore all will be defined, and all re-summations are permissible.

Let $\phi_1, \phi_2, \ldots$ and $\psi_1, \psi_2, \ldots$ be two complete orthonormal sets. We define

$$\Sigma(\mathsf{A}; \phi_\mu, \psi_\nu) = \sum_{\mu,\nu=1}^{\infty} |(\mathsf{A}\phi_\mu, \psi_\nu)|^2$$

By THEOREM $7\boldsymbol{\gamma}$ in **II.2**, this is equal to

$$\sum_{\mu=1}^{\infty} \|\mathsf{A}\phi_\mu\|^2$$

i.e., $\Sigma(\mathsf{A}; \phi_\mu, \psi_\nu)$ depends only apparently on the ψ_ν. Furthermore (assuming $\mathsf{A}\phi_\mu$ and $\mathsf{A}^*\psi_\nu$ to be defined)

$$\begin{aligned}\Sigma(\mathsf{A}; \phi_\mu, \psi_\nu) = \sum_{\mu,\nu=1}^{\infty} |(\mathsf{A}\phi_\mu, \psi_\nu)|^2 = \sum_{\mu,\nu=1}^{\infty} |(\phi_\mu, \mathsf{A}^*\psi_\nu)|^2 = \sum_{\mu,\nu=1}^{\infty} |(\mathsf{A}^*\psi_\nu, \phi_\mu,)|^2 \\ = \Sigma(\mathsf{A}^*; \psi_\nu, \phi_\mu)\end{aligned}$$

Therefore the dependence on the ϕ_μ is also only apparent, because this is the case on the right side of the formula. Consequently, $\Sigma(\mathsf{A}; \phi_\mu, \psi_\nu)$ depends in general only on A. We then call it simply $\Sigma(\mathsf{A})$. By the above proofs

$$\Sigma(\mathsf{A}) = \sum_{\mu=1}^{\infty} \|\mathsf{A}\phi_\mu\|^2 = \sum_{\mu,\nu=1}^{\infty} |(\mathsf{A}\phi_\mu, \psi_\nu)|^2$$

and $\Sigma(\mathsf{A}) = \Sigma(\mathsf{A}^*)$. Therefore $\mathrm{Tr}(\mathsf{A}^*\mathsf{A})$ is correctly re-defined as $\Sigma(\mathsf{A})$.

We now prove independently several properties of $\Sigma(\mathsf{A})$ which also follow from general properties of $\mathrm{Tr}\,\mathsf{A}$ as previously defined.

From the definition it follows in general that $\Sigma(\mathsf{A}) \geqslant 0$ and that for $\Sigma(\mathsf{A}) = 0$ all $\mathsf{A}\phi_\mu$ must vanish, from which it follows as before that $\mathsf{A} = \mathsf{O}$. That is, if $\mathsf{A} \neq \mathsf{O}$ then $\Sigma(\mathsf{A}) > 0$.

Obviously $\Sigma(a\mathsf{A}) = |a|^2\Sigma(\mathsf{A})$. If $\mathsf{A}^*\mathsf{B} = \mathsf{O}$ then

$$\begin{aligned}\|(\mathsf{A}+\mathsf{B})\phi_\mu\|^2 - \|\mathsf{A}\phi_\mu\|^2 - \|\mathsf{B}\phi_\mu\|^2 &= (\mathsf{A}\phi_\mu, \mathsf{B}\phi_\mu) + (\mathsf{B}\phi_\mu, \mathsf{A}\phi_\mu) \\ &= 2\mathrm{Re}(\mathsf{A}\phi_\mu, \mathsf{B}\phi_\mu) \\ &= 2\mathrm{Re}(\phi_\mu, \mathsf{A}^*\mathsf{B}\phi_\mu) = 0\end{aligned}$$

so, after summation $\sum_{\mu=1}^{\infty}$,

$$\Sigma(\mathsf{A}+\mathsf{B}) = \Sigma(\mathsf{A}) + \Sigma(\mathsf{B})$$

This relation does not change if we interchange A, B. Therefore it is also valid for $\mathsf{B}^*\mathsf{A} = \mathsf{O}$. Furthermore, we can replace A, B in it by $\mathsf{A}^*, \mathsf{B}^*$. Then $\mathsf{B}\mathsf{A}^* = \mathsf{O}$ or $\mathsf{A}\mathsf{B}^* = \mathsf{O}$ are likewise sufficient. For Hermitian A (or B) we can therefore write $\mathsf{B}\mathsf{A} = \mathsf{O}$ (or $\mathsf{A}\mathsf{B} = \mathsf{O}$).

If E projects onto the closed linear manifold $\mathfrak{M}$ then, for the $\psi_1, \ldots, \psi_k$, $\chi_1, \ldots, \chi_\ell$ considered in the determination of $\operatorname{Tr}\mathsf{E}$, we have

$$\Sigma(\mathsf{E}) = \sum_{\mu=1}^{k} \|\mathsf{E}\psi_\mu\|^2 + \sum_{\mu=1}^{\ell} \|\mathsf{E}\chi_\mu\|^2 = \sum_{\mu=1}^{k} \|\psi_\mu\|^2 + \sum_{\mu=1}^{\ell} \|0\|^2$$
$$= \sum_{\mu=1}^{k} 1 + 0 = k$$

So $\Sigma(\mathsf{E})$ also is the dimension of $\mathfrak{M}$ (which, because $\mathsf{E}^*\mathsf{E} = \mathsf{E}\mathsf{E}^* = \mathsf{E}$, is just what one would expect).

For two definite (Hermitian) operators A, B our $\operatorname{Tr}\mathsf{A}\mathsf{B}$ is now reducible to Σ. That is, there are two operators A', B' of the same category with $\mathsf{A}'^2 = \mathsf{A}$, $\mathsf{B}'^2 = \mathsf{B}$[114]—we call them $\sqrt{\mathsf{A}}, \sqrt{\mathsf{B}}$. We have the formal relations

[114] The precise proposition runs as follows: If A is hypermaximal and definite, then there exists one and only one operator A' of the same category with $\mathsf{A}'^2 = \mathsf{A}$. We prove the existence. Let $\mathsf{A} = \int_{-\infty}^{+\infty} \lambda\, d\mathsf{E}(\lambda)$ be the eigenvalue representation of A. Since A is definite, then $\mathsf{E}(\lambda)$ is constant for $\lambda < 0$ (and therefore equals 0 by $\overline{\mathbf{S}}_1$). For otherwise, $\mathsf{E}(\lambda_2) - \mathsf{E}(\lambda_1) \neq \mathsf{O}$ for suitable $\lambda_1 < \lambda_2 < 0$. Therefore an f can be chosen with $[\mathsf{E}(\lambda_2) - \mathsf{E}(\lambda_1)]f = f$. But it follows from this, as we have deduced several times previously, that

$$\mathsf{E}(\lambda) = \begin{cases} f & \text{for} \quad \lambda \geqslant \lambda_2 \\ 0 & \text{for} \quad \lambda \leqslant \lambda_1 \end{cases}$$

Therefore

$$(\mathsf{A}f, f) = \int_{-\infty}^{+\infty} \lambda\, d(\mathsf{E}(\lambda)f, f) = \int_{\lambda_1}^{\lambda_2} \lambda\, d(\mathsf{E}(\lambda)f, f)$$
$$\leqslant \int_{\lambda_1}^{\lambda_2} \lambda_2\, d(\mathsf{E}(\lambda)f, f)$$
$$= \lambda_2([\mathsf{E}(\lambda_2) - \mathsf{E}(\lambda_1)]f, f) = \lambda_2(f, f) < 0$$

Consequently

$$\mathsf{A} = \int_{-\infty}^{+\infty} \lambda\, d\mathsf{E}(\lambda) = \int_{0}^{+\infty} \lambda\, d\mathsf{E}(\lambda) = \int_{0}^{+\infty} \mu^2\, d\mathsf{E}(\mu^2)$$

and $\mathsf{A}' = \int_0^{+\infty} \mu\, d\mathsf{E}(\mu^2)$ yields the desired result. We may observe that we have deduced from the property of definiteness that $\mathsf{E}(\lambda) = \mathsf{O}$ for $\lambda < 0$, and since definiteness clearly follows from this, the fact that the entire spectrum is $\geqslant 0$ is characteristic for definiteness.

$$\begin{aligned}\mathrm{Tr}(\mathsf{AB}) &= \mathrm{Tr}(\sqrt{\mathsf{A}}\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}\cdot\sqrt{\mathsf{B}}) = \mathrm{Tr}(\sqrt{\mathsf{B}}\cdot\sqrt{\mathsf{A}}\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}) \\ &= \mathrm{Tr}((\sqrt{\mathsf{A}}\sqrt{\mathsf{B}})^*(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}})) \\ &= \Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}})\end{aligned}$$

This $\Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}})$, by reason of its own definition and without consideration of its relation to the trace, has all the properties one expects of $\mathrm{Tr}\,\mathsf{AB}$, namely:

$$\begin{aligned}\Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}) &= \Sigma(\sqrt{\mathsf{B}}\sqrt{\mathsf{A}}) \\ \Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}+\mathsf{C}}) &= \Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}) + \Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{C}}) \\ \Sigma(\sqrt{\mathsf{A}+\mathsf{B}}\sqrt{\mathsf{C}}) &= \Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{C}}) + \Sigma(\sqrt{\mathsf{B}}\sqrt{\mathsf{C}})\end{aligned}$$

The first follows from the fact that $\Sigma(\mathsf{XY})$ is symmetric in X, Y:

$$\Sigma(\mathsf{XY}) = \sum_{\mu,\nu=1}^{\infty} |(\mathsf{XY}\phi_\mu, \psi_\nu)|^2 = \sum_{\mu,\nu=1}^{\infty} |(\mathsf{Y}\phi_\mu, \mathsf{X}\psi_\nu)|^2$$

The second follows from the third by reason of the first property. Therefore this third property is the only one which need be proved; *i.e.*, that $\Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}})$ is additive in A. But this can be seen if we write $\Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}})$ as

$$\begin{aligned}\Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}) &= \sum_{\mu=1}^{\infty} \|\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}\,\phi_\mu\|^2 = \sum_{\mu=1}^{\infty} (\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}\,\phi_\mu, \sqrt{\mathsf{A}}\sqrt{\mathsf{B}}\,\phi_\mu) \\ &= \sum_{\mu=1}^{\infty} (\sqrt{\mathsf{A}}\cdot\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}\,\phi_\mu, \sqrt{\mathsf{B}}\,\phi_\mu) = \sum_{\mu=1}^{\infty} (\mathsf{A}\sqrt{\mathsf{B}}\,\phi_\mu, \sqrt{\mathsf{B}}\,\phi_\mu)\end{aligned}$$

In this way, we have established a rigorous foundation for the concept of trace to the extent which was desired.

In addition, the last formula permits the following conclusion: it A, B are definite then $\mathsf{AB} = \mathsf{O}$ is a consequence of $\mathrm{Tr}\,\mathsf{AB} = 0$. For the latter implies that $\Sigma(\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}) = 0$ and therefore that $\sqrt{\mathsf{A}}\sqrt{\mathsf{B}} = \mathsf{O}$ (see the discussion on page 114 and also the considerations given above with regard to Σ). Therefore

$$\mathsf{AB} = \sqrt{\mathsf{A}}\cdot\sqrt{\mathsf{A}}\sqrt{\mathsf{B}}\cdot\sqrt{\mathsf{B}} = \mathsf{O}$$

For a definite Hermitian operator A the calculation with the trace is correct even in its original form. Indeed, let $\phi_1, \phi_2, \ldots$ be a complete orthonormal set. Then

$$\sum_{\mu=1}^{\infty} (\mathsf{A}\phi_\mu, \phi_\mu)$$

(the sum which should define the trace) is a sum with all terms non-negative, and is therefore either convergent or divergent to $+\infty$. Two cases are then possible: either the sum is infinite for each choice of $\phi_1, \phi_2, \ldots$, and therefore

the trace is actually defined independently of $\phi_1, \phi_2, \ldots$ and equals $+\infty$, or the sum is finite for at least one choice of $\phi_1, \phi_2, \ldots$; say $\overline{\phi}_1, \overline{\phi}_2, \ldots$. Then—since

$$\Big(\sum_{\mu=1}^{\infty}(\mathsf{A}\overline{\phi}_\mu, \overline{\phi}_\mu)\Big)^2 = \sum_{\mu,\nu=1}^{\infty}(\mathsf{A}\overline{\phi}_\mu, \overline{\phi}_\mu)(\mathsf{A}\overline{\phi}_\nu, \overline{\phi}_\nu) \geqslant \sum_{\mu,\nu=1}^{\infty}|(\mathsf{A}\overline{\phi}_\mu, \overline{\phi}_\nu)|^2 = \Sigma(\mathsf{A})$$

—$\Sigma(\mathsf{A})$ is also finite, and is equal to some C^2. If $\psi_1, \psi_2, \ldots$ is any complete orthonormal set, then

$$\Sigma(\mathsf{A}) = \sum_{\mu=1}^{\infty}\|\mathsf{A}\psi_\mu\|^2 = C^2, \quad \|\mathsf{A}\psi_1\|^2 \leqslant C^2, \quad \|\mathsf{A}\psi_1\| \leqslant C$$

Since each ψ with $\|\psi\| = 1$ can be chosen as the ψ_1 of such a system, it follows from $\|\psi\| = 1$ that $\|\mathsf{A}\psi\| \leqslant C$. In general then, $\|\mathsf{A}f\| \leqslant C \cdot \|f\|$: for $f = 0$ this is obvious, while for $f \neq 0$ it suffices to set $\psi = \frac{1}{\|f\|}\cdot f$. Consequently A satisfies the condition **Co** from **II.9**. It is therefore a continuous operator. But actually even more is true.

Because of the finite nature of $\Sigma(\mathsf{A})$, A belongs to the class of so-called *totally continuous* operators. Hilbert showed that the eigenvalue problem for such an operator is solvable in the original form; *i.e.*, that a complete orthogonal set $\psi_1, \psi_2, \ldots$ with $\mathsf{A}\psi_\mu = \lambda_\mu\psi_\mu$ exists (and for $\mu \to \infty$, $\lambda_\mu \to 0$).[115] Because

[115] See the reference in Note 64. A direct proof runs as follows: Let

$$\lambda_0 < \lambda_1 < \cdots < \lambda_n \quad : \quad \begin{cases} \text{all} \leqslant -\epsilon \text{ or} \geqslant +\epsilon \\ \mathsf{E}(\lambda_0) \neq \mathsf{E}(\lambda_1) \neq \cdots \neq \mathsf{E}(\lambda_n) \end{cases}$$

Then $\mathsf{E}(\lambda_\nu) - \mathsf{E}(\lambda_{\nu-1}) \neq 0$, therefore $\phi_\nu \neq 0$ can be chosen with

$$[\mathsf{E}(\lambda_\nu) - \mathsf{E}(\lambda_{\nu-1})]\phi_\nu = \phi_\nu$$

It follows from this that

$$\mathsf{E}(\lambda)\phi = \begin{cases} \phi_\nu & \text{for} \quad \lambda \geqslant \lambda_\nu \\ 0 & \text{for} \quad \lambda \leqslant \lambda_{\nu-1} \end{cases}$$

and we can even make $\|\phi_\nu\| = 1$. It follows from the above that $(\phi_\mu, \phi_\nu) = 0$ for $\mu \neq \nu$. The $\phi_1, \ldots \phi_n$ consequently form an orthogonal set, and we can extend it to a complete one: $\phi_1, \ldots \phi_n, \phi_{n+1}, \ldots$. We have $(\nu = 1, \ldots, n)$

$$\begin{aligned} \|\mathsf{A}\phi_\nu\|^2 = \int_{-\infty}^{+\infty}\lambda^2 d\|\mathsf{E}(\lambda)\phi_\nu\|^2 &= \int_{\lambda_{\nu-1}}^{\lambda_\nu}\lambda^2 d\|\mathsf{E}(\lambda)\phi_\nu\|^2 \\ &\geqslant \int_{\lambda_{\nu-1}}^{\lambda_\nu}\epsilon^2\, d\|\mathsf{E}(\lambda)\phi_\nu\|^2 \\ &= \epsilon^2\Big(\|\mathsf{E}(\lambda_\nu)\phi_\nu\|^2 - \|\mathsf{E}(\lambda_\nu)\phi_{\nu-1}\|^2\Big) \\ &= \epsilon^2\|\phi_\nu\|^2 = \epsilon^2 \end{aligned}$$

the operator is definite, $\lambda_\mu = (\mathsf{A}\psi_\mu, \psi_\mu) \geqslant 0$, and furthermore

$$\sum_{\mu=1}^{\infty} \lambda_\mu^2 = \sum_{\mu=1}^{\infty} \|\mathsf{A}\psi_\mu\|^2 = \Sigma(\mathsf{A}) = C^2$$

If $\phi_1, \phi_2, \ldots$ is any complete orthonormal set then

$$\begin{aligned}\sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\mu) &= \sum_{\mu=1}^{\infty}\Big(\sum_{\nu=1}^{\infty}(\mathsf{A}\phi_\mu, \psi_\nu)(\psi_\nu, \phi_\mu)\Big) \\ &= \sum_{\mu=1}^{\infty}\Big(\sum_{\nu=1}^{\infty}(\phi_\mu, \mathsf{A}\psi_\nu)(\psi_\nu, \phi_\mu)\Big) \\ &= \sum_{\mu=1}^{\infty}\Big(\sum_{\nu=1}^{\infty}\lambda_\nu(\phi_\mu, \psi_\nu)(\psi_\nu, \phi_\mu)\Big) = \sum_{\mu=1}^{\infty}\Big(\sum_{\nu=1}^{\infty}\lambda_\nu|(\phi_\mu, \psi_\nu)|^2\Big)\end{aligned}$$

Since all terms are $\geqslant 0$ we may rearrange the summations:

$$\begin{aligned}\sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\mu) = \sum_{\mu,\nu=1}^{\infty}\lambda_\nu|(\phi_\mu, \psi_\nu)|^2 &= \sum_{\nu=1}^{\infty}\lambda_\nu\Big(\sum_{\mu=1}^{\infty}|(\phi_\mu, \psi_\nu)|^2\Big) \\ &= \sum_{\nu=1}^{\infty}\lambda_\nu\|\phi_\nu\|^2 = \sum_{\nu=1}^{\infty}\lambda_\nu\end{aligned}$$

In this case, therefore, $\sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu, \phi_\mu)$ is again independent of $\phi_1, \phi_2, \ldots$, and is actually equal to the sum of the eigenvalues. Since the sum is finite for $\overline{\phi}_1, \overline{\phi}_2, \ldots$ it is therefore always finite. That is, $\mathrm{Tr}\,\mathsf{A}$ is again unique, but this time it is finite. Calculation with the trace is therefore justified in both cases.

We now give several estimates relative to $\mathrm{Tr}\,\mathsf{A}$ and $\Sigma(\mathsf{A})$. For all A with finite $\Sigma(\mathsf{A})$, $\|\mathsf{A}f\| \leqslant \sqrt{\Sigma(\mathsf{A})}\|f\|$; for all definite (Hermitian) A with finite $\mathrm{Tr}\,\mathsf{A}$, $\|\mathsf{A}f\| \leqslant \mathrm{Tr}\,\mathsf{A} \cdot \|f\|$. Now let A again be definite, with $\mathrm{Tr}\,\mathsf{A} = 1$. For an appropriate ϕ with $\|\phi\| = 1$, $\|\mathsf{A}\phi\| \geqslant 1 - \epsilon$ or $(\mathsf{A}\phi, \phi) \geqslant 1 - \epsilon$. It suffices to consider the second case, since the first follows from the second because $(\mathsf{A}\phi, \phi) \leqslant \|\mathsf{A}\phi\| \cdot \|\phi\| = \|\mathsf{A}\phi\|$ (put $(1-\epsilon)^2 \geqslant 1 - 2\epsilon$ in place of $1 - \epsilon$, therefore 2ϵ in place of ϵ).

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and therefore

$$\sum_{\mu=1}^{\infty}\|\mathsf{A}\phi_\mu\|^2 \begin{cases} \geqslant \sum_{\mu=1}^{n}\|\mathsf{A}\phi_\mu\|^2 \geqslant n\epsilon^2 \\ = \Sigma(\mathsf{A}) = C^2 \end{cases}$$

i.e., $n \leqslant C^2/\epsilon^2$. Then, for $|\lambda| \geqslant \epsilon$, $\mathsf{E}(\lambda)$ can in general assume only $\leqslant 2 \cdot C^2/\epsilon^2$ many different values. It can therefore change only in a finite number of places, the remainder being made up of constancy intervals. That is, for $|\lambda| \geqslant \epsilon$ only a discrete spectrum exists. Since this holds for all $\epsilon > 0$, only a pure discrete spectrum is present in general.

Let ψ be orthogonal to ϕ, $\|\psi\| = 1$. Then we can find a complete orthonormal set $\chi_1, \chi_2, \chi_3 \ldots$ with $\chi_1 = \phi$, $\chi_2 = \psi$. Therefore

$$\sum_{\mu=1}^{\infty} \|\mathsf{A}\chi_\mu\|^2 \begin{cases} = \Sigma(\mathsf{A}) \leqslant [\operatorname{Tr}\mathsf{A}]^2 = 1 \\ \\ \geqslant \|\mathsf{A}\phi\|^2 + \|\mathsf{A}\psi\|^2 \geqslant 1 - 2\epsilon + \|\mathsf{A}\psi\|^2 \end{cases}$$

$$\|\mathsf{A}\psi\|^2 \leqslant 2\epsilon, \qquad |\mathsf{A}\psi\| \leqslant \sqrt{2\epsilon}$$

For an arbitrary f orthogonal to ϕ it follows that $\|\mathsf{A}f\| \leqslant \sqrt{2\epsilon}\,\|f\|$. (For $f = 0$ this is obvious. Otherwise, $\psi = \frac{1}{\|f\|} \cdot f$.) If we now remember that $(\mathsf{A}f, g) = (f, \mathsf{A}g)$ then we obtain $|(\mathsf{A}f, g)| \leqslant \sqrt{2\epsilon}\|f\| \cdot \|g\|$ if either f or g is orthogonal to ϕ.

Now let f, g be arbitrary, and write

$$f = \alpha\phi + f', \qquad g = \beta\phi + g'$$

where f', g' are orthogonal to ϕ and $\alpha = (f, \phi),\ \beta = (g, \phi)$. Then

$$(\mathsf{A}f, g) = \alpha\bar{\beta}(\mathsf{A}\phi, \phi) + \alpha(\mathsf{A}\phi, g') + \bar{\beta}(\mathsf{A}f', \phi) + (\mathsf{A}f', g')$$

Therefore, if we set $(\mathsf{A}\phi, \phi) = c$,

$$|(\mathsf{A}f, g) - c\alpha\bar{\beta}| \leqslant |\alpha| \cdot |(\mathsf{A}\phi, g')| + |\beta| \cdot |(\mathsf{A}f', \phi)| + |(\mathsf{A}f', g')|$$

and according to the above estimates

$$\begin{aligned} |(\mathsf{A}f, g) - c\alpha\bar{\beta}| &\leqslant \sqrt{2\epsilon} \cdot \big\{ |\alpha| \cdot \|g'\| + |\beta| \cdot \|f'\| + \|f'\| \cdot \|g'\| \big\} \\ &\leqslant \sqrt{2\epsilon} \cdot \big(|\alpha| + \|f'\| \big) \big(|\beta| + \|g'\| \big) \\ &\leqslant 2\sqrt{2\epsilon} \cdot \sqrt{|\alpha|^2 + \|f'\|^2} \sqrt{|\beta|^2 + \|g'\|^2} \\ &= 2\sqrt{2\epsilon} \cdot \|f\| \cdot \|g\| \end{aligned}$$

On the other hand,

$$(\mathsf{A}f, g) - c\alpha\bar{\beta} = (\mathsf{A}f, g) - c(f, \phi)(\phi, g) = ((\mathsf{A} - c\mathsf{P}_{[\phi]})f, g)$$

In general, then, $|((\mathsf{A} - c\mathsf{P}_{[\phi]})f, g)| \leqslant 2\sqrt{2\epsilon} \cdot \|f\| \cdot \|g\|$. Therefore, as we know from **II.9**,

$$\|((\mathsf{A} - c\mathsf{P}_{[\phi]})f\| \leqslant 2\sqrt{2\epsilon} \cdot \|f\|$$

For $f = \phi$ this implies that

$$\|\mathsf{A}\phi - c\phi\| \leqslant \sqrt{2\epsilon}$$

$$c = \|c\phi\| \begin{cases} \leqslant \quad \|\mathsf{A}\phi - c\phi\| + \|\mathsf{A}\phi\| \leqslant \quad 2\sqrt{2\epsilon} + \ 1 \\ \\ \geqslant -\|\mathsf{A}\phi - c\phi\| + \|\mathsf{A}\phi\| \geqslant -2\sqrt{2\epsilon} + (1 - \epsilon) \end{cases}$$

$$1 - (\epsilon + 2\sqrt{2\epsilon}) \leqslant c \leqslant 1 + 2\sqrt{2\epsilon} \quad : \quad (c \text{ is real and } \geqslant 0)$$

Consequently

$$\begin{aligned}\|((\mathsf{A}-\mathsf{P}_{[\phi]})f\| &\leqslant \|((\mathsf{A}-c\mathsf{P}_{[\phi]})f\| + \|(c-1)\mathsf{P}_{[\phi]}f\| \\ &\leqslant 2\sqrt{2\epsilon}\cdot\|f\| + \big(\epsilon+2\sqrt{2\epsilon}\,\big)\|\mathsf{P}_{[\phi]}f\| \\ &\leqslant \big(\epsilon+4\sqrt{2\epsilon}\,\big)\cdot\|f\|\end{aligned}$$

For $\epsilon\to 0$ therefore A converges uniformly to $\mathsf{P}_{[\phi]}$.

In conclusion, let us consider $\mathrm{Tr}\,\mathsf{A}$ and $\mathrm{Tr}\,\mathsf{B}$ in the realizations F_Z and F_Ω of $\mathfrak{R}_\infty$ (see **I.4** and **II.3**), since physical applications occur in these cases.

In F_Z (set of all $x_1, x_2, \ldots$ with finite $\sum_{\nu=1}^{\infty}|x_\nu|^2$) A may be described by a matrix$\{a_{\mu\nu}\}$:

$$\mathsf{A}\{x_1,\ldots,x_n\} = \{y_1,\ldots,y_n\} \quad : \quad y_\mu = \sum_{\nu=1}^{\infty} a_{\mu\nu}x_\nu$$

In terms of the complete orthonormal set

$$\phi_1 = \{1,0,0,\ldots\},\quad \phi_2 = \{0,1,0,\ldots\},\quad \ldots$$

we have $\mathsf{A}\phi_\mu = \{a_{1\mu}, a_{2\mu},\ldots\} = \sum_{\rho=1}^{\infty} a_{\rho\mu}\phi_\rho$. Therefore $(\mathsf{A}\phi_\mu,\phi_\mu) = a_{\mu\mu}$ and $\|\mathsf{A}\phi_\mu\|^2 = \sum_{\rho=1}^{\infty}|a_{\rho\mu}|^2$. From this it follows immediately that

$$\mathrm{Tr}\,\mathsf{A} = \sum_{\mu=1}^{\infty} a_{\mu\mu}, \qquad \Sigma(\mathsf{A}) = \sum_{\mu,\nu=1}^{\infty}|a_{\mu\nu}|^2$$

In F_Ω (set of all $f(\mathsf{P})$ defined in Ω with finite $\int_\Omega |f(\mathsf{P})|^2 dv$) let us consider only the integral operators

$$\mathsf{A}f(\mathsf{P}) = \int_\Omega a(\mathsf{P},\mathsf{P}')f(\mathsf{P}')dv'$$

where $a(\mathsf{P},\mathsf{P}')$ is a two-variable function defined in Ω, the "kernel" of A (see **I.4**). Let $\phi_1(\mathsf{P}), \phi_2(\mathsf{P},\ldots$ be any complete orthonormal set; then

$$\mathrm{Tr}\,\mathsf{A} = \sum_{\mu=1}^{\infty}(\mathsf{A}\phi_\mu(\mathsf{P}),\phi_\mu(\mathsf{P})) = \sum_{\mu=1}^{\infty}\int_\Omega\Big[\int_\Omega a(\mathsf{P},\mathsf{P}')f(\mathsf{P}')dv'\Big]\overline{\phi_\mu(\mathsf{P})}\,dv$$

and because in general (THEOREM $7\boldsymbol{\beta}$ in **II.2**, applied to $\overline{g(\mathsf{P})}$)

$$\sum_{\mu=1}^{\infty}\Big(\int_\Omega \overline{g(\mathsf{P}')}\;\overline{\phi_\mu(\mathsf{P}')}\,dv'\Big)\phi_\mu(\mathsf{P}) = \overline{g(\mathsf{P})}$$

$$\sum_{\mu=1}^{\infty}\Big(\int_\Omega g(\mathsf{P}')\;\phi_\mu(\mathsf{P}')\,dv'\Big)\overline{\phi_\mu(\mathsf{P})} = g(\mathsf{P})$$

hold, we have

$$\mathrm{Tr}\,\mathsf{A} = \int_\Omega a(\mathsf{P},\mathsf{P})\,dv$$

Furthermore

$$\Sigma(\mathsf{A}) = \sum_{\mu=1}^{\infty} \int_\Omega \Big| \int_\Omega a(\mathsf{P},\mathsf{P}')\phi_\mu(\mathsf{P}')\,dv' \Big|^2 dv$$

and therefore—because [THEOREM $7\boldsymbol{\gamma}$ in **II.2**]

$$\begin{aligned}\sum_{\mu=1}^{\infty} \Big| \int_\Omega g(\mathsf{P}')\phi_\mu(\mathsf{P}')dv' \Big|^2 &= \sum_{\mu=1}^{\infty} \Big| \int_\Omega \overline{g(\mathsf{P}')}\ \overline{\phi_\mu(\mathsf{P}')}dv' \Big|^2 \\ &= \int_\Omega |\overline{g(\mathsf{P}')}|^2 dv' \\ &= \int_\Omega |g(\mathsf{P}')|^2 dv'\end{aligned}$$

—it is also true that

$$\Sigma(\mathsf{A}) = \int_\Omega \int_\Omega |a(\mathsf{P},\mathsf{P}')|^2 dv dv'$$

We see that $\mathrm{Tr}\,\mathsf{A}$, $\Sigma(\mathsf{A})$ accomplish what was sought before by the use of mathematically doubtful artifices: in the transition from F_Z to F_Ω, $\sum_{\mu=1}^{\infty} \cdots$ is replaced by $\int_\Omega \cdots dv$.

With this we have concluded our mathematical treatment of Hermitian operators. The reader who is interested in the mathematics will find more on this subject in the literature relating to these topics.[116]

[116] In addition to the original papers mentioned in the course of the preceding discussion, the foremost reference is the encyclopedia article of Hellinger and Toeplitz referred to in Note 33.

CHAPTER III

THE QUANTUM STATISTICS

1. THE STATISTICAL ASSERTIONS OF QUANTUM MECHANICS

Let us now return to the analysis of the quantum mechanical theories, which was interrupted by the mathematical considerations of Chapter II. At that time we discussed only how quantum mechanics makes possible the determination of all possible values of one particular physical quantity—energy. These values are the eigenvalues of the energy operator (*i.e.*, the numbers of its spectrum). On the other hand, no mention was made about the values of other quantities, as well as regarding the causal or statistical relations among the values of several quantities. The statements of the theory relative to this problem should now be considered. We shall take as a basis the wave mechanical method of description since the equivalence of the two theories has already been established.

In the Schrödinger formalism, it is evident that everything which can be said about the state of a system must be derived from its wave function $\phi(q_1, \ldots, q_k)$. (We suppose that the system has k degrees of freedom and employs $q_1, \ldots, q_k$ as the coordinates of its configuration.) Actually, this does not restrict us to the stationary states of the system (quantum orbits in which ϕ is an eigenfunction of H: $\mathsf{H}\phi = \lambda\phi$, see **I.3**), but also admits all other states of the system; *i.e.*, wave functions which vary according to the Schrödinger time-dependent differential equation $\mathsf{H}\phi = i\hbar\frac{\partial}{\partial t}\phi$ (see **I.2**). What pronouncements can now be made regarding a system which is in the state ϕ?

First of all, we observe that ϕ was normalized (**I.3**) by

$$\int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k = 1$$

i.e., (in our present terminology) as a point of the Hilbert space $\mathcal{R}_\infty$ of all

$f(q_1, \ldots, q_k)$ with finite

$$\int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} |f(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k$$

(in an F_Ω!) it is normalized by $\|\phi\| = 1$. In other words, it must lie on the surface of the unit sphere in Hilbert space.[117] We already know that a constant (meaning independent of $q_1, \ldots, q_k$) factor in ϕ is physically meaningless. (This means that the substitution of $a\phi$ for ϕ—a a complex number—is of no physical consequence. To preserve normalization it must be the case that $|a| = 1$.) Furthermore, it should in this regard be pointed out that while ϕ is dependent on time t as well as the coordinates $q_1, \ldots, q_k$ of the configuration space of our system, nevertheless the Hilbert space involves only the $q_1, \ldots, q_k$ (because the normalization is related to these alone). Hence the dependence on t is not to be considered in forming the Hilbert space. Instead of this, it is rather to be regarded as a parameter. Consequently, ϕ—as a point in $\mathfrak{R}_\infty$—depends on t but is, on the other hand, independent of the $q_1, \ldots, q_k$. Indeed, as a point in $\mathfrak{R}_\infty$, it represents the entire functional dependence. Because of this, we shall occasionally indicate the parameter t in ϕ (when ϕ is viewed as a point in $\mathfrak{R}_\infty$) by writing ϕ_t.

Let us now consider the state $\phi = \phi(q_1, \ldots, q_k)$. The statistical assertions which can be made are as follows: The system is at the point $q_1, \ldots, q_k$ of the configuration space with the probability density $|\phi(q_1, \ldots, q_k)|^2$; *i.e.*, the probability that it is in the volume V of the configuration space is

$$\int \cdots \int_V |\phi(q_1, \ldots, q_k)|^2 dv$$

(This is one of the first and simplest examples by means of which the statistical character of quantum mechanics was recognized.[118] In addition, the relationship between this statement and Schrödinger's charge distribution assumption (see **I.2**) is manifest.) Furthermore, if the energy of the system has the operator H, and if this operator has eigenvalues $\lambda_1, \lambda_2, \ldots$ and eigenfunctions $\phi_1, \phi_2, \ldots$, then the probability of the energy eigenvalue λ_n in the state ϕ is equal to

$$\left| \int \cdots \int \phi(q_1, \ldots, q_k) \overline{\phi_n(q_1, \ldots, q_k)}\, dq_1 \ldots dq_k \right|^2$$

(see the papers mentioned in Note 118). We now want to join these two statements, and put them in a unified form.

[117] By geometric analogy, the sphere with center ϕ_0 and radius r is (in $\mathfrak{R}_\infty$) the set of points f with $\|f - \phi_0\| \leqslant r$, its interior the set with $\|f - \phi_0\| < r$ and its outer surface the set with $\|f - \phi_0\| = r$. For the unit sphere, $\phi_0 = 0, r = 1$.

[118] The first statistical statements of the behavior of a system in the state ϕ originated with M. Born, and were treated in more detail by Dirac and by Jordan. See the references in Note 8 and Note 2.

Let V be a the k-dimensional cube

$$\begin{aligned} q_1' < q_1 \leqslant q_1'' \\ q_2' < q_2 \leqslant q_2'' \\ \vdots \\ q_k' < q_k \leqslant q_k'' \end{aligned}$$

We denote the intervals $\{q_1', q_1''\}$, $\{q_2', q_2''\}$, ..., $\{q_k', q_k''\}$ by $I_1, I_2, \ldots, I_k$ respectively. The $q_1, q_2, \ldots, q_k$ have the operators $q_1\cdot, q_2\cdot, \ldots, q_k\cdot$ respectively. The resolutions of the identity belonging to these operators are defined as follows (see **II.8**): we call the resolution belonging to $q_j\cdot$ $(j = 1, \ldots, k)$ $\mathsf{E}_j(\lambda)$ and stipulate that

$$\mathsf{E}_j(\lambda) f(q_1, q_2, \ldots, q_k) = \begin{cases} f(q_1, q_2, \ldots, q_k) & \text{for} \quad q_j \leqslant \lambda \\ 0 & \text{for} \quad q_j > \lambda \end{cases}$$

We introduce the following general notation: If $\mathsf{F}(\lambda)$ is a resolution of the identity and I is the interval $\{\lambda', \lambda''\}$ then $\mathsf{F}(I) = \mathsf{F}(\lambda'') - \mathsf{F}(\lambda')$ (which for $\lambda' \leqslant \lambda''$, $\mathsf{F}(\lambda') \leqslant \mathsf{F}(\lambda'')$ is a projection operator). The probability therefore that the system lies in the above V—*i.e.*, that q_1 lies in I_1, ... , q_k lies in I_k—is given by

$$\begin{aligned} &\int_{I_1} \cdots \int_{I_k} |\phi(q_1, \ldots, q_k)|^2 dq_1 \ldots dq_k \\ &\qquad = \int \cdots \int \left| \mathsf{E}_1(I_1) \cdots \mathsf{E}_k(I_k) \phi(q_1, \ldots, q_k) \right|^2 dq_1 \ldots dq_k \end{aligned}$$

(because $\mathsf{E}_1(I_1) \cdots \mathsf{E}_k(I_k) \phi(q_1, \ldots, q_k) = \phi(q_1, \ldots, q_k)$ for q_1 in I_1, ... , q_k in I_k, and is otherwise 0); *i.e.*,

$$= \| \mathsf{E}_1(I_1) \cdots \mathsf{E}_k(I_k) \|^2$$

In the second case, let us consider the probability that the energy lies in the interval $I = \{\lambda', \lambda''\}$. The resolution of the identity, $\mathsf{E}(\lambda)$, is defined (see **II.8**) by

$$\mathsf{E}(\lambda) = \sum_{\lambda_n \leqslant \lambda} \mathsf{P}_{[\phi_n]}$$

Therefore

$$\mathsf{E}(I) = \mathsf{E}(\lambda'') - \mathsf{E}(\lambda') = \sum_{\lambda' < \lambda_n \leqslant \lambda''} \mathsf{P}_{[\phi_n]}$$

But since only the $\lambda_1, \lambda_2, \ldots$ appear as values of the energy, this latter probability is the sum of the probabilities of all λ_n with $\lambda' < \lambda_n \leqslant \lambda''$. Therefore

$$\sum_{\lambda' < \lambda_n \leqslant \lambda''} \Big| \int \cdots \int \phi(q_1, \ldots, q_k) \overline{\phi_n(q_1, \ldots, q_k)}\, dq_1 \ldots dq_k \Big|^2$$
$$= \sum_{\lambda' < \lambda_n \leqslant \lambda''} |(\phi, \phi_n)|^2$$
$$= \sum_{\lambda' < \lambda_n \leqslant \lambda''} (\mathsf{P}_{[\phi_n]}\phi, \phi)$$
$$= \Big(\Big\{ \sum_{\lambda' < \lambda_n \leqslant \lambda''} \mathsf{P}_{[\phi_n]} \Big\} \phi, \phi \Big) = (\mathsf{E}(I)\phi, \phi) = \|\mathsf{E}(I)\phi\|^2$$

In both cases we have then obtained a result which can be formulated as follows:

> **P.** The probability that in the state ϕ the operators $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$[119] take on values from the respective intervals $I_1, \ldots, I_\ell$ is
>
> $$\|\mathsf{E}_1(I_1) \cdots \mathsf{E}_\ell(I_\ell)\phi\|^2$$
>
> where $\mathsf{E}_1(\lambda), \ldots, \mathsf{E}_\ell(\lambda)$ are the resolutions of the identity belonging to $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ respectively.

The first case corresponds to $\ell = k$, $\mathsf{R}_1 = q_1\cdot, \ldots, \mathsf{R}_k = q_k\cdot$, the second to $\ell = 1$, $\mathsf{R}_1 = \mathsf{H}$. We shall now assume this statement **P** to be generally valid. It actually contains all the statistical assertions of quantum mechanics which have been made thus far.

However, a limitation of its validity is necessary. Since the order of the $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ is entirely arbitrary in the problem, it must be arbitrary in the result. That is, all the $\mathsf{E}_1(I_1), \ldots, \mathsf{E}_\ell(I_\ell)$ or equivalently all the $\mathsf{E}_1(\lambda_1), \ldots, \mathsf{E}_\ell(\lambda_\ell)$ must commute. By **II.10** this means that the $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ commute with each other. This condition is satisfied for $q_1\cdot, \ldots, q_k\cdot$, while for $\ell = 1$, $\mathsf{R}_1 = \mathsf{H}$ it is vacuously satisfied.

Consequently, we postulate **P** for all commuting $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$. Then $\mathsf{E}_1(I_1), \ldots, \mathsf{E}_\ell(I_\ell)$ commute, so $\mathsf{E}_1(I_1) \cdots \mathsf{E}_\ell(I_\ell)$ is a projection (THEOREM 14 in **II.4**) and the probability in question becomes

$$P = \|\mathsf{E}_1(I_1) \cdots \mathsf{E}_\ell(I_\ell)\phi\|^2 = \big(\mathsf{E}_1(I_1) \cdots \mathsf{E}_\ell(I_\ell)\phi, \phi\big)$$

(THEOREM 12 in **II.4**).

[119] We shall speak more expressly in **IV.1** about this correspondence, which allows each physical quantity to correspond to a Hermitian operator. For the present, we know only (by reason of **I.2**) that the operators $q_1\cdot, \ldots, q_k\cdot$ correspond to the coordinates, the operators $\frac{\hbar}{i}\frac{\partial}{\partial q_1}, \ldots, \frac{\hbar}{i}\frac{\partial}{\partial q_k}$ to the momenta, and the "energy operator" H to the energy.

Before we go any further we must verify a few properties of **P** which must hold in any reasonable statistical theory.

1°. The order of the propositions is irrelevant.

2°. Vacuous propositions can be inserted at will.

These are propositions where the interval $I_j = \{\infty, +\infty\}$, and they give rise only to a factor $\mathsf{E}_j(I_j) = \mathsf{E}_j(+\infty) - \mathsf{E}_j(-\infty) = \mathsf{I} - \mathsf{O} = \mathsf{I}$.

3°. The addition theorem of probability holds.

That is, if we resolve an interval I_j into two intervals I_j', I_j'' then the old probability is the sum of the two new probabilities. For let I_j, I_j', I_j'' be $\{\lambda', \lambda''\}$, $\{\lambda', \lambda\}, \{\lambda, \lambda''\}$ respectively. Then

$$\mathsf{E}(\lambda'') - \mathsf{E}(\lambda') = \big(\mathsf{E}(\lambda) - \mathsf{E}(\lambda')\big) + \big(\mathsf{E}(\lambda'' - \mathsf{E}(\lambda)\big)$$

i.e., $\mathsf{E}(I_j) = \mathsf{E}(I_j') + \mathsf{E}(I_j'')$ which, by reason of the second of the preceding formulations of **P** (which is linear in $\mathsf{E}_1(I_1) \cdots \mathsf{E}_j(I_j) \cdots \mathsf{E}_\ell(I_\ell)$) gives the additivity of the probabilities.

4°. For absurd propositions (one I_j empty), $P = 0$ because then the corresponding $\mathsf{E}_j(I_j) = \mathsf{O}$. For truly trivial propositions (all $I_j = \{-\infty, +\infty\}$), $P = 1$ because then all $\mathsf{E}_j(I_j) = \mathsf{I}$, $P = \|\phi\|^2 = 1$. We always have $0 \leqslant P \leqslant 1$ because of THEOREM 13 in **II.4**.

Finally, we observe that **P** contains the assertion that a quantity R_j can take on as values only its eigenvalues; *i.e.*, the numbers of its spectrum. For if the interval $I_j = \{\lambda', \lambda''\}$ lies outside of the spectrum then $\mathsf{E}_j(\lambda)$ is constant in it, and therefore

$$\mathsf{E}_j(I_j) = \mathsf{E}_j(\lambda'') - \mathsf{E}(\lambda') = \mathsf{O}$$

from which it follows that $P = 0$.

We shall now set $\ell = 1$ and denote R_1 by R. Let $\mathcal{R}$ be the physical quantity to which R corresponds (see Note 119). Let $F(\lambda)$ be any function. The expectation value of $F(\mathcal{R})$ is then to be calculated.

For this purpose, we divide the interval $\{-\infty, +\infty\}$ into a sequence of subintervals $\{\lambda_n, \lambda_{n+1}\}$, $n = 0, \pm 1, \pm 2, \ldots$. The probability that $\mathcal{R}$ lies in $\{\lambda_n, \lambda_{n+1}\}$ is

$$(\{\mathsf{E}(\lambda_{n+1}) - \mathsf{E}(\lambda_n)\}\phi, \phi) = (\mathsf{E}(\lambda_{n+1})\phi, \phi) - (\mathsf{E}(\lambda_n)\phi, \phi)$$

and the expectation value of $F(\mathcal{R})$ is consequently

$$\sum_{-\infty}^{+\infty} F(\lambda_n')\big\{(\mathsf{E}(\lambda_{n+1})\phi, \phi) - (\mathsf{E}(\lambda_n)\phi, \phi)\big\}$$

if λ_n' is an appropriate intermediate value from $\{\lambda_n, \lambda_{n+1}\}$. But if we choose

the subdivisions $\ldots, \lambda_{-2}, \lambda_{-1}, \lambda_0, \lambda_1, \lambda_2, \ldots$ closer and closer together this sum converges to the Stieltjes integral

$$\int_{-\infty}^{+\infty} F(\lambda)\, d(\mathsf{E}(\lambda)\phi, \phi)$$

which therefore provides a description of the expectation value in question. But by reason of the general definition of operator functions in **II.8** this integral is equal to $(F(\mathsf{R})\phi, \phi)$. Consequently, we have

> **$\mathbf{E}_1$.** Let $\mathcal{R}$ be any physical quantity, R its operator (see Note 119), and $F(\lambda)$ an arbitrary function. Then, for the expectation value of $F(\mathcal{R})$ in the state ϕ, we have
>
> $$\mathrm{Exp}(F(\mathcal{R}); \phi) = (F(\mathsf{R})\phi, \phi)$$

In particular, if we set $F(\lambda) = \lambda$, then:

> **$\mathbf{E}_2$.** Let $\mathcal{R}$, R be as above. Then for the expectation value of $\mathcal{R}$ in the state ϕ, we have
>
> $$\mathrm{Exp}(\mathcal{R}; \phi) = (\mathsf{R}\phi, \phi)$$

We look now to the relations among **P**, $\mathbf{E}_1$ and $\mathbf{E}_2$. We shall deduce $\mathbf{E}_1$ from **P** and $\mathbf{E}_2$ from $\mathbf{E}_1$.

Let the operator that corresponds to the physical quantity $F(\mathcal{R})$ be denoted S. Then a comparison of $\mathbf{E}_1$, $\mathbf{E}_2$ gives

$$(\mathsf{S}\phi, \phi) = (F(\mathsf{R})\phi, \phi)$$

for all states ϕ; *i.e.*, for all ϕ with $\|\phi\| = 1$. Consequently, in general,

$$(\mathsf{S}f, f) = (F(\mathsf{R})f, f)$$

(obvious for $f = 0$, while otherwise $\phi = \frac{1}{\|f\|} \cdot f$) and therefore

$$(\mathsf{S}f, g) = (F(\mathsf{R})f, g)$$

(replace f by $\frac{f+g}{2}$ else by $\frac{f-g}{2}$ and subtract; this gives equality of the real parts; if, g instead of f, g gives equality of the imaginary parts). Therefore $\mathsf{S} = F(\mathsf{R})$. We formulate this important result as follows:

> **F.** If the quantity $\mathcal{R}$ has the operator R, then the quantity $F(\mathcal{R})$ must have the operator $F(\mathsf{R})$.

Because of **F**, now $\mathbf{E}_1$ clearly follows from $\mathbf{E}_2$. Consequently (under the assumption of **F**), $\mathbf{E}_1$ and $\mathbf{E}_2$ are equivalent assertions, and we shall now show that they are also equivalent to **P**. Since they follow from **P** we need only show that **P** follows from $\mathbf{E}_1$ or $\mathbf{E}_2$.

Let $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ be commuting operators belonging to the respective quantities $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$. By **II.10** they are functions of a Hermitian operator R:

$$\mathsf{R}_1 = F_1(\mathsf{R}), \quad \ldots \quad , \mathsf{R}_\ell = F_\ell(\mathsf{R})$$

We may assume that R also belongs to a quantity $\mathcal{R}$. (We therefore make the assumption that a (hypermaximal) operator R belongs to each $\mathcal{R}$ and conversely. See Note 119 and **IV.2**.) Then, by **F**,

$$\mathcal{R}_1 = F_1(\mathcal{R}), \quad \ldots \quad , \mathcal{R}_\ell = F_\ell(\mathcal{R})$$

Now let $I_1, \ldots, I_\ell$ be the intervals involved in **P**, and let $G_j(\lambda)$ be defined

$$G_j(\lambda) = \begin{cases} 1 & \text{for } \lambda \text{ in } I_j \\ 0 & \text{otherwise} \end{cases} \quad : \quad j = 1, \ldots, \ell$$

We set

$$H(\lambda) = G_1(F_1(\lambda)) \cdots G_\ell(F_\ell(\lambda))$$

and form the quantity

$$\mathcal{S} = H(\mathcal{R})$$

If $\mathcal{R}_j$ lies in I_j—*i.e.*, if $F_j(\mathcal{R})$ lies in I_j—then $G_j(F_j(\mathcal{R}))$ equals 1, otherwise it equals 0. $\mathcal{S} = H(\mathcal{R})$ is therefore equal to 1 if each $\mathcal{R}_j$ lies in its I_j $(j = 1, \ldots, \ell)$, and is otherwise equal to 0. The expectation value of $\mathcal{S}$ is therefore equal to the probability P that $\mathcal{R}_1$ lies in I_1, ... , $\mathcal{R}_\ell$ lies in I_ℓ., Hence

$$\begin{aligned} P = \mathrm{Exp}(\mathcal{S}, \phi) &= (H(\mathsf{R})\phi, \phi) \\ &= (G_1(F_1(\mathsf{R})) \cdots G_\ell(F_\ell(\mathsf{R}))\phi, \phi) \\ &= (G_1(\mathsf{R}_1) \cdots G_\ell(\mathsf{R}_\ell)\phi, \phi) \end{aligned}$$

Let the resolution of the identity belonging to R_j again be called $\mathsf{E}_j(\lambda)$, and let I_j be the interval $\{\lambda_j', \lambda_j''\}$. Then, by reason of the discussion at the end of **II.8**, and with the notation used there,

$$\begin{aligned} G_j(\lambda) &= e_{\lambda_j''}(\lambda) - e_{\lambda_j'}(\lambda) \\ G_j(\mathsf{R}_j) &= e_{\lambda_j''}(\mathsf{R}_j) - e_{\lambda_j'}(\mathsf{R}_j) \\ &= \mathsf{E}_j(\lambda_j'') - \mathsf{E}_j(\lambda_j') = \mathsf{E}_j(I_j) \end{aligned}$$

we have

$$P = (\mathsf{E}_1(I_1) \cdots \mathsf{E}_\ell(I_\ell)\phi, \phi)$$

But this is precisely **P**.

Because of the simplicity of their form, $\mathbf{E}_2$, **F** are especially suited to be considered as the foundations upon which the entire theory is built. We saw that **P**—the most general probability assertion possible—follows from these.

But the statement **P** has two striking features:

1. **P** is statistical, and not causal; *i.e.*, it does not tell us what values $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$ have in the states ϕ, but only with what probabilities they take on all possible values.

2. The problem of **P** cannot be answered for arbitrary quantities $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$, but only for those whose operators $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ commute with one another.

Our next problem is to discuss the significance of these two facts.

2. THE STATISTICAL INTERPRETATION

Classical mechanics is a causal discipline; *i.e.*, if we know exactly the state of a classical system—for which, with k degrees of freedom, $2k$ numbers are necessary: the k space coordinates $q_1, \ldots, q_k$ and their k time derivatives $\partial q_1/\partial t, \ldots, \partial q_k/\partial t$ or, in place of these, the k momenta $p_1, \ldots, p_k$—then we can give the value of each physical quantity (energy, torque, etc.) uniquely and with numerical exactness. Nevertheless, there also exists a statistical method for approaching classical mechanical problems, but this is, as it were, a luxury or extra addition. That is, if we do not know all $2k$ variables $q_1, \ldots, q_k, p_1, \ldots, p_k$ but only several of them (and some of those perhaps only approximately), we—by averaging over the unknown variables—may at least be able to formulate statistical assertions about the physical quantities of interest. The same holds for the preceding or subsequent states of the system: if we know $q_1, \ldots, q_k$, $p_1, \ldots, p_k$ at time $t = t_0$ then, by means of the classical equations of motion, we can calculate (causally) the state for every other time; but if we know only some of the variables we must average over the rest, and we can then make only statistical statements about the state at other times.[120]

The statistical statements which we found in quantum mechanics have a different character. Here, for k degrees of freedom, the state is described by the wave function $\phi(q_1, \ldots, q_k)$; *i.e.*, by a point ϕ in $\mathcal{R}_\infty$, suitably realized ($\|\phi\| = 1$, and a numerical factor of absolute value 1 is unimportant). Although we believe that after having specified ϕ we know the state of the system completely, nevertheless only statistical statements can be made concerning the values of the physical quantities involved.

[120] The kinetic theory of gases furnishes a good illustration of the points at issue. A mole (32 g) of oxygen contains $6 \cdot 10^{23}$ oxygen molecules, and, if we observe that each oxygen molecule is composed of two oxygen atoms (whose inner structure we shall neglect, so that they can be treated as mass points with three degrees of freedom), one such mole is a system with $2{\cdot}3{\cdot}6{\cdot}10^{23} = 36{\cdot}10^{23} = k$ degrees of freedom. Its behavior can therefore be described causally by $2k$ variables, but gas theory uses only two: pressure and temperature, which are certain complicated functions of these $2k$ independent variables. Consequently, only statistical (probability) observations can be made. That these are in many cases nearly causal (*i.e.*, the probabilities are near 0 or 1) does not alter the fundamental nature of the situation.

On the other hand, this statistical character is limited to statements about the values of physical quantities, while the preceding and subsequent states ϕ_t can be calculated causally from $\phi_{t_0} = \phi$. The time-dependent Schrödinger equation (see **I.2**) makes this possible:

$$\phi_{t_0} = \phi \quad : \quad \tfrac{\hbar}{i}\tfrac{\partial}{\partial t}\phi_t = -\mathsf{H}\phi_t$$

determine the entire path of ϕ_t. The solution of this differential equation can be explicitly rendered

$$\phi_t = e^{-\frac{i}{\hbar}(t-t_0)\mathsf{H}}\phi$$

where the operator $e^{-\frac{i}{\hbar}(t-t_0)\mathsf{H}}$ is unitary.[121] (In this formula H was assumed to be independent of time, but even with a time-dependent H the evolved state ϕ_t is uniquely determined, since the differential equation is of first degree. In this case, however, there are no simple solution formulas.)

If we want to explain the non-causal character of the connection between ϕ and the values of physical quantities following the pattern of classical mechanics, then this interpretation is clearly the proper one: In reality, ϕ does not determine the state exactly. In order to know this state absolutely, additional numerical data are necessary. That is, the system has other characteristics or coordinates in addition to ϕ. If we were to know all of these we could then give the values of all physical quantities exactly and with certainty. On the other hand, with the use of ϕ alone, just as in classical mechanics when only some of the $q_1, \ldots, q_k, p_1, \ldots, p_k$ are known, only statistical statements are possible. Of course, this concept is only hypothetical. It is an attempt whose utility depends upon whether or not it actually succeeds in finding the additional coordinates contributing to ϕ, and in building, with their help, a causal theory which is in agreement with experiment, and which gives the statistical assertions of quantum mechanics when only ϕ is given (and an averaging is performed over the other coordinates).

---

[121] If $F_t(\lambda)$ is a time-dependent function, $\frac{\partial}{\partial t}F_t(\lambda) = G_t(\lambda)$ and H is a Hermitian operator, then $\frac{\partial}{\partial t}F_t(\mathsf{H}) = G_t(\mathsf{H})$ because $\frac{\partial}{\partial t}$ is obtained by subtraction, division and passage to the limit. For

$$F_t(\lambda) = e^{-\frac{i}{\hbar}(t-t_0)\lambda}$$

this gives

$$\tfrac{\partial}{\partial t}e^{-\frac{i}{\hbar}(t-t_0)\mathsf{H}} = -\tfrac{i}{\hbar}\mathsf{H}\cdot e^{-\frac{i}{\hbar}(t-t_0)\mathsf{H}}$$

which yields the desired differential equation when applied to ϕ.

Because $|F_t(\lambda)| = 1$, $F_t(\lambda)\cdot\overline{F_t(\lambda)} = 1$ we have $F_t(\mathsf{H})\cdot[F_t(\mathsf{H})]^* = 1$; *i.e.*, our

$$F_t(\mathsf{H}) = e^{-\frac{i}{\hbar}(t-t_0)\mathsf{H}}$$

is unitary. Since it is obviously I at $t = t_0$, $\phi_{t_0} = \phi$ is also satisfied.

It is customary to call these hypothetical additional coordinates "hidden parameters" or "hidden coordinates," since they must play a hidden role, in addition to the ϕ which alone have been uncovered by investigation thus far. Explanations by means of hidden parameters have (in classical mechanics) reduced many apparently statistical relations to the causal foundations of mechanics. An example of this is the kinetic theory of gases (see Note 120).

Whether or not an explanation of this type, by means of hidden parameters, is possible for quantum mechanics is a much discussed question. The view that it will sometime be answered in the affirmative has at present some prominent representatives. If it were correct, it would brand the present form of the theory provisional, since then the description of states would be essentially incomplete.

We shall show later (**IV.2**) that an introduction of hidden parameters is certainly not possible without a basic change in the present theory. For the present, let us emphasize only these two things: (1) ϕ has an entirely different appearance and role from the $q_1, \ldots, q_k, p_1, \ldots, p_k$ complex in classical mechanics, and (2) the time dependence of ϕ is causal and not statistical: ϕ_{t_0} determines all ϕ_t uniquely, as we saw above.

Until a more precise analysis of the statements of quantum mechanics enables us to prove objectively the possibility of introducing hidden parameters (a problem discussed in the place quoted above), we shall abandon this possible explanation. We therefore adopt the opposite point of view. That is, we admit as a fact that the natural laws which govern elementary processes (*i.e.*, the laws of quantum mechanics) are of a statistical nature. (The causality of the macroscopic world can in any event be simulated by the leveling action which is manifest whenever many elementary processes operate simultaneously; *i.e.*, by the "law of large numbers." See the remarks at the end of Note 120 and Note 175.) Accordingly, we recognize **P** (or $\mathbf{E}_2$) as the most far reaching pronouncement on elementary processes.

This concept of quantum mechanics, which accepts its statistical expression as the actual form of the laws of nature, and which abandons the principle of causality, is the so-called "statistical interpretation." It is due to M. Born,[122] and is the only consistently enforceable interpretation of quantum mechanics today—*i.e.*, of the sum of our experience relative to elementary processes. It is this interpretation to which we shall conform in the following (until we can proceed to a detailed and fundamental discussion of the situation).

3. SIMULTANEOUS MEASURABILITY AND MEASURABILITY IN GENERAL

The second of the "striking" circumstances to which we drew attention at the end of **III.1** was connected with the fact that **P** provided information not

[122] Z. Physik **37** (1926). The entire subsequent development (see Note 2) rests on this concept.

only about the probabilities with which a quantity $\mathcal{R}$ took on given numerical values, but also about the probability interrelations of several quantities $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$. **P** specified the probability that these quantities took on certain given values simultaneously (more precisely: that these quantities lay in certain intervals $I_1, \ldots, I_\ell$, the presumption being that all refer to the same state ϕ). But these quantities $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$ were subject to a characteristic limitation: their operators $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ had to commute pairwise. In the case of non-commuting $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ on the other hand, **P** gave no information regarding the probability interrelations of the $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$. In this case, **P** could be used only to determine the probability distribution of each of these quantities by itself, without consideration of the others.

The most obvious remedy would be to assume that this reflects an incompleteness in **P**, and that there must exist a more general formula which gives back **P** as a special case. Because even if quantum mechanics furnishes only statistical information regarding nature, the least we can expect of it is that it describes not only the statistics of individual quantities, but also the relations among several such quantities.

But—contrary to this concept, which appears reasonable at first glance—we shall soon see that such a generalization of **P** is not possible, and that, in addition to the formal reasons (intrinsic to the structure of the mathematical tools of the theory), weighty physical grounds also suggest this type of limitation. The necessity of this limitation and its physical meaning will give us an important insight into the nature of elementary processes.

In order to be clear on this point we must investigate more precisely what the process of measurement of a quantity $\mathcal{R}$—about which **P** makes a (probability) statement—means quantum mechanically.

First, let us refer to an important experiment which Compton and Simon carried out prior to the formulation of quantum mechanics.[123] In this experiment, light was scattered by electrons, and the scattering process was controlled in such a way that the scattered light and scattered electrons were subsequently intercepted, and their energy and momenta measured. That is, there ensued collisions between light quanta and electrons, and the observer, since he measured the paths after collision, could determine whether or not the laws of elastic collision were satisfied. (We need consider only elastic collisions, since we do not believe that energy can be absorbed by electrons and light quanta in any form other than as kinetic energy. According to all experiments, both appear to have uniquely constituted structures. The collision calculation must naturally be carried out relativistically.[123]) Such a mathematical calculation was in fact possible because the paths before collision were known, and those after the collision were observed. Therefore the collision problem was entirely determined. In order to determine the process

[123] Phys. Rev. **26** (1925). See also the comprehensive treatment of Bothe in *Handbuch der Physik*, Vol. 23 ("Quanta"), Berlin, 1926, Chapter 3, particularly §73.

mechanically, two of these four paths, and the "central line" of the collision (the direction of momentum transfer) suffices. In any case, therefore, knowledge of three paths is sufficient, and the fourth acts as a check. The experiment gave complete confirmation of the mechanical laws of collision.

This result can also be formulated as follows, provided we admit the validity of the laws of collision, and regard the paths before collision as known. The measurement of either the light quantum or the electron after collision suffices to determine the position and the central line of the collision. The Compton-Simon experiment now shows that these two observations give the same result.

More generally, the experiment shows that the same physical quantity (namely, any coordinate of the place of collision or of the central line) is measured in two different ways (by capture of the light quantum and of the electron), and the result is always the same.

These two measurements do not occur entirely simultaneously. The light quantum and the electron do not arrive at once, and by suitable arrangement of the measurement apparatus either process may be observed first. The time difference is usually about 10^{-9} to 10^{-10} seconds. We call the first measurement M_1 and the second M_2. $\mathcal{R}$ is the quantity measured. We then have the following situation: Although the entire arrangement is of such a type that, prior to the measurement, we can make only statistical statements regarding $\mathcal{R}$, *i.e.*, regarding M_1, M_2 (see the reference in Note 123), the statistical correlation between M_1 and M_2 is perfectly sharp (causal): the $\mathcal{R}$ value of M_1 is certainly equal to that of M_2. Before the measurements of M_1, M_2, therefore, both results were completely undetermined; after M_1 has been performed (but not M_2) the result of M_2 is already determined, causally and uniquely.

We can formulate the principle that is involved as follows: by nature, three degrees of causality or non-causality may be distinguished. First, the $\mathcal{R}$ value could be entirely statistical; *i.e.*, the result of a measurement could be predicted only statistically, and if a second measurement were made immediately after the first one this would also have a dispersion, without regard to the value found initially; for example, its dispersion might be equal to the original one.[124] Second, it is conceivable that the value of $\mathcal{R}$ may have a dispersion in the first measurement, but that immediately subsequent measurement is constrained to give a result which agrees with that of the first. Third, $\mathcal{R}$ could be determined causally at the outset.

The Compton-Simon experiment shows that only the second case is possible in a statistical theory. Therefore, if the system is initially found in a state in which the values of $\mathcal{R}$ cannot be predicted with certainty, then this state is transformed by the measurement M of $\mathcal{R}$ (in the example above, M_1) into

[124] A statistical theory of elementary processes was erected by Bohr, Kramers and Slater on these basic concepts. See Z. Physik **24** (1924), as well as the references cited in Note 123. The Compton-Simon experiment serves to refute this view.

another state: namely, into one in which the value of $\mathcal{R}$ is uniquely determined. Moreover, the new state, into which M places the system, depends not only upon the arrangement of M but also upon the result of the measurement M (which could not be predicted causally in the original state), because the value of $\mathcal{R}$ in this new state must actually be equal to this M-result.

Now let $\mathcal{R}$ be a quantity whose operator R has a pure discrete spectrum $\lambda_1, \lambda_2, \ldots$ with the respective eigenfunctions $\phi_1, \phi_2, \ldots$ which then form a complete orthonormal set. In addition, let each eigenvalue be simple (*i.e.*, of multiplicity 1: see **II.6**); *i.e.*, $\lambda_\mu \neq \lambda_\nu$ for $\mu \neq \nu$. Let us assume that we have measured $\mathcal{R}$ and found the value λ^*. What is the state of the system after the measurement?

By virtue of the foregoing discussion, this state must be such that a new measurement of $\mathcal{R}$ gives the result λ^* with certainty. (Of course, this measurement must be made immediately because after τ seconds ϕ has changed to

$$e^{-\frac{i}{\hbar}\tau \mathsf{H}}\phi$$

See **III.2**; H is the energy operator.)

This question, as to when the measurement of $\mathcal{R}$ in the state ϕ gives the value λ^* with certainty, we shall now answer in general, without limiting assumptions on the operator R.

Let $\mathsf{E}(\lambda)$ be the resolution of the identity corresponding to R, and I an interval $\{\lambda', \lambda''\}$. Our assumption can also be formulated this way: that $\mathcal{R}$ lies in I with probability 0 if this does not contain λ^*, and with probability 1 if I does contain λ^*; *i.e.*, if $\lambda' < \lambda^* \leqslant \lambda''$.

By **P** this means that $\|\mathsf{E}(I)\phi\|^2 = 1$ or (since $\|\phi\| = 1$) $\|\mathsf{E}(I)\phi\| = \|\phi\|$. Since $\mathsf{E}(I)$ is a projection, and $\mathsf{I} - \mathsf{E}(I)$ is also (THEOREM 13, **II.4**), we have

$$\begin{aligned} \|\phi - \mathsf{E}(I)\phi\| = \|\phi\|^2 - \|\mathsf{E}(I)\phi\|^2 &= 0 \\ \phi - \mathsf{E}(I)\phi &= 0 \\ \mathsf{E}(\lambda'')\phi - \mathsf{E}(\lambda')\phi = \mathsf{E}(I)\phi &= \phi \end{aligned}$$

$\lambda' \to -\infty$ gives $\mathsf{E}(\lambda'')\phi = \phi$ while $\lambda'' \to +\infty$ gives $\mathsf{E}(\lambda')\phi = 0$ (see $\mathbf{S}_1$, **II.7**). Therefore

$$\mathsf{E}(\lambda)\phi = \begin{cases} \phi & \text{for} \quad \lambda \geqslant \lambda^* \\ 0 & \text{for} \quad \lambda < \lambda^* \end{cases}$$

But by **II.8** this is characteristic for $\mathsf{R}\phi = \lambda^*\phi$.

Another way of proving $\mathsf{R}\phi = \lambda^*\phi$ rests on $\mathbf{E}_1$ (*i.e.*, $\mathbf{E}_2$). That $\mathcal{R}$ has the value λ^* with certainty means that $(\mathcal{R} - \lambda^*)^2$ has the expectation value 0. That is, the operator $F(\mathsf{R}) = (\mathsf{R} - \lambda^*\mathsf{I})^2$ obtained from $F(\lambda) = (\lambda - \lambda^*)^2$ has that expectation value. We must then have

$$\begin{aligned} ((\mathsf{R} - \lambda^*\mathsf{I})^2\phi, \phi) = ((\mathsf{R} - \lambda^*\mathsf{I})\phi, (\mathsf{R} - \lambda^*\mathsf{I})\phi) &= \|(\mathsf{R} - \lambda^*\mathsf{I})\phi\|^2 \\ &= \|\mathsf{R}\,\phi - \lambda^*\phi\|^2 = 0 \end{aligned}$$

i.e., $\mathsf{R}\phi = \lambda^*\phi$.

For the special case that we considered originally we thus have $\mathsf{R}\phi = \lambda^*\phi$. As discussed in **II.6**, this has the consequence that λ^* must be equal to λ_μ (because $\|\phi\| = 1$, $\phi \neq 0$) and $\phi = a\phi_\mu$. Since $\|\phi\| = \|\phi_\mu\| = 1$, $|a|$ must equal 1, and therefore a can be neglected without altering the state. Therefore: $\lambda^* = \lambda_\mu$, $\phi = \phi_\mu$ for some $\mu = 1, 2, \ldots$. (The λ^*-assertion could have been obtained directly from **P**, but not the assertion regarding ϕ!)

Under the above assumptions on R, a measurement of $\mathcal{R}$ then has the consequence of changing the state ψ into one of the states $\phi_1, \phi_2, \ldots$ which are connected with the respective results of measurement $\lambda_1, \lambda_2, \ldots$. The probabilities of these changes are therefore equal to the measurement probabilities for $\lambda_1, \lambda_2, \ldots$, and can therefore be calculated from **P**.

The probability that the value of $\mathcal{R}$ lies in I is then $\|\mathsf{E}(I)\psi\|^2$ by **P**. Hence, if we observe that by **II.8** $\mathsf{E}(I) = \sum_{\lambda_n \text{in } I} \mathsf{P}_{[\phi_n]}$, we have

$$P = \|\mathsf{E}(I)\psi\|^2 = (\mathsf{E}(I)\psi, \psi) = \sum_{\lambda_n \text{ in } I} (\mathsf{P}_{[\psi_n]}\psi, \psi) = \sum_{\lambda_n \text{ in } I} |(\psi, \phi_n)|^2$$

One should therefore suspect that the probability for λ_n equals $|(\psi, \phi_n)|^2$. If we can so choose I that it contains a unique λ_m which is just λ_n, then this follows directly from the above formula. Otherwise (*i.e.*, if the other λ_m are dense near λ_n) we can, for example, argue as follows: let $F(\lambda) = 1$ for $\lambda = \lambda_n$ and be otherwise 0. Then the desired probability P_n is the expectation value of $F(\mathcal{R})$, and hence by $\mathbf{E}_2$ (or $\mathbf{E}_1$) is $(F(\mathsf{R})\psi, \psi)$. Now by definition

$$(F(\mathsf{R})\psi, \psi) = \int_{-\infty}^{+\infty} F(\lambda)\, d(\|\mathsf{E}(\lambda)\psi\|^2)$$

and if we recall the definition of the Stieltjes integral we can easily see that this equals 0 if $\mathsf{E}(\lambda)$ is continuous (in λ) for $\lambda = \lambda_n$, and in general the discontinuity for the (monotonic increasing) λ-function $\|\mathsf{E}(\lambda)\psi\|^2$ is at the point $\lambda = \lambda_n$. But this is equal to $\|\mathsf{P}_{\mathcal{M}}\psi\|^2$, where $\mathcal{M}$ is the closed linear manifold spanned by all solutions of $\mathsf{R}\psi = \lambda_n\psi$ (see **II.8**). In the present case, $\mathcal{M} = [\phi_n]$ and therefore

$$P_n = \|\mathsf{P}_{[\phi_n]}\psi\|^2 = |(\psi, \phi_n)|^2$$

We have then answered the question as to what happens in the measurement of a quantity $\mathcal{R}$ under the above assumptions for its operator R. To be sure, the "how" remains unexplained for the present. This discontinuous transition from ψ to one of the states $\phi_1, \phi_2, \ldots$ (which are independent of ψ because ψ enters only into the respective probabilities $P_n = |(\psi, \phi_n)|^2$, $n = 1, 2, \ldots$) is certainly not of the type described by the time-dependent Schrödinger equation. This latter always results in a continuous change of ψ, in which the final result is uniquely determined and is dependent on ψ (see the discussion in **III.2**). We shall attempt to bridge this chasm later (see **VI**).[125]

[125] That these jumps are related to the "quantum jumps" concept of the older Bohr theory was recognized by Jordan; Z. Physik **40** (1924).

Let us retain the assumption that R has a pure discrete spectrum but abandon the requirement that the eigenvalues are simple. Then we can again form the $\phi_1, \phi_2, \ldots$ and $\lambda_1, \lambda_2, \ldots$, but duplications may now occur among the λ_n. After a measurement of $\mathcal{R}$ a state ϕ with $\mathsf{R}\phi = \lambda^*\phi$ is certainly present (λ^* is the result of the measurement). As a consequence, λ^* is equal to one of the λ_n, but we can say only the following of ϕ: let those λ_n that equal λ^* be $\lambda_{n_1}, \lambda_{n_2}, \ldots$ (their number may be either finite or infinite). Then

$$\phi = \sum_\nu a_\nu \phi_\nu$$

(If there are infinitely many n_ν then $\sum_\nu |a_\nu|^2$ must be finite.) Two such ϕ represent the same state if they differ by no more than a numerical factor; *i.e.*, if the ratio $a_1 : a_2 : \cdots$ is the same. Therefore, as soon as more than one n_ν exists; *i.e.*, if the eigenvalue λ^* is multiple, then the state ϕ after the measurement is not uniquely determined by knowledge of the result of the measurement.

We calculate the probability of λ^* (by $\mathbf{P}$ or $\mathbf{E}_1$ or $\mathbf{E}_2$) exactly as before. It is

$$P(\lambda^*) = \sum_{\lambda_n = \lambda^*} |(\psi, \phi_n)|^2 = \sum_\nu |(\psi, \phi_{n_\nu})|^2$$

If R has no pure discrete spectrum the situation is this: All solutions f of $\mathsf{R}f = \lambda f$ span a closed linear manifold $\mathfrak{M}_\lambda$; all $\mathfrak{M}_\lambda$ together form an additional $\overline{\mathfrak{M}}$, and it is characteristic for the non-existence of a pure discrete spectrum that $\overline{\mathfrak{M}} \neq \mathfrak{R}_\infty$; *i.e.*, that $\overline{\mathfrak{R}} = \mathfrak{R}_\infty - \overline{\mathfrak{M}} \neq \mathfrak{O}$. (See **II.8** for this, as well as for what follows.) $\mathfrak{M}_\lambda$ is at best $\neq \mathfrak{O}$ for a sequence of λ. These form the discrete spectrum of R. If we measure $\mathcal{R}$ in the state ψ then the probability that the result of the measurement will be λ^* is

$$P(\lambda^*) = \|\mathsf{P}_{\mathfrak{M}_{\lambda^*}}\psi\|^2 = (\mathsf{P}_{\mathfrak{M}_{\lambda^*}}\psi, \psi)$$

This is best proved by the line of argument used above, which is based on $\mathbf{E}_2$ (or $\mathbf{E}_1$) and on the function

$$F(\lambda) = \begin{cases} 1 & \text{for} \quad \lambda = \lambda^* \\ 0 & \text{for} \quad \lambda \neq \lambda^* \end{cases}$$

The probability that the value of $\mathcal{R}$ will be some λ^* of the discrete spectrum Λ of R is then

$$P = \sum_{\lambda^* \text{ in } \Lambda} (\mathsf{P}_{\mathfrak{M}_{\lambda^*}}\psi, \psi) = (\mathsf{P}_{\overline{\mathfrak{M}}}\psi, \psi) = \|\mathsf{P}_{\overline{\mathfrak{M}}}\psi\|^2$$

which we can also see directly with the aid of the function

$$F(\lambda) = \begin{cases} 1 & \text{for} \quad \lambda^* \text{ from } \Lambda \\ 0 & \text{otherwise} \end{cases}$$

However, if we measure $\mathcal{R}$ exactly, then afterwards a state ϕ with $\mathsf{R}\phi = \lambda^*\phi$ must be present, and therefore the result of measurement must belong to Λ; the probability of obtaining an exact measurement is therefore (at most) $\|\mathsf{P}_{\overline{\mathcal{M}}}\,\psi\|^2$. But this number is not always 1, and for ψ of $\overline{\mathcal{R}}$ it is in fact 0; therefore an exact measurement is not always possible.

We have seen that a quantity $\mathcal{R}$ can always (*i.e.*, for each state ψ) be measured exactly if and only if it possesses a pure discrete spectrum. If it possesses none, then it can be measured with only limited accuracy; *i.e.*, the number continuum can be divided into intervals

$$\dots, I^{(-2)}, I^{(-1)}, I^{(0)}, I^{(+1)}, I^{(+2)}, \dots$$

(Let the division points be

$$\dots, \lambda^{(-2)}, \lambda^{(-1)}, \lambda^{(0)}, \lambda^{(+1)}, \lambda^{(+2)}, \dots \quad : \quad I^{(n)} = \{\lambda^{(n)}, \lambda^{(n+1)}\}$$

The maximum interval-length $\epsilon = \mathrm{Max}(\lambda^{(n+1)} - \lambda^{(n)})$—the maximal spacing of the division points—is then the measure of accuracy.) The interval in which $\mathcal{R}$ lies can be determined by a process which we pursue mathematically: Let $F(\lambda)$ be the following function (λ'_n is some intermediate value from $I^{(n)}$, which is arbitrary for each $n = 0, \pm1, \pm2, \dots$ but will be considered to be fixed):

$$F(\lambda) = \lambda'_n \text{ if } \lambda \text{ lies in } I^{(n)}$$

Then the approximate measurement of $\mathcal{R}$ is equivalent to the exact measurement of $F(\mathcal{R})$. Now

$$\begin{aligned} F(\mathsf{R}) = \int_{-\infty}^{+\infty} F(\lambda) d\mathsf{E}(\lambda) &= \sum_{n=-\infty}^{+\infty} \int_{\lambda^{(n)}}^{\lambda^{(n+1)}} F(\lambda) d\mathsf{E}(\lambda) \\ &= \sum_{n=-\infty}^{+\infty} \lambda'_n \int_{\lambda^{(n)}}^{\lambda^{(n+1)}} d\mathsf{E}(\lambda) = \sum_{n=-\infty}^{+\infty} \lambda'_n \mathsf{E}(I^{(n)}) \end{aligned}$$

The equation $F(\mathsf{R})f = \lambda'_n f$ clearly holds for all f of the closed linear manifold belonging to $\mathsf{E}(I^{(n)})$; *i.e.*, to $F(\mathsf{R})\mathcal{M}_{\lambda'_n}$, which contains that closed manifold. Consequently

$$\mathsf{P}_{\mathcal{M}_{\lambda'_n}} \geqslant \mathsf{E}(I^{(n)})$$

and therefore

$$\begin{aligned} \mathsf{P}_{\overline{\mathcal{M}}} \geqslant \sum_{n=-\infty}^{\infty} \mathsf{P}_{\mathcal{M}_{\lambda'_n}} &\geqslant \sum_{n=-\infty}^{\infty} \mathsf{E}(I^{(n)}) \\ &= \sum_{n=-\infty}^{\infty} \left(\mathsf{E}(\lambda^{(n+1)}) - \mathsf{E}(\lambda^{(n)})\right) = \mathsf{I} - \mathsf{O} = \mathsf{I} \end{aligned}$$

From this it follows that

$$\sum_{n=-\infty}^{\infty} \mathsf{P}_{\mathcal{M}_{\lambda'_n}} = \mathsf{P}_{\overline{\mathcal{M}}} = \mathsf{I}, \qquad \mathsf{P}_{\mathcal{M}_{\lambda'_n}} = \mathsf{E}(I^{(n)})$$

i.e., that $F(\mathsf{R})$ has a pure discrete spectrum, and that this consists of λ'_n.

Therefore $F(\mathcal{R})$ is exactly measurable, and the probability that its value is λ'_n—*i.e.*, that the value of $\mathcal{R}$ lies in $I^{(n)}$—is

$$\|\mathsf{P}_{\mathfrak{M}_{\lambda'_n}}\psi\|^2 = \|\mathsf{E}(I^{(n)})\psi\|^2$$

in agreement with the statement **P** for $\mathcal{R}$.

This result can also be interpreted physically, and it demonstrates that the theory is in good agreement with the ordinary intuitive physical point of view.

In the method of observation of classical mechanics (without any quantum conditions) we assign to each quantity $\mathcal{R}$ in each state a completely determined value. At the same time, however, we recognize that every conceivable measuring apparatus, as a consequence of the imperfections of human means of observation (which result in the reading of the position of a pointer, or of locating the blackening of a photographic plate, with only limited accuracy), can furnish this value only with a certain (never vanishing) margin of error. This margin of error can, by sufficient refinement of the method of measurement, be made arbitrarily close to zero—but it is never exactly zero. One expects that this will also be true in quantum theory for those quantities $\mathcal{R}$ which, according to the pictures that were customarily made of such things (especially before the discovery of quantum mechanics), are not quantized; this expectation pertains, for example, to the cartesian coordinates of an electron (which can take on every value between $-\infty$ and $+\infty$, and whose operators have continuous spectra). On the other hand, for those quantities which (according to our intuitive picture of them) are "quantized" the reverse is true: since these are capable of assuming only discrete values it suffices to observe them with just sufficient precision that no doubt can exist as to which of these "quantized" values is occurring. That value is then as good as "observed" with absolute precision. For example, if we know of a hydrogen atom that it contains less energy than is necessary for the second-lowest energy level, then we know its energy content with absolute precision: it is in the lowest energy state.

This division into quantized and unquantized quantities corresponds, as the analysis of the matrix theory has already shown (see **I.2** and **II.6**), to the division of quantities $\mathcal{R}$ with operators R which do/don't have pure discrete spectra. It was for the former—and only for those—that we found measurements of absolute precision to be possible; the latter, we found, can be observed only with arbitrarily good (but never absolute) precision.[126]

In addition, it should be observed that the introduction of an eigenfunction which is "improper"—*i.e.*, which does not belong to Hilbert space (mentioned in the preface as well as in **I.3**; see also **II.8**, especially the Notes 84, 86)—gives

[126] In all such cases we make the supposition that the structure of the observed system—and of the measuring apparatus (*i.e.*, all the ambient force fields, etc.)—is known exactly, and that only the state (*i.e.*, the values of the coordinates) is sought. If these (idealized) assumptions do not prove to be correct then additional sources of indeterminacy are of course present.

a less good approach to reality than our treatment here. For such a method assumes the existence of states in which quantities with continuous spectra take on certain values exactly, although this never occurs. Although such idealizations have often been advanced, we believe that it is necessary to discard them on these grounds, additional to the grounds provided by the fact of their mathematical untenability.

With this we have brought to a tentative conclusion our discussion of the processes which occur in the measurement of a single quantity, and can apply ourselves to the problems posed by the simultaneous measurement of several quantities.

First, let $\mathcal{R}$, $\mathcal{S}$ be two quantities with the respective operators R, S. We shall assume that they are simultaneously measurable. What follows from this?

We begin by assuming exact measurability so that R, S must have pure discrete spectra: $\lambda_1, \lambda_2, \dots$ and $\mu_1, \mu_2, \dots$ respectively. Let the corresponding complete orthonormal sets of eigenfunctions be $\phi_1, \phi_2, \dots$ and $\psi_1, \psi_2, \dots$.

In order to discuss the simplest case first, we shall assume that one of the operators—say R—has simple eigenvalues; *i.e.*, $\lambda_m \neq \lambda_n$ for $m \neq n$.

If we measure $\mathcal{R}$, $\mathcal{S}$ simultaneously then a state is subsequently present in which $\mathcal{R}$ as well as $\mathcal{S}$ has the previously measured values with certainty. These values are (say) $\lambda_{\bar{m}}$, $\lambda_{\bar{n}}$. The state which then exists must satisfy the relations $\mathsf{R}\psi = \lambda_{\bar{m}}\psi$, $\mathsf{S}\psi = \lambda_{\bar{n}}\psi$. From the first of these if follows that $\psi = \phi_{\bar{m}}$ (except for a numerical factor which we can neglect), while from the second $\psi = \sum_\nu a_\nu \psi_{n_\nu}$ if $\mu_{n_1}, \mu_{n_2}, \dots$ are all μ_n equal to $\mu_{\bar{n}}$. If the initial state was ϕ then $\lambda_{\bar{m}}$, $\phi_{\bar{m}}$ has the probability $|(\phi, \phi_{\bar{m}})|^2$. For $\phi = \phi_m$ therefore $\bar{m} = m$ is certain, so that we can say for each m that ϕ_m can be developed $\sum_\nu a_\nu \psi_{n_\nu}$ with equal μ_{n_ν}; *i.e.*, $\mathsf{S}\phi_m = \bar{\mu}\phi_m$ with $\bar{\mu} = \mu_{n_1} = \mu_{n_2} = \cdots$. For $f = \phi_m$ consequently $\mathsf{RS}f = \mathsf{SR}f$ (both are equal to $\lambda_m \bar{\mu} \cdot \phi_m$). Therefore this also holds for these; *i.e.*, for all f. Therefore R, S commute.

If R, S are not continuous then we argue as follows: The resolutions of the identity $\mathsf{E}(\lambda), \mathsf{F}(\mu)$ belonging to R, S are defined by

$$\mathsf{E}(\lambda) = \sum_{\lambda_m \leqslant \lambda} \mathsf{P}_{[\phi_m]}, \qquad \mathsf{F}(\mu) = \sum_{\mu_n \leqslant \mu} \mathsf{P}_{[\psi_n]}$$

Consequently

$$\mathsf{E}(\lambda)\phi_m = \begin{cases} \phi_m & \text{for} \quad \lambda \geqslant \lambda_m \\ 0 & \text{for} \quad \lambda < \lambda_m \end{cases}$$

$$\mathsf{F}(\mu)\phi_m = \begin{cases} \phi_m & \text{for} \quad \mu \geqslant \bar{\mu} \\ 0 & \text{for} \quad \mu < \bar{\mu} \end{cases}$$

Therefore in any case $\mathsf{E}(\lambda)\mathsf{F}(\mu)\phi_m = \mathsf{F}(\mu)\mathsf{E}(\lambda)\phi_m$ for all ϕ_m. The commutativity of $\mathsf{E}(\lambda), \mathsf{F}(\mu)$ follows from this, just as above, and therefore (by **II.10**) also the commutativity of R, S.

But according to **II.10** there exists a complete orthonormal set of eigenfunctions common to R, S; *i.e.*, we may assume $\phi_m = \psi_m$. Since $\lambda_m \neq \lambda_n$ for $m \neq n$, we can set up a function $F(\lambda)$ with

$$F(\lambda) = \begin{cases} \mu_n \quad \text{for} \quad \lambda = \lambda_n \ : \ n = 1, 2, \ldots \\ \text{arbitrary elsewhere} \end{cases}$$

Then $\mathsf{S} = F(\mathsf{R})$; *i.e.*, $\mathcal{S} = F(\mathcal{R})$. That is: $\mathcal{R}$, $\mathcal{S}$ are not only measurable simultaneously but each measurement of $\mathcal{R}$ is also one of $\mathcal{S}$, since $\mathcal{S}$ is a function of $\mathcal{R}$; *i.e.*, is determined causally by $\mathcal{R}$.[127]

We now proceed to the more general case where nothing is assumed concerning the multiplicity of the eigenvalues of R, S. In this case we use an essentially different method.

First let us consider the quantity $\mathcal{R} + \mathcal{S}$. A simultaneous measurement of $\mathcal{R}$, $\mathcal{S}$ is also a measurement of $\mathcal{R} + \mathcal{S}$ because addition of the results of the measurements gives the value of $\mathcal{R} + \mathcal{S}$. Consequently, the expectation value of $\mathcal{R} + \mathcal{S}$ in each state ψ is the sum of the expectation values of $\mathcal{R}$ and of $\mathcal{S}$. It should be noted that this holds independently of whether $\mathcal{R}$, $\mathcal{S}$ are statistically independent, or whether (and which) correlations exist between them, because the law

Expectation value of the sum = Sum of the expectation values

holds in general, as is well known. Therefore, if T is the operator of $\mathcal{R} + \mathcal{S}$ then this expectation value is on the one hand $(\mathsf{T}\psi, \psi)$ and on the other

$$(\mathsf{R}\psi, \psi) + (\mathsf{S}\psi, \psi) = ((\mathsf{R} + \mathsf{S})\psi, \psi)$$

i.e., for all ψ

$$(\mathsf{T}\psi, \psi) = ((\mathsf{R} + \mathsf{S})\psi, \psi)$$

Therefore $\mathsf{T} = \mathsf{R} + \mathsf{S}$. Consequently $\mathcal{R} + \mathcal{S}$ has the operator $\mathsf{R} + \mathsf{S}$.[128] In the same way we can show that $a\mathcal{R} + b\mathcal{S}$ (a, b real numbers) has the operator $a\mathsf{R} + b\mathsf{S}$. (This also follows from the first formula if we substitute $\mathcal{R}$, $\mathcal{S}$ and R, S in the functions $F(\lambda) = a\lambda, G(\mu) = b\mu$.)

A simultaneous measurement of $\mathcal{R}$, $\mathcal{S}$ is also a measurement of

$$\frac{\mathcal{R} + \mathcal{S}}{2}, \quad \left(\frac{\mathcal{R} + \mathcal{S}}{2}\right)^2, \quad \frac{\mathcal{R} - \mathcal{S}}{2}, \quad \left(\frac{\mathcal{R} - \mathcal{S}}{2}\right)^2$$

$$\left(\frac{\mathcal{R} + \mathcal{S}}{2}\right)^2 - \left(\frac{\mathcal{R} - \mathcal{S}}{2}\right)^2 = \mathcal{R} \cdot \mathcal{S}$$

[127] The latter proposition can be verified with the aid of **P**. The resolutions of the identity which belong to R and S may be formed by **II.8**.

[128] We have proved this law, according to which the operator of $\mathcal{R} + \mathcal{S}$ is the sum of the operators of $\mathcal{R}$ and $\mathcal{S}$, for simultaneously measurable $\mathcal{R}$, $\mathcal{S}$. See what is said at the end of **IV.1** and **IV.2**.

Operators of these quantities (if we also make use of the fact that if T is the operator of $\mathcal{T}$ then $F(\mathsf{T})$ is the operator of $F(\mathcal{T})$ and hence $\mathcal{T}^2$ has the operator T^2) are therefore

$$\begin{aligned}\frac{\mathsf{R}+\mathsf{S}}{2}, \quad \Big(\frac{\mathsf{R}+\mathsf{S}}{2}\Big)^2 &= \frac{\mathsf{R}^2+\mathsf{S}^2+\mathsf{RS}+\mathsf{SR}}{4}\\ \frac{\mathsf{R}-\mathsf{S}}{2}, \quad \Big(\frac{\mathsf{R}-\mathsf{S}}{2}\Big)^2 &= \frac{\mathsf{R}^2+\mathsf{S}^2-\mathsf{RS}-\mathsf{SR}}{4}\\ \Big(\frac{\mathsf{R}+\mathsf{S}}{2}\Big)^2 - \Big(\frac{\mathsf{R}-\mathsf{S}}{2}\Big)^2 &= \frac{\mathsf{RS}+\mathsf{SR}}{2}\end{aligned}$$

That is, $\mathcal{R}\cdot\mathcal{S}$ has the operator $\frac{1}{2}(\mathsf{RS}+\mathsf{SR})$. This also holds for all $F(\mathcal{R})$, $F(\mathcal{S})$ (which are also measured), and therefore $F(\mathcal{R})\cdot G(\mathcal{S})$ has the operator

$$\frac{F(\mathsf{R})\,G(\mathsf{S})+G(\mathsf{S})\,F(\mathsf{R})}{2}$$

Now let $\mathsf{E}(\lambda),\mathsf{F}(\mu)$ be the resolutions of the identity corresponding to R, S. Furthermore, let

$$F(\lambda)=\begin{cases}1 & \text{for} \quad \lambda\leqslant\bar{\lambda}\\ 0 & \text{for} \quad \lambda>\bar{\lambda}\end{cases} \quad : \quad G(\mu)=\begin{cases}1 & \text{for} \quad \mu\leqslant\bar{\mu}\\ 0 & \text{for} \quad \mu>\bar{\mu}\end{cases}$$

As we know, $F(\mathsf{R})=\mathsf{E}(\bar{\lambda}), G(\mathsf{S})=\mathsf{F}(\bar{\mu})$ so $F(\mathcal{R})\cdot G(\mathcal{S})$ has the operator $\frac{1}{2}(\mathsf{EF}+\mathsf{FE})$ (for brevity we replace $\mathsf{E}(\bar{\lambda}),\mathsf{F}(\bar{\mu})$ by E,F). Since $F(\mathcal{R})$ is always either 0 or 1 we have $F(\mathcal{R})^2=F(\mathcal{R})$ and therefore

$$F(\mathcal{R})\cdot\big(F(\mathcal{R})\cdot G(\mathcal{S})\big)=F(\mathcal{R})\cdot G(\mathcal{S})$$

Let us now apply our multiplication formula to $F(\mathcal{R})$ and $F(\mathcal{R})\cdot G(\mathcal{S})$ (both of which are simultaneously measurable). We then obtain the operator

$$\frac{\mathsf{E}\,\frac{\mathsf{EF}+\mathsf{FE}}{2}+\frac{\mathsf{EF}+\mathsf{FE}}{2}\mathsf{E}}{2}=\frac{\mathsf{E}^2\mathsf{F}+2\mathsf{EFE}+\mathsf{FE}^2}{4}=\frac{\mathsf{EF}+\mathsf{FE}+2\mathsf{EFE}}{4}$$

for this product. This must equal $\frac{1}{2}(\mathsf{EF}+\mathsf{FE})$, from which it follows that

$$\mathsf{EF}+\mathsf{FE}=2\cdot\mathsf{EFE}$$

Multiplication on the left by E gives

$$\mathsf{E}^2\mathsf{F}+\mathsf{EFE}=2\cdot\mathsf{E}^2\mathsf{FE}, \qquad \mathsf{EF}+\mathsf{EFE}=2\cdot\mathsf{EFE}, \qquad \mathsf{EF}=\mathsf{EFE}$$

while multiplication on the right by E gives

$$\mathsf{EFE}+\mathsf{FE}^2=2\cdot\mathsf{EFE}^2, \qquad \mathsf{EFE}+\mathsf{FE}=2\cdot\mathsf{EFE}, \qquad \mathsf{FE}=\mathsf{EFE}$$

Therefore $\mathsf{EF}=\mathsf{FE}$. That is, all $\mathsf{E}(\bar{\lambda}),\mathsf{F}(\bar{\mu})$ commute. Consequently R,S again commute.

It was established in **II.10** that the requirement that R, S be commutative is the same as the requirement that there exists a Hermitian operator T of which R and S are functions: $\mathsf{R} = F(\mathsf{T}), \mathsf{S} = G(\mathsf{T})$. If this operator belongs to the quantity $\mathcal{T}$ then $\mathcal{R} = F(\mathcal{T})$, $\mathcal{S} = G(\mathcal{T})$. However, this condition is also sufficient for simultaneous measurability, because a measurement of $\mathcal{T}$ (an absolutely exact one because $\mathcal{T}$ has a pure discrete spectrum: see **II.10**) measures simultaneously the functions $\mathcal{R}$, $\mathcal{S}$. The commutativity of R, S is therefore a necessary and sufficient condition.

If several variables $\mathcal{R}, \mathcal{S}, \ldots$ (but a finite number) are given, if their operators are $\mathsf{R}, \mathsf{S}, \ldots$ and if absolutely exact measurement is again required, then the situation with regard to simultaneous measurability is as follows. If all quantities $\mathcal{R}, \mathcal{S}, \ldots$ are simultaneously measurable then all pairs formed from them must also be simultaneously measurable. That is, all operators $\mathsf{R}, \mathsf{S}, \ldots$ must commute pairwise. Conversely, if all $\mathsf{R}, \mathsf{S}, \ldots$ commute with each other then by **II.10** there exists an operator T of which all are functions: $\mathsf{R} = F(\mathsf{T}), \mathsf{S} = G(\mathsf{T}), \ldots$. And therefore the corresponding $\mathcal{T}$: $\mathcal{R} = F(\mathcal{T})$, $\mathcal{S} = G(\mathcal{T}), \ldots$. An exact measurement of $\mathcal{T}$ ($\mathcal{T}$ has again a pure discrete spectrum: see again **II.10**) is consequently a simultaneous measurement of $\mathcal{R}, \mathcal{S}, \ldots$ That is, the commutativity of $\mathsf{R}, \mathsf{S}, \ldots$ is necessary and sufficient for the simultaneous measurability of $\mathcal{R}, \mathcal{S}, \ldots$.

Now let us consider such measurements which are not absolutely exact, but only of some (arbitrarily great) previously given accuracy. Then $\mathsf{R}, \mathsf{S}, \ldots$ no longer need have discrete spectra.

Since the limited accuracy measurements of $\mathcal{R}, \mathcal{S}, \ldots$ are in effect the same as absolutely exact measurements of $F(\mathcal{R}), G(\mathcal{S}), \ldots$, where $F(\lambda), G(\lambda), \ldots$ are certain functions the manner of whose formation was described at the beginning of this section (in the discussion of a single measurement, of course, only $F(\lambda)$ was given), we can infer that $\mathcal{R}, \mathcal{S}, \ldots$ are certainly measurable simultaneously if all the $F(\mathcal{R}), G(\mathcal{S}), \ldots$ are measurable simultaneously (with, of course, absolute accuracy). But the latter is equivalent to the commutativity of $F(\mathsf{R}), G(\mathsf{S}), \ldots$, and this follows from that of $\mathsf{R}, \mathsf{S}, \ldots$. Therefore the commutativity of $\mathsf{R}, \mathsf{S}, \ldots$ is in any case sufficient.

Conversely, if $\mathcal{R}, \mathcal{S}, \ldots$ are taken to be simultaneously measurable, then we proceed as follows. A sufficiently exact measurement of $\mathcal{R}$ permits us to determine whether its value is $> \bar{\lambda}$ or $\leqslant \bar{\lambda}$ (see our definition of "limited accuracy," discussed in Note 126). So if $F(\lambda)$ is defined

$$F(\lambda) = \begin{cases} 1 & \text{for} \quad \lambda \leqslant \bar{\lambda} \\ 0 & \text{for} \quad \lambda > \bar{\lambda} \end{cases}$$

then $F(\mathcal{R})$ is measurable with absolute accuracy. Correspondingly, if

$$G(\mu) = \begin{cases} 1 & \text{for} \quad \mu \leqslant \bar{\mu} \\ 0 & \text{for} \quad \mu > \bar{\mu} \end{cases}$$

then $G(\mathcal{S})$ is measurable with absolute accuracy, and moreover: both quantities are measurable simultaneously. Therefore $R(\mathsf{R}), G(\mathsf{S})$ commute. Now let $\mathsf{E}(\lambda)$ and $\mathsf{F}(\mu)$ be the resolutions of the identity belonging to R, S. Then $F(\mathsf{R}) = \mathsf{E}(\bar{\lambda})$, $G(\mathsf{S}) = \mathsf{F}(\bar{\mu})$ and therefore $\mathsf{E}(\bar{\lambda}), \mathsf{F}(\bar{\mu})$ commute (for all $\bar{\lambda}, \bar{\mu}$). Consequently, R, S commute. And, since this must hold for each pair of operators R, S, all R, S must commute pairwise. Therefore this condition is also necessary.

We therefore see that the characteristic conditions for the simultaneous measurability of a (finite) number of quantities $\mathcal{R}, \mathcal{S}, \ldots$ is the commutativity of their operators $\mathsf{R}, \mathsf{S}, \ldots$. In fact, this holds for absolutely exact as well as for arbitrarily exact measurements. In the first case, however, it is also required that the operators possess pure discrete spectra, as is characteristic of absolutely exact measurements.

We have now produced the mathematical proof that **P** makes the most extensive statement that is in general possible in this theory (*i.e.*, in any theory that includes **P**). This is due to the fact that it presumes only the commutativity of the operators $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$. Without this condition, nothing can be said concerning the results of simultaneous measurements of $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$ since simultaneous measurements of these quantities are then in general not possible.

4. UNCERTAINTY RELATIONS

In the foregoing sections we have obtained important information about the measuring process involving a single quantity, or several simultaneously measurable ones. We must now develop the procedure for quantities which are not simultaneously measurable if we are interested in their statistics in the same system (in the same state ϕ).

Therefore, let two such quantities $\mathcal{R}$, $\mathcal{S}$ as well as their (non-commuting) operators R, S be given. In spite of this assumption, states ϕ may exist in which both quantities have sharply defined (*i.e.*, dispersionless) values—*i.e.*, eigenfunctions common to both—but no complete orthonormal set can be formed from these, since then R, S would commute. (See the construction given in **II.8** for the corresponding resolutions of the identity $\mathsf{E}(\lambda), \mathsf{F}(\lambda)$. If $\phi_1, \phi_2, \ldots$ is the complete orthonormal set mentioned then both $\mathsf{E}(\lambda)$ and $\mathsf{F}(\lambda)$ are $\mathsf{P}_{[\phi_\rho]}$ sums, and therefore commute since the $\mathsf{P}_{[\phi_\rho]}$ do.) What this means can easily be seen: the closed linear manifold $\mathcal{M}$ spanned by these ϕ must be smaller than $\mathcal{R}_\infty$ because were this equal to $\mathcal{R}_\infty$ then the desired complete orthonormal set could be built up exactly as was done in the beginning of **II.6** for the case of a single operator.

For the states of $\mathcal{M}$ our $\mathcal{R}$, $\mathcal{S}$ are simultaneously measurable. This can be shown most readily by indicating a model for this simultaneous measurement. Since the common eigenfunctions of R, S span $\mathcal{M}$ there is also an orthonormal set of such ϕ: $\phi_1, \phi_2, \ldots$ spanning $\mathcal{M}$ (*i.e.*, complete in $\mathcal{M}$). (This is also obtained by the method of construction described previously in **II.6**.) We extend $\phi_1, \phi_2, \ldots$

to a complete set $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$ by the addition of an orthonormal set $\psi_1, \psi_2, \ldots$ which spans $\mathfrak{R}_\infty - \mathfrak{M}$. Now let $\lambda_1, \lambda_2, \ldots, \mu_1, \mu_2, \ldots$ be distinct numbers and let T be defined by

$$\mathsf{T}\Big(\sum_m x_m\phi_m + \sum_n y_n\psi_n\Big) = \sum_m \lambda_m x_m\phi_m + \sum_n \mu_n y_n\psi_n$$

where $\mathcal{T}$ is the corresponding quantity.

A measurement of $\mathcal{T}$ produces (as we know from **III.3**) one of the states $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$. If a ψ_m results (which can sensed by observing that the result of the measurement is a λ_m) then we also know the values of $\mathcal{R}$ and $\mathcal{S}$ because $\mathcal{R}$, $\mathcal{S}$ have sharply defined values in ϕ_m by our assumptions, and we can predict with certainty that in an immediate measurement of $\mathcal{R}$ or $\mathcal{S}$ these respective values will be found. On the other hand, if ψ_n is the result then we know nothing of the sort (ψ_n does not lie in $\mathfrak{M}$; therefore $\mathcal{R}$, $\mathcal{S}$ are not sharply defined in ψ_n). The probability of finding ψ_n is, as we know, $(\mathsf{P}_{[\psi_n]}\phi, \phi)$, and the probability of finding some ψ_n $(n = 1, 2, \ldots)$ is

$$\sum_n (\mathsf{P}_{[\psi_n]}\phi, \phi) = (\mathsf{P}_{\mathfrak{R}_\infty - \mathfrak{M}}\phi, \phi) = \|\mathsf{P}_{\mathfrak{R}_\infty - \mathfrak{M}}\phi\|^2 = \|\phi - \mathsf{P}_{\mathfrak{M}}\phi\|^2$$

If ϕ belongs to $\mathfrak{M}$—*i.e.*, if $\phi = \mathsf{P}_{\mathfrak{M}}\phi$—then this probability is 0; *i.e.*, $\mathcal{R}$, $\mathcal{S}$ are measured simultaneously with certainty.[129]

Since we are now interested in non-simultaneously measurable quantities we shall now assume the existence of the extreme case $\mathfrak{M} = \mathfrak{O}$; *i.e.*, we shall assume that $\mathcal{R}$, $\mathcal{S}$ are not simultaneously measurable in any state because no eigenstates common to $\mathcal{R}$, $\mathcal{S}$ exist.

If R, S have resolutions of the identity $\mathsf{E}(\lambda), \mathsf{F}(\lambda)$ and the system is in state ϕ then, as we know from **III.1**, the expectation values of $\mathcal{R}$, $\mathcal{S}$ are

$$\rho = (\mathsf{R}\phi, \phi), \qquad \sigma = (\mathsf{S}\phi, \phi)$$

and their dispersions—*i.e.*, the expectation values of $(\mathcal{R} - \rho)^2$, $(\mathcal{S} - \sigma)^2$ (see the discussion of absolutely precise measurements in **III.3**)—are

$$\epsilon^2 = ((\mathsf{R} - \rho \cdot \mathsf{I})\phi, \phi) = \|(\mathsf{R} - \rho \cdot \mathsf{I})\phi\|^2 = \|\mathsf{R}\phi - \rho\phi\|^2$$
$$\eta^2 = ((\mathsf{S} - \sigma \cdot \mathsf{I})\phi, \phi) = \|(\mathsf{S} - \sigma \cdot \mathsf{I})\phi\|^2 = \|\mathsf{S}\phi - \sigma\phi\|^2$$

[129] The further detailed discussion of the "simultaneous measurability for ϕ of $\mathfrak{M}$" for $\mathcal{R}$, $\mathcal{S}$ which are not measurable with absolute precision (continuous spectra) is left to the reader. This can be carried out in the same way as in the treatment of **III.3**.

After a familiar transformation[130] this becomes

$$\epsilon^2 = \|\mathsf{R}\phi\|^2 - (\mathsf{R}\phi,\phi)^2, \qquad \eta^2 = \|\mathsf{S}\phi\|^2 - (\mathsf{S}\phi,\phi)^2$$

From $\|\phi\| = 1$ and the Schwarz inequality (THEOREM 1, **II.1**) it follows that both of these expressions are $\geqslant 0$. There now arises the question: Since ϵ and η cannot both be zero, but ϵ alone can be made arbitrarily small, and η likewise ($\mathcal{R}$, $\mathcal{S}$ are measurable separately with arbitrary exactness, and perhaps even with absolute exactness), must there be relations between ϵ and η which prevent their becoming arbitrarily small simultaneously, and what would be the form of such relations?

The existence of such relations was discovered by Heisenberg.[131] They are of great importance for the knowledge of the uncertainties in the description of nature produced by quantum mechanics. They are consequently known as the uncertainty relations. We shall first derive the most important relation of this type mathematically, and then return to its fundamental meaning, and its connection with experiment.

In matrix theory, operators P, Q with the commutation property

$$\mathsf{PQ} - \mathsf{QP} = \tfrac{\hbar}{i}\mathsf{I}$$

play an important role: they were, for example, assigned to the coordinate and its conjugate momentum (see **I.2**) or, more generally, to any two quantities which were canonically conjugate in classical mechanics (see, for example, the papers mentioned in Note 2). Let us examine any two such Hermitian operators P, Q with

$$\mathsf{PQ} - \mathsf{QP} = a \cdot \mathsf{I}$$

(From $(\mathsf{PQ} - \mathsf{QP})^* = \mathsf{QP} - \mathsf{PQ}$ we have $(a \cdot \mathsf{I})^* = \bar{a} \cdot \mathsf{I} = -a \cdot \mathsf{I}$ giving $\bar{a} = -a$: a is pure imaginary. This operator equation is not necessarily understood to entail equality of the domains of definition of the two sides: $\mathsf{PQ} - \mathsf{QP}$ need not

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[130] The operator calculation is the following:

$$\begin{aligned}\epsilon^2 &= ((\mathsf{R} - \rho \cdot \mathsf{I})^2\phi, \phi) \\ &= (\mathsf{R}^2\phi, \phi) - 2\rho \cdot (\mathsf{R}\phi, \phi) + \rho^2 \\ &= \|\mathsf{R}\phi\|^2 - 2 \cdot (\mathsf{R}\phi, \phi)^2 + (\mathsf{R}\phi, \phi)^2 \\ &= \|\mathsf{R}\phi\|^2 - (\mathsf{R}\phi, \phi)^2\end{aligned}$$

and similarly for η^2.

[131] Z. Physik **43** (1927). These considerations were extended by Bohr, Naturwiss. **16** (1928). The mathematical discussion that follows was first undertaken by Kennard, Z. Physik **44** (1927), and was given by Robertson in its present form.

make sense everywhere.) For each ϕ then

$$\begin{aligned} 2\mathrm{Im}(\mathsf{P}\phi, \mathsf{Q}\phi) &= -i[(\mathsf{P}\phi, \mathsf{Q}\phi) - (\mathsf{Q}\phi, \mathsf{P}\phi)] \\ &= -i[(\mathsf{QP}\phi, \phi) - (\mathsf{PQ}\phi, \phi)] \\ &= (i[\mathsf{PQ} - \mathsf{QP}]\phi, \phi) \\ &= ia \cdot \|\phi\|^2 \end{aligned}$$

Let $a \neq 0$; then we have (by THEOREM 1, **II.1**)

$$\|\phi\|^2 = -\tfrac{2i}{a}\,\mathrm{Im}(\mathsf{P}\phi, \mathsf{Q}\phi) \leqslant \tfrac{2}{|a|}|(\mathsf{P}\phi, \mathsf{Q}\phi)| \leqslant \tfrac{2}{|a|}\|\mathsf{P}\phi\| \cdot \|\mathsf{Q}\phi\|$$

and therefore, for $\|\phi\| = 1$,

$$\|\mathsf{P}\phi\| \cdot \|\mathsf{Q}\phi\| \geqslant \tfrac{1}{2}|a|$$

Since $\mathsf{P} - \rho\cdot\mathsf{I}$, $\mathsf{Q} - \sigma\cdot\mathsf{I}$ satisfy that same commutation relation, we have by that same argument

$$\|\mathsf{P}\phi - \rho\cdot\phi\| \cdot \|\mathsf{Q}\phi - \sigma\cdot\phi\| \geqslant \tfrac{1}{2}|a|$$

and if we introduce the mean values and dispersions

$$\begin{aligned} \rho &= (\,\mathsf{P}\phi, \phi), \qquad & \epsilon^2 &= \|\,\mathsf{P}\phi - \rho\cdot\phi\|^2 \\ \sigma &= (\mathsf{Q}\phi, \phi), \qquad & \eta^2 &= \|\mathsf{Q}\phi - \rho\cdot\phi\|^2 \end{aligned}$$

then this becomes

U $$\epsilon\eta \geqslant \tfrac{1}{2}|a|$$

In order for the equality sign to hold it is necessary and sufficient that the $\leqslant$ inequalities encountered in the derivation all be equalities. With $\mathsf{P}' = \mathsf{P} - \rho\cdot\mathsf{I}$, $\mathsf{Q}' = \mathsf{Q} - \sigma\cdot\mathsf{I}$ we then have

$$-i\tfrac{|a|}{a}\,\mathrm{Im}(\mathsf{P}'\phi, \mathsf{Q}'\phi) = |(\mathsf{P}'\phi, \mathsf{Q}'\phi)| = \|\mathsf{P}'\phi\| \cdot \|\mathsf{Q}'\phi\|$$

By THEOREM 1, **II.1**, the second equation means that $\mathsf{P}'\phi$ and $\mathsf{Q}'\phi$ differ by only a constant factor, and since $\|\mathsf{P}'\phi\| \cdot \|\mathsf{Q}'\phi\| \geqslant \frac{1}{2}|a| > 0$ implies $\mathsf{P}'\phi \neq 0$, $\mathsf{Q}'\phi \neq 0$ it must be the case that $\mathsf{P}'\phi = c \cdot \mathsf{Q}'\phi$, $c \neq 0$. But the first equation means that $(\mathsf{P}'\phi, \mathsf{Q}'\phi) = c\|\mathsf{Q}'\phi\|^2$ is pure imaginary, and in fact that its i-coefficient has the same sign as $-i|a|/a$ (a real!); *i.e.*, opposite to that of a. Therefore $c = i\gamma$, γ real and $\lessgtr 0$ for $ia \lessgtr 0$, respectively. Consequently

Eq $$\mathsf{P}'\phi = i\gamma \cdot \mathsf{Q}'\phi \quad : \quad \gamma \text{ real, and } \lessgtr 0 \text{ for } ia \lessgtr 0$$

The definitions of ρ, σ entail $(\mathsf{P}'\phi, \phi) = 0, (\mathsf{Q}'\phi, \phi) = 0$. Since $(\mathsf{P}'\phi, \phi) = i\gamma(\mathsf{Q}'\phi, \phi)$ follows from **Eq** and is real on the left but imaginary on the right, the expressions on both left and right must vanish, so the desired equations actually hold automatically. We have yet to determine ϵ, η. We have the relations

$$\epsilon : \eta = \|\mathsf{P}'\phi\| : \|\mathsf{Q}'\phi\| = |c| = |\gamma|, \qquad \epsilon\eta = \tfrac{1}{2}|a|$$

Therefore, since ϵ, η are both positive,

$$\epsilon = \sqrt{\frac{|a||\gamma|}{2}}, \qquad \eta = \sqrt{\frac{|a|}{2|\gamma|}}$$

For the quantum mechanical case $a = \hbar/i$ we get from **U**

U′ $$\epsilon\eta \geqslant \tfrac{1}{2}\hbar$$

We discuss **Eq** in the case where P, Q are the operators of the Schrödinger theory: $\mathsf{P} = \frac{\hbar}{i}\frac{\partial}{\partial q}$, $\mathsf{Q} = q\cdot$. (See **I.2**. We assume that a mechanical system with one degree of freedom is under consideration, and that the single coordinate is q.) Then **Eq** becomes

$$\Big(\frac{\hbar}{i}\frac{\partial}{\partial q} - \rho\Big)\phi = i\gamma(q-\sigma)\phi$$

where because $ia = \hbar > 0$ we have $\gamma > o$. Therefore

$$\frac{\partial}{\partial q}\phi = \tfrac{1}{\hbar}\big\{-\gamma q + \gamma\sigma + i\rho\big\}\phi$$

which gives

$$\begin{aligned}\phi &= \exp\Big[\tfrac{1}{\hbar}\int^q \{-\gamma q + \gamma\sigma + i\rho\}dq\Big] \\ &= C\cdot\exp\big[\tfrac{1}{\hbar}\big\{-\tfrac{1}{2}\gamma q^2 + \gamma\sigma q + i\rho q\big\}\big] \\ &= C'\cdot\exp\big[-\tfrac{1}{2}(\gamma/\hbar)(q-\sigma)^2\big]\cdot\exp\big[i(\rho/\hbar)q\big]\end{aligned}$$

Since $\gamma > 0$, $\|\phi\|^2 = \int_{-\infty}^{+\infty}|\phi(q)|^2dq$ is indeed finite, and C' is obtained from $\|\phi\| = 1$:

$$\begin{aligned}\|\phi\|^2 = \int_{-\infty}^{+\infty}|\phi(q)|^2dq &= |C'|^2\int_{-\infty}^{+\infty}\exp\big[-(\gamma/\hbar)(q-\sigma)^2\big]dq \\ &= |C'|^2\sqrt{\hbar/\gamma}\cdot\int_{-\infty}^{+\infty}e^{-x^2}dx \\ &= |C'|^2\sqrt{\hbar/\gamma}\cdot\sqrt{\pi} \\ &= |C'|^2\sqrt{h/2\gamma} = 1 \quad \text{where} \quad h = 2\pi\hbar \\ \therefore \qquad |C'| &= \Big(\frac{2\gamma}{h}\Big)^{\frac{1}{4}}\end{aligned}$$

Therefore, by neglect of a physically unimportant factor of absolute value 1,

$$C' = \Big(\frac{2\gamma}{h}\Big)^{\frac{1}{4}}$$

and we have

$$\phi = \phi(q) = \Big(\frac{2\gamma}{h}\Big)^{\frac{1}{4}}\exp\Big[-\tfrac{1}{2}(\gamma/\hbar)(q-\sigma)^2 + i(\rho/\hbar)q\Big]$$

Then ϵ, η are given by

$$\epsilon = \sqrt{\tfrac{1}{2}\hbar\gamma}, \qquad \eta = \sqrt{\tfrac{1}{2}\hbar/\gamma}$$

Aside from the condition $\epsilon\eta = \frac{1}{2}\hbar$ they are therefore arbitrary, since γ varies from 0 to $+\infty$. That is, each set of four quantities $\rho, \sigma, \epsilon, \eta$ satisfying $\epsilon\eta = \frac{1}{2}\hbar$ is exactly realized by a ϕ. These ϕ were first investigated by Heisenberg, and applied to the interpretation of quantum mechanical situations. They are especially suitable for this because they represent the highest possible degree of approximation (in quantum mechanics) to classical mechanical relations (where p, q are both without dispersion!), where ϵ and η can be prescribed without restrictions. (See the reference in Note 131.)

With the foregoing considerations we have addressed only one aspect of the uncertainty relations; namely, the formal one. For a complete understanding of these relations it is still necessary to consider them from another point of view: from that of direct physical experience. For the uncertainty relations bear a more easily understandable and simpler relation to direct experience than many of the facts on which quantum mechanics was originally based, and therefore the above—entirely formal—derivation does not do them full justice. An intuitive discussion is all the more necessary since one could obtain, at first glance, an impression that a contradiction exists here with the ordinary, intuitive point of view: it will not be clear to common sense without further discussion why the position and velocity (*i.e.*, coordinate and momentum) of a material body cannot both be measured simultaneously and with arbitrarily high accuracy, provided that sufficiently refined measurement instruments were available. Therefore it is necessary to elucidate by an exact analysis of the finest measurement processes (capable of execution perhaps only in the sense of ideal measurements) that this is not the case. Actually, the well-known laws of wave optics, electrodynamics and elementary atomic processes place very great difficulties in the way of accurate measurement precisely where this is required by the uncertainty relations. And in fact, this can already be recognized if the processes in question are investigated purely classically (not quantum theoretically). This is an important point of principle. It shows that the uncertainty relations, although apparently paradoxical, do not conflict with classical experience (*i.e.*, with the area in which quantum phenomena do not call for a correction of the earlier ways of thinking)—and classical experience is the only kind which is valid independently of the correctness of quantum mechanics; indeed, the only kind directly accessible to our ordinary, intuitive way of thinking.[132]

[132] The fundamental meaning of this circumstance was emphasized by Bohr. See the reference in Note 131. Actually, the argument developed below is not entirely classical at one point: the existence of light quanta will be assumed; *i.e.*, the fact that light of frequency ν never appears in quantities of energy smaller than $h\nu$.

We are then to show that if p, q are two canonically conjugate quantities, and a system is in a state in which the value of p can be giving with accuracy ϵ (*i.e.*, by a p-measurement with an error range ϵ), then q can be known with no greater accuracy than $\eta = \frac{1}{2}\hbar : \epsilon$. Which is to say: a measurement of p with accuracy ϵ must bring about an indeterminacy $\eta = \frac{1}{2}\hbar : \epsilon$ in the value of q.

Naturally, in these qualitative considerations we cannot expect to recover each detail with perfect exactness. Thus, instead of showing that $\epsilon\eta = \frac{1}{2}\hbar$ we will be able to show only that $\epsilon\eta \sim h$ for the most precise measurement possible (*i.e.*, that it is of the same order of magnitude as h). As a typical example, we will consider the conjugate pair position (coordinate)-momentum of a particle **T**.[133]

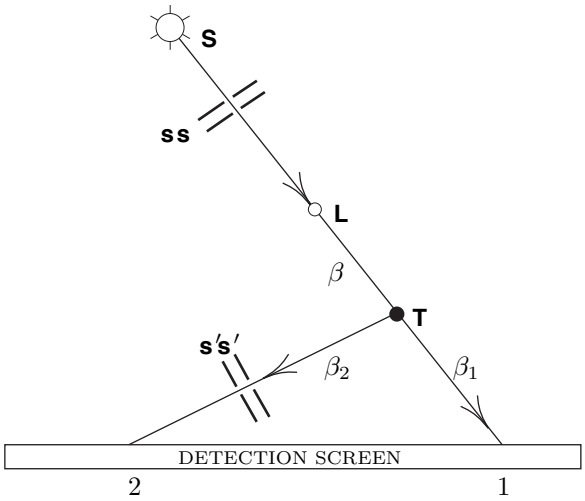

FIGURE 1: *Schematic arrangement for using columnated light* **L** *to measure the position of a particle* (*Teilchens*) **T**.

First let us investigate the determination of position. This results when one looks at **T**; *i.e.*, when **T** is illuminated and the scattered light is absorbed in the eye. Therefore, a light quantum **L** is emitted from a light source **S** in the direction of **T**, and is deflected from its straight line path $\beta\beta_1$ into $\beta\beta_2$ by collision with **T**, and at the end of its path is annihilated by absorption at the screen (which represents the eye or a photographic plate: FIGURE 1). The measurement takes place by the determination that **L** hits the screen not at 1 (the end of its undeflected path $\beta\beta_1$) but at 2 (the end of $\beta\beta_2$). But in order to be able to furnish the position of the collision (*i.e.*, of **T**) from this the directions of β and β_2 must also be known (*i.e.*, **L**'s direction before and after the collision): we achieve this by the interposition of slit systems **ss** and **s′s′**. (In this way we are actually not performing a measurement of the coordinate of **T** but obtain

[133] The following discussion is due to Heisenberg and Born. See references in Note 131.

only an answer to the question of whether or not this coordinate has a certain value, corresponding to the intersections of the directions β and β_2. This value, however, can be selected at will by appropriate arrangement of the slits. The superposition of several such determinations—*i.e.*, the use of additional slits **s′s′** —is equivalent to the complete coordinate measurement.) Now what is the accuracy of this measurement of position?

This measurement has a fundamental limitation in the laws of optical image formation. Indeed, it is impossible, with light of wavelength λ, to picture sharply objects which are smaller than λ, or even to reduce the scattering to such an extent that one can speak of a (distorted) image. To be sure, we did not require a faithful optical image, since the mere fact of the deviation of **L** suffices to determine the position of **T**. Nevertheless, the slits **ss** and **s′s′** cannot be narrower than λ, since otherwise **L** cannot pass through without appreciable diffraction. Rather, a bundle of interference lines will then occur, so that from knowledge of the slit locations nothing can be deduced concerning the directions β and β_2 of the light ray. As a consequence, it is never possible with this projectile **L** to aim and hit with an accuracy greater than λ.

The wavelength λ is then a measure of the error in measuring the coordinate: $\lambda \sim \epsilon$. Further characteristics of **L** are: its frequency ν, its energy $\overline{E}$, its momentum $\overline{p}$, and there exist the well-known relations

$$\nu = \frac{c}{\lambda}, \qquad \overline{E} = h\nu = \frac{hc}{\lambda}, \qquad \overline{p} = \frac{\overline{E}}{c} = \frac{hc}{c} = \frac{h}{\lambda}$$

where c is the velocity of light.[134] Consequently, $\overline{p} \sim h/\epsilon$. Now there is a momentum change in the (not exactly known) collision process between **L** and **T**, which is clearly of the order of magnitude of $\overline{p}$; *i.e.*, of the same order as h/ϵ. Hence there results an uncertainty $\eta \sim h/\epsilon$ in the momentum.

This would show that $\epsilon\eta \sim h$ if one detail had not been overlooked. The collision process is not really so unknown. We actually know the directions of the motion of **L** before and after (β and β_2), and therefore also its momentum, and the momentum transferred to **T** can be obtained from this. Consequently, $\overline{p}$ is not a measure of η; it is rather the directional uncertainty of the rays β and β_2 that will supply such a measure. Now in order to be able to establish more precisely the relations between the "aiming" at the small object **T** and the uncertainty of direction which is associated with it, it is appropriate to use a better focusing device than the slit **ss**—namely, a lens. Consequently, the well-known theory of the microscope must be considered. This asserts the following: in order to illuminate an element of surface with the linear extension ϵ (*i.e.*, to hit **T** with **L** with a precision ϵ), a wavelength λ and a lens aperture φ are necessary, between which the relation

$$\frac{\lambda}{2\sin\frac{1}{2}\varphi} \sim \epsilon$$

[134] See, for example, Einstein's original paper (Ann. Physik **14** (1905)) or any modern text.

exists (FIGURE 2).[135] The uncertainty of the **tt**-component of the momentum of **L** therefore rests upon the fact that its direction lies between $-\frac{1}{2}\varphi$ and $+\frac{1}{2}\varphi$, but is otherwise unknown. Consequently, the error amounts to

$$2\sin\tfrac{1}{2}\varphi\cdot\overline{p}=\frac{\lambda}{\epsilon}\cdot\frac{h}{\lambda}=\frac{h}{\epsilon}$$

But this is the correct measure for η. Therefore we again have $\eta\sim h/\epsilon$; *i.e.*, $\epsilon\eta\sim h$.

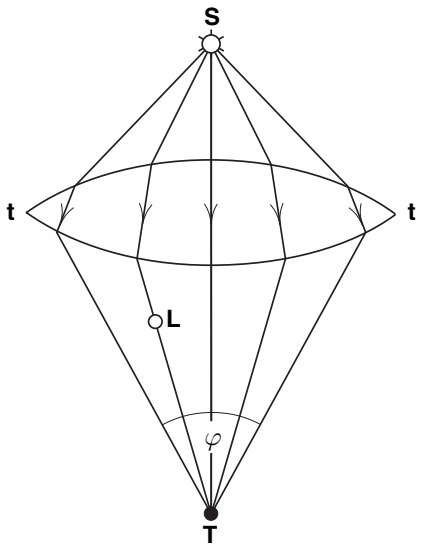

FIGURE 2: *Refinement of the coordinate-measurement set-up shown in the preceding figure.*

This example shows the mechanism of the uncertainty principle very clearly: in order to aim more accurately, we need a large eye (large aperture φ) and very short wavelength radiation; *i.e.*, very uncertain (and large) momentum for the light quantum, which produces collisions (Compton effect) with the observed object **T** that are out of control by a wide margin. In this way they cause the dispersion in **T**'s momentum.

Let us also consider the complementary measurement process: the measurement of the velocity (momentum). It should first be noted that the

[135] For the theory of the microscope, see for example *Handbuch der Physik*, Berlin, 1927, Volume 18, Chapter 2·*G*. In very precise measurements, ϵ—and therefore λ—is very small; *i.e.*, γ-rays or light of still shorter wavelength are to be used. A normal lens fails under such circumstances. The only type which could be used would be one whose molecules are neither shattered by these γ-rays nor knocked out of position by them. Since the existence of such molecules, or particles, encroaches on no known natural law, their use is possible for the purposes of an idealized experiment.

natural procedure for the measurement of the velocity of **T** is to measure its position at two times, say 0 and t, and divide the change in coordinates by t. In this case, however, the velocity in the time interval $[0, t]$ must be constant; if it changes, then this change is a measure of the deviation between the mean velocity (thus calculated) and the actual velocity (say instantaneously at t); *i.e.*, a measure of the uncertainty in the measurement. The same holds for the measurement of the momentum. Now if the coordinate measurements are obtained with precision ϵ this does not actually affect the precision of the measurement of the mean momentum, since t can be chosen arbitrarily large. Nevertheless, it does produce momentum changes of the order of h/ϵ, and therefore an uncertainty relative to the final momentum (in its relationship to the mean momentum mentioned above) of $\eta \sim h/\epsilon$. A different (more favorable) result can therefore only obtain—if at all—from momentum measurements which are not connected with position measurement. Such measurements are entirely possible, and are frequently used in astronomy. They rely on the Doppler effect, and we shall now consider this effect.

The Doppler effect is the following, as is well known. Light which is emitted from a body **T** moving with velocity v, and which is emitted with frequency ν_0 (measured on the moving body), is actually measured by the observer at rest as having a different frequency ν, which can be calculated from the relation $(\nu - \nu_0)/\nu_0 = (v/c)\cos\varphi$. ($\varphi$ is the angle between the direction of motion and the direction of emission. This formula is non-relativistic; *i.e.*, it is valid only for small values of v/c, but this limitation could easily be corrected.) Determination of the velocity is therefore possible if ν is observed and ν_0 is known—perhaps because it refers to a particular spectral line of a known element. More exactly, the component of velocity in the direction of the observation (light emission direction)

$$v\cos\varphi = \frac{c(\nu - \nu_0)}{\nu}$$

is measured, or equivalently: the corresponding component of momentum

$$p' = p\cos\varphi = \frac{mc(\nu - \nu_0)}{\nu_0}$$

where m is the mass of the body **T**. The dispersion of p' evidently depends on the dispersion $\Delta\nu$ of ν. Therefore

$$\eta \sim \frac{mc\,\Delta\nu}{\nu_0} \sim mc\,\frac{\Delta\nu}{\nu}$$

The momentum of **T** is of course changed when **T** emits a light quantum of frequency ν (and therefore of momentum $\overline{p} = h\nu/c$), but the uncertainty $h\Delta\nu/c$ of this quantity can ordinarily be neglected in comparison with $mc\,\frac{\Delta\nu}{\nu}$.[136]

[136] $mc\,\frac{\Delta\nu}{\nu}$ large in comparison to $h\frac{\Delta\nu}{c}$ means that ν is small in comparison to mc^2/h; *i.e.*, $\overline{E} = h\nu$ is small compared to mc^2. That is, the energy of the light quantum **L** is small in comparison to the relativistic rest energy of **T**—an assumption which is unavoidable for non-relativistic calculation.

Frequency ν is measured by any interference method, but this type of measurement will give an absolutely sharp ν-value only with a purely monochromatic wave train. Such a wave train has the form

$$a\sin[2\pi(\lambda^{-1}q-\nu t)+\alpha]$$

(here q is the coordinate, t the time, a the amplitude, α the phase: this expression may refer to any component of the electric or magnetic field strength) which extends infinitely in both space and time. To avoid this we must replace the preceding expression—which can also be written

$$a\sin[2\pi\nu(q/c-t)+\alpha]$$

since $\lambda = c/\nu$—by another, $F(q/c-t)$, which is non-zero only in a finite argument interval. If the light field has this form, then Fourier analysis supplies

$$F(x)=\int_0^{+\infty} a_\nu \sin(2\pi\nu x+\alpha_\nu)\,d\nu$$

and the interference picture shows all frequencies ν for which $a_\nu \neq 0$. In fact, the frequency interval $[\nu,\nu+d\nu]$ has the relative intensity $a_\nu^2\,d\nu$. The dispersion of ν—*i.e.*, $\Delta\nu$—is to be calculated from this distribution.

If our wave train has the length τ in x, *i.e.*, in t and q the respective lengths are τ and $c\tau$, then it can be seen that the ν-dispersion is $\sim\tau^{-1}$.[137] An indeterminacy of the position now results from this method of measurement because **T** undergoes recoil $h\nu/c$ (in the direction of observation) from individual light emission; *i.e.*, a velocity change $h\nu/mc$ results. Since the emission process takes time τ, we cannot localize the time of this change in velocity more accurately than τ. Hence an indeterminacy of position $\epsilon\sim(h\nu/mc)\tau$ results. Therefore

$$\epsilon\sim\frac{h\nu}{mc}\,\tau,\qquad \eta\sim mc\,\frac{\Delta\nu}{\nu}=\frac{mc}{\nu}\,\frac{1}{\tau},\qquad \epsilon\eta\sim h$$

So we again have $\epsilon\eta\sim h$.

If **T** is not self-luminous, as we assumed here, but scatters other light (*i.e.*, if it is illuminated) the calculation proceeds in a similar fashion.

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[137] Let, for example, $F(x)$ be a finite monochromatic wave train of frequency ν_0 extending from 0 to τ:

$$F(x)=\begin{cases}\alpha\sin 2\pi\nu_0 x & \text{for}\quad 0\leqslant x\leqslant\tau\\ 0 & \text{otherwise}\end{cases}$$

(To achieve continuity at the junction, $\sin 2\pi\nu_0\tau$ must vanish there; *i.e.*, $\nu_0=\frac{n}{2\tau}:n=1,2,3,\ldots$) Then, on the basis of the known inversion formulae of

5. PROJECTIONS AS PROPOSITIONS

As in **III.1**, let us consider a physical system **S** with k degrees of freedom, the configuration space of which is described by k coordinates $q_1, \ldots, q_k$ (see also **I.2**). All physical quantities $\mathcal{R}$ which can be formed in the system **S** are, in the manner of classical mechanics, functions of $q_1, \ldots, q_k$ and the conjugate momenta $p_1, \ldots, p_k$: $\mathcal{R} = \mathcal{R}(q_1, \ldots, q_k, p_1, \ldots, p_k)$ (for example, the energy is the Hamiltonian function $H(q_1, \ldots, q_k, p_1, \ldots, p_k)$). In quantum mechanics on the other hand, as we already pointed out in **III.1**, the quantities $\mathcal{R}$ correspond one-to-one to hypermaximal Hermitian operators R. In particular, $q_1, \ldots, q_k$

---

the Fourier integral (see the reference in Note 87), $a_\nu^2 = b_\nu^2 + c_\nu^2$ with

$$\begin{aligned}
\left.\begin{matrix} b_\nu \\ c_\nu \end{matrix}\right\} &= 2\int_{-\infty}^{+\infty} F(x) \begin{matrix}\cos \\ \sin\end{matrix} 2\pi\nu x \, dx = 2a\int_0^\tau \sin 2\pi\nu_0 x \cdot \begin{matrix}\cos \\ \sin\end{matrix} 2\pi\nu x \, dx \\
&= \pm a\int_0^\tau \left(\begin{matrix}\sin \\ \cos\end{matrix} \pi(\nu+\nu_0)x - \begin{matrix}\sin \\ \cos\end{matrix} \pi(\nu-\nu_0)x\right) dx \\
&= -a\left[\frac{\begin{matrix}\cos \\ \sin\end{matrix} \pi(\nu+\nu_0)x}{\pi(\nu+\nu_0)} - \frac{\begin{matrix}\cos \\ \sin\end{matrix} \pi(\nu-\nu_0)x}{\pi(\nu-\nu_0)}\right]_0^\tau \\
&= \begin{cases} -a\left[\dfrac{(-1)^n \cos\pi\nu\tau - 1}{\pi(\nu+\nu_0)} - \dfrac{(-1)^n \cos\pi\nu\tau - 1}{\pi(\nu-\nu_0)}\right] \\ -a\left[\dfrac{(-1)^n \sin\pi\nu\tau}{\pi(\nu+\nu_0)} - \dfrac{(-)^n \sin\pi\nu\tau}{\pi(\nu-\nu_0)}\right] \end{cases} \\
&= \begin{cases} \dfrac{-2a\nu_0[1-(-1)^n\cos\pi\nu\tau]}{\pi(\nu^2-\nu_0^2)} \\ \dfrac{2a\nu_0(-1)^n \sin\pi\nu\tau}{\pi(\nu^2-\nu_0^2)} \end{cases}
\end{aligned}$$

Therefore

$$a_\nu = \frac{2a\nu_0\sqrt{2-2(-1)^n\cos\pi\nu\tau}}{\pi(\nu^2-\nu_0^2)} = \frac{4a\nu_0\left|\begin{matrix}\sin \\ \cos\end{matrix} \frac{1}{2}\pi\nu\tau\right|}{\pi(\nu^2-\nu_0^2)} = \frac{4a\nu_0|\sin(\nu-\nu_0)\tau|}{\pi(\nu^2-\nu_0^2)}$$

As we see, the frequencies in the neighborhood of $\nu = \nu_0$ are most strongly represented, and the greatest part of the energy in the wave train falls in that frequency interval in which $\pi(\nu-\nu_0)\tau$ has moderate values. Therefore the dispersion of $\nu - \nu_0$ (or, which is the same thing, that of ν) has the order of magnitude τ^{-1}. Exact calculation of the expression

$$\frac{\int_0^\infty a_\nu{}^2(\nu-\nu_0)^2 d\nu}{\int_0^\infty a_\nu{}^2 d\nu}$$

gives the same result.

correspond to the operators $\mathsf{Q}_1 = q_1\cdot, \ldots, \mathsf{Q}_k = q_k\cdot$ and $p_1, \ldots, p_k$ to the operators $\mathsf{P}_1 = (\hbar/i)\frac{\partial}{\partial q_1}, \ldots, \mathsf{P}_k = (\hbar/i)\frac{\partial}{\partial q_k}$. It has already been noted in the case of the Hamiltonian function (**I.2**) that is not possible in general to define

$$\mathsf{R} = \mathcal{R}(\mathsf{Q}_1, \ldots, \mathsf{Q}_k, \mathsf{P}_1, \ldots, \mathsf{P}_k)$$

because of the non-commutativity of the $\mathsf{Q}_\ell, \mathsf{P}_\ell$. Nevertheless, without being able to give any final and complete rules regarding the relationship between the functions $\mathcal{R}(q_1, \ldots, q_k, p_1, \ldots, p_k)$ and the operators R, we stated the following special rules in **III.1** and **III.2**:

> **L.** If the operators R, S correspond to the simultaneously observable quantities $\mathcal{R}, \mathcal{S}$ then the operator $a\mathsf{R} + b\mathsf{S}$ (a and b real numbers) corresponds to the quantity $a\mathcal{R} + b\mathcal{S}$.
>
> **F.** If the operator R corresponds to the quantity $\mathcal{R}$ then the operator $F(\mathsf{R})$ corresponds to the quantity $F(\mathcal{R})$, where $F(\lambda)$ is an arbitrary real function.

L, **F** permit a certain generalization, which runs as follows:

> **F*.** If the operators $\mathsf{R}, \mathsf{S}, \ldots$ correspond to the simultaneously observable quantities $\mathcal{R}, \mathcal{S}, \ldots$ (which are consequently commutative; we assume that their number is finite) then the operator $F(\mathsf{R}, \mathsf{S}, \ldots)$ corresponds to the quantity $F(\mathcal{R}, \mathcal{S}, \ldots)$.

By way of proof, we shall assume that $F(\lambda, \mu, \ldots)$ is a real polynomial in $\lambda, \mu, \ldots$ so that the meaning of $F(\mathsf{R}, \mathsf{S}, \ldots)$ may be clear ($\mathsf{R}, \mathsf{S}, \ldots$ commutative), although **F*** could be established for arbitrary $F(\lambda, \mu, \ldots)$ (for the definition of the general $F(\mathsf{R}, \mathsf{S}, \ldots)$ see the reference in Note 94). Now since every polynomial is obtained by repetition of the three operations $a\lambda, \lambda + \mu, \lambda\mu$ it suffices to consider these, and since $\lambda\mu = \frac{1}{4}[(\lambda + \mu)^2 - (\lambda - \mu)^2]$—*i.e.*, is equal to

$$\tfrac{1}{4} \cdot (\lambda + \mu)^2 + (-\tfrac{1}{4}) \cdot (\lambda + (-1) \cdot \mu)^2$$

—we can replace these three operations by $a\lambda, (\lambda + \mu), \lambda^2$. But the first two fall under **L** and the latter under **F**. So **F*** is proved.

On the other hand, **L** is extended in quantum mechanics even to the case where $\mathcal{R}, \mathcal{S}$ are not simultaneously measurable. We shall discuss this issue later (in **IV.1**), but at present limit ourselves to the observation that even the meaning of $a\mathcal{R} + b\mathcal{S}$ for $\mathcal{R}, \mathcal{S}$ not simultaneously measurable is not yet clear.

Apart from the physical quantities $\mathcal{R}$ there exists another category of concepts that are important objects of physics—namely, the *properties* of the states of the system **S**. Some such properties are: that a certain quantity $\mathcal{R}$ takes a value λ. Or that the value of $\mathcal{R}$ is positive. Or that the values of two simultaneously observable quantities $\mathcal{R}, \mathcal{S}$ are λ and μ respectively. Or that the sum of the squares of these values is > 1, etc. We have denoted quantities

by $\mathcal{R}, \mathcal{S}, \ldots$ and will denote their properties by $\mathfrak{E}, \mathfrak{F}, \ldots$. The hypermaximal operators $\mathsf{R}, \mathsf{S}, \ldots$ correspond to the quantities. What now corresponds to the properties?

To each property $\mathfrak{E}$ we can assign a quantity which we define as follows: each measurement which distinguishes between the presence or absence of $\mathfrak{E}$ is considered to comprise a measurement of this property, such that its value is 1 if $\mathfrak{E}$ is verified, and 0 in the opposite case. This quantity which corresponds to $\mathfrak{E}$ will also be denoted $\mathfrak{E}$.

Such quantities take on only the values 0 and 1, and conversely: each quantity $\mathcal{R}$ which is capable of only these two values corresponds to a property $\mathfrak{E}$, which is evidently this: "the value of $\mathcal{R}$ is $\neq 0$." The quantities $\mathfrak{E}$ that correspond to properties are therefore characterized by this behavior.

That $\mathfrak{E}$ takes on only the values 0 and 1 can also be formulated as follows: Substituting $\mathfrak{E}$ into the polynomial $F(\lambda) = \lambda - \lambda^2$ makes it vanish identically. If $\mathfrak{E}$ has the operator E then $F(\mathfrak{E})$ has the operator $F(\mathsf{E}) = \mathsf{E} - \mathsf{E}^2$; *i.e.*, the condition is that $\mathsf{E} - \mathsf{E}^2 = \mathsf{O}$ or $\mathsf{E}^2 = \mathsf{E}$. In other words: the operator E of $\mathfrak{E}$ is a projection.

The projections E therefore correspond to the properties $\mathfrak{E}$ (through the agency of the corresponding quantities $\mathfrak{E}$ which we just defined). If we introduce, along with the projections E, the closed linear manifolds $\mathcal{M}$ belonging to them ($\mathsf{E} = \mathsf{P}_{\mathcal{M}}$) then the closed linear manifolds $\mathcal{M}$ correspond equally to the properties $\mathfrak{E}$.

Relations among corresponding $\mathfrak{E}$, E and $\mathcal{M}$ will be examined now in detail.

If, in a state ϕ, we want to determine whether or not a property $\mathfrak{E}$ is verified, then we must measure the quantity $\mathfrak{E}$ and ascertain whether its value is 1 or 0 (these processes are identical by definition). The probability of the former, *i.e.*, that $\mathfrak{E}$ is verified, is consequently equal to the expectation value of $\mathfrak{E}$

$$(\mathsf{E}\phi, \phi) = \|\mathsf{E}\phi\|^2 = \|\mathsf{P}_{\mathcal{M}}\phi\|^2$$

and that of the latter; *i.e.*, that $\mathfrak{E}$ is not verified, is equal to the expectation value of $1 - \mathfrak{E}$

$$((\mathsf{I} - \mathsf{E})\phi, \phi) = \|(\mathsf{I} - \mathsf{E})\phi\|^2 = \|\phi - \mathsf{P}_{\mathcal{M}}\phi\|^2$$

(The sum, of course, is equal to (ϕ, ϕ); *i.e.*, to 1.) Consequently, $\mathfrak{E}$ is certainly present or certainly absent according as the second or first probability is equal to zero; *i.e.*, according as $\mathsf{P}_{\mathcal{M}}\phi = \phi$ or $\mathsf{P}_{\mathcal{M}}\phi = 0$. That is, according as ϕ belongs to $\mathcal{M}$ or is orthogonal to $\mathcal{M}$; *i.e.*, according as ϕ belongs to $\mathcal{M}$ or to $\mathcal{R}_\infty - \mathcal{M}$.

$\mathcal{M}$ can therefore be defined as the set of all ϕ which possess the property $\mathfrak{E}$ with certainty. (Such ϕ are found actually only in the subset of $\mathcal{M}$ that lies on the surface $\|\phi\| = 1$. $\mathcal{M}$ itself is obtained by multiplying these ϕ with positive constants and the adjunction of 0.)

If we call the property opposite that of $\mathfrak{E}$ (the denial of $\mathfrak{E}$) "not $\mathfrak{E}$," then it follows immediately from the above that if E, $\mathcal{M}$ belong to $\mathfrak{E}$, then $\mathsf{I}-\mathsf{E}$ and $\mathcal{R}_\infty - \mathcal{M}$ belong to "not $\mathfrak{E}$."

As with quantities, there arises here also the question of the simultaneous measurability (or rather, the simultaneous decidability) of properties. It is clear that properties $\mathfrak{E}$, $\mathfrak{F}$ are simultaneously decidable if and only if the corresponding quantities $\mathfrak{E}$, $\mathfrak{F}$ are simultaneously measurable (whether with arbitrarily great or with absolute accuracy is unimportant, since they admit only of the values $0, 1$); *i.e.*, if E, F commute. The same holds for several properties $\mathfrak{E}$, $\mathfrak{F}$, $\mathfrak{G}$, ...

From properties $\mathfrak{E}$, $\mathfrak{F}$ which are simultaneously decidable we can form the additional properties "$\mathfrak{E}$ and $\mathfrak{F}$" and "$\mathfrak{E}$ or $\mathfrak{F}$." The quantity corresponding to "$\mathfrak{E}$ and $\mathfrak{F}$" is 1 if those corresponding to $\mathfrak{E}$ and to $\mathfrak{F}$ are both 1, and it is 0 if one (or both) of these is 0. Hence, it is the product of these quantities. By F^* its operator is the product of the operators of $\mathfrak{E}$ and $\mathfrak{F}$; *i.e.*, EF. By THEOREM 14, **II.4** the corresponding closed linear manifold $\mathcal{P}$ is the set common to $\mathcal{M}$, $\mathcal{N}$.

On the other hand, "$\mathfrak{E}$ or $\mathfrak{F}$" can be written

"not [(not $\mathfrak{E}$) and (not $\mathfrak{F}$)]"

and therefore its operator is

$$\mathsf{I} - (\mathsf{I}-\mathsf{E})(\mathsf{I}-\mathsf{F}) = \mathsf{E}+\mathsf{F}-\mathsf{EF}$$

(which, because of its origin, is also a projection). Since $\mathsf{F}-\mathsf{EF}$ is a projection, the linear manifold belonging to $\mathsf{E}+\mathsf{F}-\mathsf{EF}$ is $\mathcal{M}+(\mathcal{N}-\mathcal{P})$ (THEOREM 14, **II.4**). It is a subset of $\{\mathcal{M}, \mathcal{N}\}$ and evidently embraces $\mathcal{M}$, whence (by symmetry) also $\mathcal{N}$, and therefore all of $\{\mathcal{M}, \mathcal{N}\}$. Consequently, it is equal to $\{\mathcal{M}, \mathcal{N}\}$ and this, since it is closed, is equal to $[\mathcal{M}, \mathcal{N}]$.

If $\mathfrak{E}$ is a property which is always present (*i.e.*, empty) then the corresponding quantity is identically 1; *i.e.*, $\mathsf{E} = \mathsf{I}$, $\mathcal{M} = \mathcal{R}_\infty$. If, on the other hand, $\mathfrak{E}$ is never present (*i.e.*, impossible) then the corresponding quantity is identically 0; *i.e.*, $\mathsf{E} = \mathsf{O}$, $\mathcal{M} = \mathcal{O}$. If two properties $\mathfrak{E}$, $\mathfrak{F}$ are incompatible then they must at any rate be simultaneously decidable, and "$\mathfrak{E}$ in addition to $\mathfrak{F}$" must be impossible; *i.e.*, E, F commute: $\mathsf{EF} = \mathsf{O}$. But since $\mathsf{EF} = \mathsf{O}$ implies commutativity (THEOREM 14, **II.4**), this by itself is characteristic. If E, F are presumed to be commutative then $\mathsf{EF} = \mathsf{O}$ means merely that the subset common to $\mathcal{M}$ and $\mathcal{N}$ consists only of $\mathcal{O}$. However, the commutativity of E,F does not follow from this alone. Indeed, $\mathsf{EF} = \mathsf{O}$ is equivalent to all $\mathcal{M}$ being orthogonal to all $\mathcal{N}$.

If $\mathfrak{R}$ is a quantity with operator R to which belongs the resolution of the identity $\mathsf{E}(\lambda)$, then the operator of the property "$\mathfrak{R}$ lies in the interval $I = \{\lambda', \mu'\}$" $(\lambda' \leqslant \mu')$ is $\mathsf{E}(\mu') - \mathsf{E}(\lambda')$. To say this it suffices to observe that the probability

of the above proposition is $\big((\mathsf{E}(\mu')-\mathsf{E}(\lambda'))\phi,\phi\big)$ (see **P** in **II.1**). Phrased another way: the quantity belonging to the property in question is $\mathfrak{E}=F(\mathfrak{R})$, where

$$F(\lambda)=\begin{cases}1 & \text{for} \quad \lambda'<\lambda\leqslant\mu'\\ 0 & \text{otherwise}\end{cases}$$

and $F(\mathsf{R})=\mathsf{E}(\mu')-\mathsf{E}(\lambda')$ (see **II.8** or **III.1**). We called this operator $\mathsf{E}(I)$ in **III.1**.

Summarizing, we have thus obtained the following information about the relations among properties $\mathfrak{E}$, their projections E and the closed linear manifolds of these projections:

α) In the state ϕ the property $\mathfrak{E}$ is or is not present with the probabilities

$$(\mathsf{E}\phi,\phi)=\|\mathsf{E}\phi\|^2=\|\mathsf{P}_{\mathcal{M}}\phi\|^2$$

and

$$((\mathsf{I}-\mathsf{E})\phi,\phi)=\|(\mathsf{I}-\mathsf{E})\phi\|^2=\|\phi-\mathsf{P}_{\mathcal{M}}\phi\|^2$$

respectively.

β) $\mathfrak{E}$ is certainly present or certainly absent for the ϕ of $\mathcal{M}$ and $\mathcal{R}_\infty-\mathcal{M}$ respectively, and only for these.

γ) For the simultaneous decidability of several properties $\mathfrak{E},\mathfrak{F},\dots$ the commutativity of their operators $\mathsf{E},\mathsf{F},\dots$ is characteristic.

δ) If $\mathsf{E},\mathcal{M}$ belong to $\mathfrak{E}$ then $\mathsf{I}-\mathsf{E},\mathcal{R}_\infty-\mathcal{M}$ belong to "not $\mathfrak{E}$."

ε) If $\mathsf{E},\mathcal{M}$ belong to $\mathfrak{E}$ and $\mathsf{F},\mathcal{N}$ belong to $\mathfrak{F}$ and if $\mathfrak{E},\mathfrak{F}$ can be decided simultaneously, then EF and the common part of $\mathcal{M},\mathcal{N}$ belong to "$\mathfrak{E}$ and $\mathfrak{F}$," while $\mathsf{E}+\mathsf{F}-\mathsf{EF}$, $\{\mathcal{M},\mathcal{N}\}$ (this is equal to $[\mathcal{M},\mathcal{N}]$) belong to "$\mathfrak{E}$ or $\mathfrak{F}$."

η) $\mathfrak{E}$ always holds if $\mathsf{E}=\mathsf{I}$ (which is to say: if $\mathcal{M}=\mathcal{R}_\infty$); it never holds if $\mathsf{E}=\mathsf{O}$ (which is to say: if $\mathcal{M}=\mathcal{O}$).

θ) $\mathfrak{E},\mathfrak{F}$ are incompatible if $\mathsf{EF}=\mathsf{O}$ (which is to say: if all $\mathcal{M}$ is orthogonal to all $\mathcal{N}$).

ζ) Let $\mathcal{R}$ be a quantity, R is operator, and I an interval. Let $\mathsf{E}(\lambda)$ be the resolution of the identity belonging to R, $I=\{\lambda',\mu'\}$, $(\lambda'\leqslant\mu')$, $\mathsf{E}(I)=\mathsf{E}(\mu')-\mathsf{E}(\lambda')$ (see **III.1**). Then the operator $\mathsf{E}(I)$ belongs to the property "$\mathfrak{R}$ lies in I."

From ***α*** – ***ζ*** we can derive the earlier probability statements $\mathbf{P},\mathbf{E}_1,\mathbf{E}_2$, as well as the statements of **III.3** on simultaneous measurability. It is clear that the latter are equivalent to ***γ***; **P** follows from ***α***, ***ε***, ***ζ*** and has $\mathbf{E}_1,\mathbf{E}_1$ as consequences.

As can be seen, the relation between the properties of a physical system on the one hand, and the projections on the other, makes possible a sort of logical calculus involving those concepts. However, in contrast to the concepts

of ordinary logic, this system is extended by the concept of "simultaneous decidability" which is characteristic for quantum mechanics.

Moreover, the calculus of these propositions, based on projections, has the advantage over the calculus of quantities, which is based on the totality of (hypermaximal) Hermitian operators, in that the concept of "simultaneous decidability" represents a refinement of the concept of "simultaneous measurability." For example: In order for the questions "does $\mathcal{R}$ lie in I?" and "does $\mathcal{S}$ lie in J?" (here $\mathcal{R}, \mathcal{S}$ have operators R, S of which the respective resolutions of the identity are $\mathsf{E}(\lambda), \mathsf{F}(\mu)$ and $I = \{\lambda', \lambda''\}, J = \{\mu', \mu''\}$) to be simultaneously decidable we require (by $\boldsymbol{\gamma}, \boldsymbol{\zeta}$) only that the operators

$$\mathsf{E}(I) = \mathsf{E}(\lambda'') - \mathsf{E}(\lambda') \qquad \text{and} \qquad \mathsf{F}(J) = \mathsf{F}(\mu'') - \mathsf{F}(\mu')$$

commute. For simultaneous measurability of $\mathcal{R}, \mathcal{S}$, however, the commutativity of all $\mathsf{E}(\lambda)$ with all $\mathsf{F}(\mu)$ is necessary.

6. RADIATION THEORY

We have obtained once again the statistical statements of quantum mechanics developed in **I.2**, substantially generalized and systematically arranged—with one exception. We are lacking the Heisenberg expression for the transition probability from one stationary state of a quantized system to another—although this played an important role in the development of quantum mechanics (see the comments in **I.2**). Following the method of Dirac,[138] we shall now show how these transition probabilities can be derived from the ordinary statistical statements of quantum mechanics; *i.e.*, from the theory just now developed. This is all the more important since such a derivation will give us deeper insight into the mechanism of transitions of the stationary states, and into the Einstein-Bohr energy-frequency conditions. The radiation theory advanced by Dirac is one of the most beautiful achievements in the quantum mechanical field.

Let **S** be a system (say, a quantized atom) with an energy which corresponds to the Hermitian operator H_0. We represent the coordinates which describe the configuration space of **S** by a single symbol ξ (if, for example, **S** consists of ℓ particles then there are 3ℓ cartesian coordinates:

$$x_1 = q_1, y_1 = q_2, z_1 = q_3, \ldots, x_\ell = q_{3\ell-2}, y_\ell = q_{3\ell-1}, z_\ell = q_{3\ell}$$

—ξ stands for all of these together). Furthermore, we assume for simplicity that H_0 has a pure discrete spectrum: eigenvalues $w_1, w_2, \ldots$ and eigenfunctions $\phi_1(\xi), \phi_2(\xi), \ldots$ (several w_m may coincide). An arbitrary state of **S**—*i.e.*, a wave function $\phi(\xi)$—is developed according to the time-dependent Schrödinger

[138] Proc.Roy.Soc.**114**(1927). See also the presentation in Weyl, *Gruppentheorie und Quantenmechanik*, 2nd edition, p. 91 ff. Leipzig (1931).

equation (see **III.2**):

$$\frac{\hbar}{i}\frac{\partial}{\partial t}\phi_t(\xi) = -\mathsf{H}_0\,\phi_t(\xi)$$

So if at $t = t_0$

$$\phi_t(\xi) = \phi(\xi) = \sum_{k=1}^{\infty} a_k\phi_k(\xi)$$

then at general times

$$\phi_t(\xi) = \sum_{k=1}^{\infty} a_k e^{-\frac{i}{\hbar}w_k(t-t_0)}\phi_k(\xi)$$

The eigenstate $\phi_k(\xi)$ therefore evolves into $e^{-\frac{i}{\hbar}w_k(t-t_0)}\phi_k(\xi)$; *i.e.*, into itself (since the factor $e^{-\frac{i}{\hbar}w_k(t-t_0)}$ is irrelevant). Hence the $\phi_k(\xi)$ are stationary. Thus we find in general no transitions from one into another. How is it that we do nevertheless speak of such transitions? The answer is simple. We have disregarded the agent that causes these transitions—radiation. The stationary quantum orbits break down, on the basis of the original Bohr theory, only under the emission of radiation (see the reference in Note 5), but if this is neglected (as in the set-up just given) then it is quite possible that absolute and permanent stability results. We must therefore extend the system to be investigated, so that we include the radiation which may be emitted by **S**; *i.e.*, we must include, in general, all the radiation which can interact with **S** under any circumstances. If we denote by **L** the system which is formed by the radiation (*i.e.*, the electromagnetic field of classical theory, less the stationary field resulting from the electronic and nuclear charges), then it is **S** + **L** that we must investigate.

To that end, we must first accomplish the following:

1. Construct a quantum mechanical description of **L**; to accomplish that we must possess a description of the configuration space of **L**.

2. Construct the energy operator of **S** + **L**. This problem resolves into three parts:

   α) Look to the energy of **S**, which is present independently of **L**; *i.e.*, to the unperturbed energy of **S**. This is described by the operator H_0

   β) Look to the energy of **L**, which is present independently of **S**; *i.e.*, to the unperturbed energy of **L**. This is described by an operator that we will call H_1

   γ) Look to the energy associated with the interaction of **S** and **L**. This is described by an operator that we will call H_i

Clearly we have questions here which, in accord with the fundamental principles of quantum mechanics, must first be answered classically. The results so obtained can then be translated into operator form (see **I.2**). We therefore adopt (at

first) a purely classical point of view relative to the nature of the radiation: we consider it (in the sense of the electromagnetic theory of radiation) as an oscillatory state of the electromagnetic field.[139]

In order to avoid unnecessary complications (the loss of radiation in infinite space, etc.) we consider **S** and **L** to be enclosed within a very large cavity $\mathcal{H}$ of volume $\mathcal{V}$ which shall have perfectly reflecting walls. As is well known, the state of the electromagnetic field in $\mathcal{H}$ is described by electric and magnetic field strengths $\boldsymbol{E} = \{E_x, E_y, E_z\}$ and $\boldsymbol{H} = \{H_x, H_y, H_z\}$. All quantities $\{E_x, \ldots, H_z\}$ are functions of the cartesian coordinates x, y, z in $\mathcal{H}$ and of the time t. It should also be pointed out that we shall now frequently consider real space vectors $\boldsymbol{a} = \{a_x, a_y, a_z\}$, $\boldsymbol{b} = \{b_x, b_y, b_z\}$, etc. (for example $\boldsymbol{E}$, $\boldsymbol{H}$). And for these, concepts such as the inner or scalar product

$$[\boldsymbol{a}, \boldsymbol{b}] = a_x b_x + a_y b_y + a_z b_z$$

which will not be confused with the inner product (ϕ, ψ) in $\mathfrak{R}_\infty$. We denote the differential operator

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

by $\triangle$, and will denote some well-known vector operations by div, curl, grad. The vectors $\boldsymbol{E}, \boldsymbol{H}$ satisfy the Maxwell equations in the empty space $\mathcal{H}$:

$$\begin{aligned} \mathrm{div}\boldsymbol{H} &= 0, \qquad & \mathrm{curl}\,\boldsymbol{E} + \tfrac{1}{c}\tfrac{\partial}{\partial t}\boldsymbol{H} &= \boldsymbol{0} \\ \mathrm{div}\boldsymbol{E} &= 0, \qquad & \mathrm{curl}\,\boldsymbol{H} - \tfrac{1}{c}\tfrac{\partial}{\partial t}\boldsymbol{E} &= \boldsymbol{0} \end{aligned}$$

The first equation of the first row is satisfied by $\boldsymbol{H} = \mathrm{curl}\boldsymbol{A}$, where $\boldsymbol{A} = \{A_x, A_y, A_z\}$ is the so-called vector potential; its components also depend on x, y, z, t. The second equation in that row then follows from $\boldsymbol{E} = -\frac{1}{c}\frac{\partial}{\partial t}\boldsymbol{A}$ and the equations of the second row become

A $$\mathrm{div}\boldsymbol{A} = 0, \qquad \triangle\boldsymbol{A} - \tfrac{1}{c^2}\tfrac{\partial^2}{\partial t^2}\boldsymbol{A} = \boldsymbol{0}$$

(The vector potential is usually introduced in a somewhat different way in order to improve the symmetry in space and time. That the present set-up for $\boldsymbol{A}$ furnishes a general solution for Maxwell's equations—where it is to be noted that the first equation in the second row actually gives only $\frac{\partial}{\partial t}\mathrm{div}\boldsymbol{A} = 0$; *i.e.*, $\mathrm{div}\boldsymbol{A} = f(x, y, z)$—is shown in most treatments of the Maxwell theory, so will not be developed to any extent here: see the reference in Note 139.) **A** provides our starting point for the following discussion. The fact that (by assumption) the walls of $\mathcal{H}$ are reflecting is expressed by the condition that $\boldsymbol{A}$ must be perpendicular to the walls at the boundaries of $\mathcal{H}$. The well-known

[139] The interested reader will find treatments of the electromagnetic theory of radiation in any electromagnetic textbook; see, for example, Abraham and Becker, *Theorie der Electrizität*, Berlin, 1930. See these also for the following developments, which belong to the framework of the Maxwell theory.

method for finding all such $\boldsymbol{A}$'s is this: Since t nowhere enters explicitly into the problem, the most general $\boldsymbol{A}$ is a linear combination of all those solutions which are products of an $\{x, y, z\}$-dependent vector with a t-dependent scalar:

$$\boldsymbol{A} = \boldsymbol{A}(x, t, z, t) = \overline{\boldsymbol{A}}(x, y, z) \cdot \tilde{q}(t)$$

Therefore $\mathbf{A}$ gives

$\mathbf{A}_1$ $\qquad \mathrm{div}\overline{\boldsymbol{A}} = 0, \quad \triangle\overline{\boldsymbol{A}} = \eta\overline{\boldsymbol{A}}, \quad \overline{\boldsymbol{A}} \perp$ boundary at boundary of $\boldsymbol{\mathcal{H}}$

$\mathbf{A}_2$ $\qquad \dfrac{\partial^2}{\partial t^2}\tilde{q}(t) = c^2\eta \cdot \tilde{q}(t)$

Because of $\mathbf{A}_1$, η is t-independent. But because of $\mathbf{A}_2$ it is $\{x, y, z\}$-independent. Therefore η is constant.

$\mathbf{A}_1$ therefore poses an eigenvalue problem, in which η is the eigenvalue parameter and $\overline{\boldsymbol{A}}$ the general eigenfunction. The theory of this problem is fully known and we shall give only the results here:[140] $\mathbf{A}_1$ has a pure discrete spectrum, and all eigenvalues $\eta_1, \eta_2, \ldots$ (let the corresponding $\overline{\boldsymbol{A}}$ be $\overline{\boldsymbol{A}}_1, \overline{\boldsymbol{A}}_2, \ldots$) are negative, and $\eta_n \to -\infty$ as $n \to \infty$. We can normalize the complete set $\overline{\boldsymbol{A}}_1, \overline{\boldsymbol{A}}_2, \ldots$ by

$$\iiint_{\boldsymbol{\mathcal{H}}} [\overline{\boldsymbol{A}}_m, \overline{\boldsymbol{A}}_n] dx dy dz = \begin{cases} 4\pi c^2 & \text{for} \quad m = n \\ 0 & \text{for} \quad m \neq n \end{cases}$$

(We choose $4\pi c^2$ instead of the customary 1 because it will prove to be somewhat more practical later.) If we adopt the notation

$$\eta_n = -\frac{4\pi^2\rho_n^2}{c^2} < 0$$

then $\mathbf{A}_2$ gives

$$\tilde{q}_n(t) = \gamma \cos 2\pi\rho_n(t - \tau) \quad : \quad (\gamma, \tau \text{ arbitrary})$$

Therefore the general solution $\boldsymbol{A}$ can be developed

$$\begin{aligned} \boldsymbol{A} = \boldsymbol{A}(x, y, z, t) &= \sum_{n=1}^{\infty} \overline{\boldsymbol{A}}_n(x, y, z) \cdot \tilde{q}_n(t) \\ &= \sum_{n=1}^{\infty} \overline{\boldsymbol{A}}_n(x, y, z) \cdot \gamma_n \cos 2\pi\rho_n(t - \tau_n) \end{aligned}$$

where $\gamma_1, \gamma_2, \ldots, \tau_1, \tau_2, \ldots$ are arbitrary constants. The energy of the arbitrary field

$$\boldsymbol{A} = \sum_{n=1}^{\infty} \overline{\boldsymbol{A}}_n(x, y, z) \cdot \tilde{q}_n(t)$$

[140] See R. Courant and D. Hilbert, *Methoden der mathematischen Physik I*, pages 358–362, Berlin 1924.

($\boldsymbol{A}$ is now not assumed to be a solution of $\mathbf{A}$; *i.e.*, the $\tilde{q}_n(t)$ are arbitrary) can be written

$$\begin{aligned} E &= \tfrac{1}{8\pi}\iiint_{\mathcal{H}} \big([\boldsymbol{E},\boldsymbol{E}]+[\boldsymbol{H},\boldsymbol{H}]\big)dxdydz \\ &= \tfrac{1}{8\pi}\iiint_{\mathcal{H}} \Big(\tfrac{1}{c^2}[\tfrac{\partial}{\partial t}\boldsymbol{A},\tfrac{\partial}{\partial t}\boldsymbol{A}]+[\mathrm{curl}\boldsymbol{A},\mathrm{curl}\boldsymbol{A}]\Big)dxdydz \\ &= \tfrac{1}{8\pi}\sum_{m,n=1}^{\infty}\iiint_{\mathcal{H}} \Big(\tfrac{1}{c^2}\tfrac{\partial}{\partial t}\tilde{q}_m(t)\tfrac{\partial}{\partial t}\tilde{q}_n(t)[\overline{\boldsymbol{A}}_m,\overline{\boldsymbol{A}}_n] \\ &\qquad + \tilde{q}_m(t)\tilde{q}_n(t)[\mathrm{curl}\overline{\boldsymbol{A}}_m,\mathrm{curl}\overline{\boldsymbol{A}}_n]\Big)dxdydz \end{aligned}$$

Upon integrating by parts,[141] we find

$$\begin{aligned} \iiint_{\mathcal{H}}[\mathrm{curl}\overline{\boldsymbol{A}}_m,\mathrm{curl}\overline{\boldsymbol{A}}_n]dxdydz &= \iiint_{\mathcal{H}}[\mathrm{curl}\ \mathrm{curl}\overline{\boldsymbol{A}}_m,\overline{\boldsymbol{A}}_n]dxdydz \\ &= \iiint_{\mathcal{H}}[-\triangle\overline{\boldsymbol{A}}_m+\mathrm{grad}\ \mathrm{div}\overline{\boldsymbol{A}}_m,\overline{\boldsymbol{A}}_n]dxdydz \\ &= \frac{4\pi^2\rho_m^2}{c^2}\iiint_{\mathcal{H}}[\overline{\boldsymbol{A}}_m,\overline{\boldsymbol{A}}_n]dxdydz \end{aligned}$$

Therefore

$$\begin{aligned} E &= \tfrac{1}{8\pi}\sum_{m,n=1}^{\infty}\left(\tfrac{1}{c^2}\tfrac{\partial}{\partial t}\tilde{q}_m(t)\tfrac{\partial}{\partial t}\tilde{q}_n(t)+\frac{4\pi^2\rho_m^2}{c^2}\tilde{q}_m(t)\tilde{q}_n(t)\right)\cdot\iiint_{\mathcal{H}}[\overline{\boldsymbol{A}}_m,\overline{\boldsymbol{A}}_n]dxdydz \\ &= \tfrac{1}{2}\sum_{m=1}^{\infty}\Big[\Big(\tfrac{\partial}{\partial t}\tilde{q}_m(t)\Big)^2+4\pi^2\rho_m^2\Big(\tilde{q}_m(t)\Big)^2\Big] \end{aligned}$$

But we can regard the $\tilde{q}_1,\tilde{q}_2\ldots$ as coordinates describing the instantaneous state of the field; *i.e.*, as the coordinates of the configuration space of $\mathbf{L}$. The conjugate momenta $\tilde{p}_m$ (in the sense of classical mechanics!) are obtained from

---

[141] We have

$$\iiint_{\mathcal{H}}[\boldsymbol{a},\mathrm{curl}\,\boldsymbol{b}]dxdydz=\iiint_{\mathcal{H}}[\mathrm{curl}\,\boldsymbol{a},\boldsymbol{b}]dxdydz$$

because of

$$[\boldsymbol{a},\mathrm{curl}\,\boldsymbol{b}]-[\mathrm{curl}\,\boldsymbol{a},\boldsymbol{b}]=\mathrm{grad}(\boldsymbol{a}\times\boldsymbol{b})$$

(here $\boldsymbol{a}\times\boldsymbol{b}$ is the so-called outer or vector product of $\boldsymbol{a},\boldsymbol{b}$) if the normal components of $\boldsymbol{a}\times\boldsymbol{b}$ vanish on the boundary of $\mathcal{H}$. Since $\boldsymbol{a}\times\boldsymbol{b}$ is perpendicular to $\boldsymbol{a}$ and to $\boldsymbol{b}$, this is certainly the case if $\boldsymbol{a}$ or $\boldsymbol{b}$ is perpendicular to the boundary of $\mathcal{H}$. We have $\boldsymbol{a}=\mathrm{curl}\,\boldsymbol{A}_m$, $\boldsymbol{b}=\boldsymbol{A}_n$ so that the former indeed occurs.

the formula

$$E = \tfrac{1}{2}\sum_{m=1}^{\infty}\left[\left(\tfrac{\partial}{\partial t}\tilde{q}_m\right)^2 + 4\pi^2\rho_m^2\tilde{q}_m^2\right]$$

This gives (see **I.2**)

$$\tilde{p}_n = \frac{\partial E}{\partial(\frac{\partial}{\partial t}\tilde{q}_n)} = \tfrac{\partial}{\partial t}\tilde{q}_n \quad \text{whence} \quad E = \tfrac{1}{2}\sum_{n=1}^{\infty}\left[\tilde{p}_n^{\,2} + 4\pi^2\rho_m^2\tilde{q}_n^{\,2}\right]$$

and supplies classical mechanical equations of motion

$$\tfrac{\partial}{\partial t}\tilde{q}_n = +\frac{\partial E}{\partial \tilde{p}_n} = \tilde{p}_n$$
$$\tfrac{\partial}{\partial t}\tilde{p}_n = -\frac{\partial E}{\partial \tilde{q}_n} = -4\pi^2\rho_n^2\tilde{q}_n$$

which conjointly give back precisely the equations $\mathbf{A}_2$ that follow from Maxwell's equations. Consequently Jeans' theorem holds:

> The radiation field **L** can be described classically by coordinates $\tilde{q}_1, \tilde{q}_2, \ldots$ —which are connected through
>
> $$\boldsymbol{A} = \boldsymbol{A}(x,y,z) = \sum_{n=1}^{\infty}\tilde{q}_n\overline{\boldsymbol{A}}(x,y,z)$$
>
> with the instantaneous vector potential $\boldsymbol{A}$ describing the field—with the aid of energy (Hamiltonian function)
>
> $$E = \tfrac{1}{2}\sum_{n=1}^{\infty}\left[\tilde{p}_n^{\,2} + 4\pi^2\rho_m^2\tilde{q}_n^{\,2}\right]$$

A point particle of unit mass constrained to move on a straight line (coordinate $\tilde{q}$) in the presence of the potential field $C\tilde{q}^2, C = 2\pi^2\rho^2$ has energy $\frac{1}{2}[(\partial\tilde{q}/\partial t)^2 + 4\pi^2\rho^2\tilde{q}^2]$ which, since again $\tilde{p} = \partial\tilde{q}/\partial t$, can also be written $\frac{1}{2}[\tilde{p}^2 + 4\pi^2\rho^2\tilde{q}^2]$. The equation of motion of such a particle therefore reads

$$\tfrac{\partial^2}{\partial t^2}\tilde{q} + 4\pi^2\rho^2\tilde{q} = 0$$

of which the solution is $\tilde{q}(t) = \gamma\cos 2\pi\rho(t-\tau)$, $(\gamma, \tau$ arbitrary). Because of the form of its motion, such a mechanical system is called "a linear oscillator of frequency ρ." **L** may therefore be regarded as a set of linear oscillators whose frequencies are the eigenfrequencies dictated by the geometry of $\boldsymbol{\mathcal{H}}$: $\rho_1, \rho_2, \ldots$.

This "mechanical" description of the electromagnetic field is important because it can immediately be reinterpreted in the sense standard to the methods of quantum mechanics. The configuration space of **L** is described by $\tilde{q}_1, \tilde{q}_2, \ldots$ and in the expression for E the $\tilde{p}_n, \tilde{q}_n$ will be replaced by $\frac{\hbar}{i}\frac{\partial}{\partial\tilde{q}_n}$ and $\tilde{q}_n\cdot$

respectively. We will call these operators $\tilde{\mathsf{P}}_n$ and $\tilde{\mathsf{Q}}_n$. Then the questions 1 and $2\boldsymbol{\beta}$ (see again page 161) are answered, and in particular

$$\mathsf{H}_1 = \tfrac{1}{2}\sum_{n-1}^{\infty}\left(\tilde{\mathsf{P}}_n^{\,2} + 4\pi^2\rho_n^2\tilde{\mathsf{Q}}_n^{\,2}\right)$$

is the operator sought in response to $2\boldsymbol{\beta}$. $2\boldsymbol{\alpha}$ was solved previously, since we assumed H_0 to be known. There remains only $2\boldsymbol{\gamma}$, but this will be found now to cause no additional difficulties.

By classical electrodynamics, the interaction of $\mathbf{S}$ with $\mathbf{L}$ is to be calculated in the following way: Let $\mathbf{S}$ consist of ℓ particles (perhaps protons or electrons) with respective charges and masses $e_1, M_1, \ldots, e_\ell, M_\ell$ and cartesian coordinates $x_1 = q_1, y_1 = q_2, z_1 = q_3, \ldots, x_\ell = q_{3\ell-2}, y_\ell = q_{3\ell-1}, z_\ell = q_{3\ell}$ (these were previously denoted ξ) and let $p_1^x, p_1{}^y, p_1^z, \ldots, p_\ell^x, p_\ell{}^y, p_\ell^z$ denote the corresponding momenta. The interaction energy is then (in sufficient approximation)[142]

$$\sum_{\nu=1}^{\ell}\frac{e_\nu}{cM_\nu}\left[p_\nu^x A_x(x_\nu, y_\nu, z_\nu) + p_\nu^y A_y(x_\nu, y_\nu, z_\nu) + p_\nu^z A_z(x_\nu, y_\nu, z_\nu)\right]$$

The corresponding quantum operator is obtained when $p_\nu^x, p_\nu^y, p_\nu^z, x_\nu, y_\nu, z_\nu$ are replaced by operators

$$\tfrac{\hbar}{i}\tfrac{\partial}{\partial x_\nu}, \tfrac{\hbar}{i}\tfrac{\partial}{\partial y_\nu}, \tfrac{\hbar}{i}\tfrac{\partial}{\partial z_\nu}, x_\nu, y_\nu, z_\nu \quad : \quad \nu = 1, 2, \ldots, \ell$$

which we will denote $\mathsf{P}_\nu^x, \mathsf{P}_\nu^y, \mathsf{P}_\nu^z, \mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z$. We have now only to draw upon

$$\boldsymbol{A}(x, y, z) = \sum_{n=1}^{\infty}\tilde{q}_n\overline{\boldsymbol{A}}_n(x, y, z)$$

to obtain the desired H_i:

$$\mathsf{H}_i = \sum_{n=1}^{\infty}\sum_{\nu=1}^{\ell}\frac{e_\nu}{cM_\nu}\tilde{\mathsf{Q}}_n\Big[\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z) + \mathsf{P}_\nu^y\,\overline{A}_{n,y}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z) + \mathsf{P}_\nu^x\,\overline{A}_{n,z}(\mathsf{Q}_\nu^z, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z)\Big]$$

It should be observed that when we proceeded from (say) $p_\nu^x\overline{A}_{n,x}(x, y, z)$ to $\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z)$ we arbitrarily placed the operators in a certain order but might just as well have placed them in reversed order, or perhaps (to achieve Hermiticity) in symmetrized combination:

$$\tfrac{1}{2}[\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z) + \overline{A}_{n,x}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z)\mathsf{P}_\nu^x]$$

[142] See, for example, the reference in Note 138.

Fortunately, such distinctions make no difference in the present context because[143]

$$\begin{aligned}&\left[\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)+\cdots\right]-\left[\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)\mathsf{P}_\nu^x+\cdots\right]\\&=\left[\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)-\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)\mathsf{P}_\nu^x\right]+\cdots\\&=\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)+\cdots\\&=\tfrac{\hbar}{i}\mathrm{div}\overline{\boldsymbol{A}}_n(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)=0\end{aligned}$$

Thus the total energy of our system $\mathbf{S}+\mathbf{L}$—*i.e.*, its operator

$$\mathsf{H}=\mathsf{H}_0+\mathsf{H}_1+\mathsf{H}_i$$

—is now completely specified. But before we proceed further, let us note the following: $\mathbf{S}+\mathbf{L}$'s configuration space is described by the coordinates ξ (*i.e.*, $q_1,\ldots,q_{3\ell}$ which are just other names for $x_1,y_1,z_1,\ldots,x_\ell,y_\ell,z_\ell$) and $\tilde{q}_1,\tilde{q}_2,\ldots$. Therefore the wave function depends on these. But it is inconvenient formally and of doubtful validity to admit systems with infinitely many degrees of freedom, or wave functions with infinitely many arguments. Our work heretofore always assumed the number of coordinates to be finite. We shall therefore begin by considering only the first N of the $\tilde{q}_1,\tilde{q}_2,\ldots$ (namely $\tilde{q}_1,\ldots,\tilde{q}_N$, and shall limit $\boldsymbol{A}$ to linear combinations of $\overline{\boldsymbol{A}}_1,\ldots,\overline{\boldsymbol{A}}_N$), and only after we have obtained a final result based on these will we carry out the necessary transition to the limit $N\to\infty$.

So we have

$$\begin{aligned}\mathsf{H}=\mathsf{H}_0&+\tfrac{1}{2}\sum_{n=1}^{N}\left(\tilde{\mathsf{P}}_n^2+4\pi^2\rho_n^2\tilde{\mathsf{Q}}_n^2\right)\\&+\sum_{n=1}^{N}\sum_{\nu=1}^{\ell}\frac{e_\nu}{cM_\nu}\tilde{\mathsf{Q}}_n\Big[\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)\\&\qquad+\mathsf{P}_\nu^y\,\overline{A}_{n,y}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)+\mathsf{P}_\nu^x\,\overline{A}_{n,z}(\mathsf{Q}_\nu^z,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)\Big]\end{aligned}$$

It is convenient to introduce the (non-Hermitian) operators

$$\begin{aligned}\tilde{\mathsf{R}}_n&=\tfrac{1}{\sqrt{2h\rho_n}}(2\pi\rho_n\tilde{\mathsf{Q}}_n+i\tilde{\mathsf{P}}_n)\\\tilde{\mathsf{R}}_n^*&=\tfrac{1}{\sqrt{2h\rho_n}}(2\pi\rho_n\tilde{\mathsf{Q}}_n-i\tilde{\mathsf{P}}_n)\end{aligned}$$

[143] Since P_ν^x commutes with $\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z$—though not with Q_ν^x—we have to establish the following relation in order to carry out the following manipulations (we neglect superfluous indices, and replace A by F):

$$\mathsf{P}F(\mathsf{Q})-F(\mathsf{Q})\mathsf{P}=\tfrac{\hbar}{i}F'(\mathsf{Q})\quad\text{if}\quad\mathsf{P}=\tfrac{\hbar}{i}\tfrac{\partial}{\partial q},\ \mathsf{Q}=q.$$

This relation, which is of especial importance in matrix theory, can be verified most easily by direct calculation.

in place of $\tilde{\mathsf{Q}}_n$ and $\tilde{\mathsf{P}}_n$. Then

$$\tilde{\mathsf{Q}}_n = \tfrac{1}{2\pi}\sqrt{h/2\rho_n}\,(\tilde{\mathsf{R}}_n + \tilde{\mathsf{R}}_n^*)$$

and because $\tilde{\mathsf{P}}_n\tilde{\mathsf{Q}}_n - \tilde{\mathsf{Q}}_n\tilde{\mathsf{P}}_n = \frac{\hbar}{i}\mathsf{I}$

$$\tilde{\mathsf{R}}_n\tilde{\mathsf{R}}_n^* = \tfrac{1}{2h\rho_n}\,(\tilde{\mathsf{P}}_n^{\,2} + 4\pi^2\rho_n^2\tilde{\mathsf{Q}}_n^{\,2}) + \tfrac{1}{2}\cdot\mathsf{I}$$
$$\tilde{\mathsf{R}}_n^*\tilde{\mathsf{R}}_n = \tfrac{1}{2h\rho_n}\,(\tilde{\mathsf{P}}_n^{\,2} + 4\pi^2\rho_n^2\tilde{\mathsf{Q}}_n^{\,2}) - \tfrac{1}{2}\cdot\mathsf{I}$$

Therefore, in particular, $\tilde{\mathsf{R}}_n\tilde{\mathsf{R}}_n^* - \tilde{\mathsf{R}}_n^*\tilde{\mathsf{R}}_n = \mathsf{I}$ and the energy operator becomes

$$\begin{aligned}\mathsf{H} = \mathsf{H}_0 + \sum_{n=1}^{N} h\rho_n\cdot\tilde{\mathsf{R}}_n^*\tilde{\mathsf{R}}_n + \mathsf{C}\\ + \sum_{n=1}^{N}\sum_{\nu=1}^{\ell}\frac{e_\nu}{2\pi c M_\nu}\sqrt{h/2\rho_\nu}\,(\tilde{\mathsf{R}}_n + \tilde{\mathsf{R}}_n^*)\Big[\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)\\ + \mathsf{P}_\nu^y\,\overline{A}_{n,y}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z) + \mathsf{P}_\nu^x\,\overline{A}_{n,z}(\mathsf{Q}_\nu^z,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)\Big]\end{aligned}$$

in which $\mathsf{C} = \frac{1}{2}\sum_{n=1}^{N} h\rho_n\cdot\mathsf{I}$ (constant). Since an additive constant is meaningless in the expression for the energy, we can neglect C. This is all the more desirable since C becomes infinite for $N\to\infty$, and would therefore upset the proper completion of the theory.

The Hermitian operator $\tilde{\mathsf{R}}_n^*\tilde{\mathsf{R}}_n$ is hypermaximal, and in fact it has a pure discrete spectrum consisting of the numbers $0, 1, 2, \ldots$. The corresponding eigenfunctions are denoted $\psi_0^n(\tilde{q}_n), \psi_1^n(\tilde{q}_n), \psi_2^n(\tilde{q}_n)\ldots$.

(If we write $\frac{1}{2\pi}\sqrt{h/\rho_n}\,q$ in place of $\tilde{q}_n$ then

$$\frac{1}{\sqrt{2h\rho_n}}2\pi\rho_n\tilde{q}_n = 2\pi\sqrt{\rho_n/2h}\,\tilde{q}_n \text{ and } \frac{1}{\sqrt{2h\rho_n}}\,\tfrac{\hbar}{i}\tfrac{\partial}{\partial\tilde{q}_n} = \tfrac{1}{2\pi}\sqrt{h/2\rho_n}\,\tfrac{1}{i}\tfrac{\partial}{\partial\tilde{q}_n}$$

go over into $\frac{1}{\sqrt{2}}q$ and $\frac{1}{\sqrt{2}}\frac{1}{i}\frac{\partial}{\partial q}$ respectively, so that

$$\tilde{\mathsf{R}}_n = \tfrac{1}{\sqrt{2}}(q + \tfrac{\partial}{\partial q}), \qquad \tilde{\mathsf{R}}_n^* = \tfrac{1}{\sqrt{2}}(q + \tfrac{\partial}{\partial q})$$

$$\tilde{\mathsf{R}}_n\tilde{\mathsf{R}}_n^* = -\tfrac{1}{2}\tfrac{\partial^2}{\partial q^2} + \tfrac{1}{2}q^2 + \tfrac{1}{2}$$
$$\tilde{\mathsf{R}}_n^*\tilde{\mathsf{R}}_n = -\tfrac{1}{2}\tfrac{\partial^2}{\partial q^2} + \tfrac{1}{2}q^2 - \tfrac{1}{2}$$

The eigenvalue theory of these operators can be found in many treatises, for example, Courant-Hilbert, page 261, formulas (42), (43) and related subject matter, as well as page 76, formulas (60), (61); or Weyl, *Gruppentheorie und Quantenmechanik*, page 74 and thereafter.)

Since the $\psi_1(\xi), \psi_2(\xi), \ldots$ form a complete orthogonal set in ξ-space, and the $\psi_0^n(\tilde{q}_n), \psi_1^n(\tilde{q}_n), \ldots$ form one in $\tilde{q}$-space, the functions

$$\Phi_{km_1\ldots m_N}(\xi, \tilde{q}_1, \ldots, \tilde{q}_N) = \psi_k(\xi) \cdot \psi^1_{m_1}(\tilde{q}_1) \cdots \psi^N_{m_N}(\tilde{q}_N)$$

($k = 1, 2, \ldots$; $m_1, \ldots, m_M = 0, 1, 2, \ldots$) form a complete orthogonal set in $\{\xi, \tilde{q}_1, \ldots, \tilde{q}_N\}$-space; *i.e.*, in the configuration space. We can then expand $\phi = \phi(\xi, \tilde{q}_1, \ldots, \tilde{q}_N)$ as follows:

$$\begin{aligned}\phi(\xi, \tilde{q}_1, \ldots, \tilde{q}_N) &= \sum_{k=1}^{\infty} \sum_{m_1=0}^{\infty} \cdots \sum_{m_N=0}^{\infty} a_{km_1\ldots m_N} \Phi_{km_1\ldots m_N}(\xi, \tilde{q}_1, \ldots, \tilde{q}_N) \\ &= \sum_{k=1}^{\infty} \sum_{m_1=0}^{\infty} \cdots \sum_{m_N=0}^{\infty} a_{km_1\ldots m_N} \psi_k(\xi) \cdot \psi^1_{m_1}(\tilde{q}_1) \cdots \psi^N_{m_N}(\tilde{q}_N)\end{aligned}$$

It is of no significance that we enumerate the complete orthogonal set and the expansion coefficients with $N + 1$ indices $k, m_1, \ldots, m_N$ instead of one. Indeed, the considerations of **II.2** justify this conclusion. The Hilbert space of wave functions ϕ can also be interpreted as the space of $(N+1)$-fold sequences $a_{km_1\ldots m_N}$ (with finite $\sum_{k=1}^{\infty} \sum_{m_1=0}^{\infty} \cdots \sum_{m_N=0}^{\infty} |a_{km_1\ldots m_N}|^2$).

How in this latter context are we to describe the action of the operator H? In order to answer this question let us first evaluate $\mathsf{H}\Phi_{km_1\ldots m_N}$. Since H_0 operates on ξ alone, and $\psi_k(\xi)$ is an eigenfunction of H_0 with eigenvalue w_k, and since moreover $\tilde{\mathsf{R}}_n^* \tilde{\mathsf{R}}_n$ operates on $\tilde{q}_n$ alone, and $\psi_{m_n}(\tilde{q}_n)$ is the eigenfunction of $\tilde{\mathsf{R}}_n^* \tilde{\mathsf{R}}_n$ with eigenvalue m_n, we have

$$\begin{aligned}\mathsf{H}\Phi_{km_1\ldots m_N} = \Big(w_k + \sum_{n=1}^{N} h\rho_n m_n\Big)\Phi_{km_1\ldots m_N} \\ + \sum_{n=1}^{N} \sum_{\nu=1}^{\ell} \frac{e_\nu}{2\pi c M_\nu} \sqrt{\tfrac{h}{2\rho_n}} \Big[\mathsf{P}^x_\nu \, \overline{A}_{n,x}(\mathsf{Q}^x_\nu, \mathsf{Q}^y_\nu, \mathsf{Q}^z_\nu) \\ + \mathsf{P}^y_\nu \, \overline{A}_{n,y}(\mathsf{Q}^x_\nu, \mathsf{Q}^y_\nu, \mathsf{Q}^z_\nu) + \mathsf{P}^z_\nu \, \overline{A}_{n,z}(\mathsf{Q}^z_\nu, \mathsf{Q}^y_\nu, \mathsf{Q}^z_\nu)\Big] \\ \times \psi_k(\xi) \cdot \psi^1_{m_1}(\tilde{q}_1) \cdots \big(\tilde{\mathsf{R}}_n + \tilde{\mathsf{R}}_n^*\big)\psi^n_{m_n}(\tilde{q}_n) \cdots \psi^N_{m_N}(\tilde{q}_N)\end{aligned}$$

For all operators A which (like those in the $[\cdots]$ expression) affect only the variable ξ we can employ the expansion

$$\mathsf{A}\psi_k(\xi) = \sum_{j=1}^{\infty} (\mathsf{A}\psi_k, \psi_j) \cdot \psi_j(\xi) = \sum_{j=1}^{\infty} A_{kj} \cdot \psi_j(\xi)$$

in which $A_{kj} = (\mathsf{A}\psi_k, \psi_j)$. Furthermore, it is shown in the treatises cited above that

$$\begin{aligned}\tilde{\mathsf{R}}_n \psi^n_m(\tilde{q}_n) &= \begin{cases} \sqrt{m}\, \psi^n_{m-1}(\tilde{q}_n) & : \quad m = 1, 2, \ldots \\ 0 & : \quad m = 0 \end{cases} \\ \tilde{\mathsf{R}}_n^* \psi^n_m(\tilde{q}_n) &= \sqrt{m+1}\, \psi^n_{m+1}(\tilde{q}_n) \quad : \quad m = 0, 1, 2, \ldots\end{aligned}$$

Consequently

$$\begin{aligned}\mathsf{H}\Phi_{km_1\dots m_N} = \Big(w_k + \sum_{n=1}^{N} h\rho_n m_n\Big)\Phi_{km_1\dots m_N} \\ + \sum_{j=1}^{\infty}\sum_{n=1}^{N}\sqrt{\tfrac{h}{2\rho_n}}\Big\{\sum_{\nu=1}^{\ell}\frac{e_\nu}{2\pi c M_\nu}\Big(\mathsf{P}_\nu^x\,\overline{A}_{n,\nu}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^x)+\cdots\Big)_{kj}\Big\} \\ \times\big(\sqrt{m_n+1}\,\Phi_{km_1\dots m_n+1\dots m_N}+\sqrt{m_n}\,\Phi_{km_1\dots m_n-1\dots m_N}\big)\end{aligned}$$

We can now portray H as an $a_{km_1\dots m_N}$ operator: writing

$$\mathsf{H}\sum_{km_1\dots m_N} a_{km_1\dots m_N}\Phi_{a_{km_1\cdots m_N}} = \sum_{km_1\dots m_N} a'_{km_1\dots m_N}\Phi_{a_{km_1\cdots m_N}}$$

we have

$$\mathsf{H}\,a_{km_1\dots m_N} = a'_{km_1\dots m_N}$$

with

$$\begin{aligned}a'_{km_1\dots m_N} = \Big(w_k + \sum_{n=1}^{N} h\rho_n m_n\Big)a_{km_1\dots m_N} \\ + \sum_{j=1}^{\infty}\sum_{n=1}^{N}\sqrt{\tfrac{h}{2\rho_n}}\Big\{\sum_{\nu=1}^{\ell}\frac{e_\nu}{2\pi c M_\nu}\Big(\mathsf{P}_\nu^x\,\overline{A}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^x)+\cdots\Big)_{kj}\Big\} \\ \times\big(\sqrt{m_n+1}\,a_{km_1\dots m_n+1\dots m_N}+\sqrt{m_n}\,a_{km_1\dots m_n-1\dots m_N}\big)\end{aligned}$$

The discussion of H has now been carried far enough for us to undertake the transition to the limit $N\to\infty$. Since the system of indexing the $a_{km_1\dots m_N}$ changes in the process, there arises an entirely new H operator. We must introduce components $a_{km_1m_2\dots}$ with infinitely many indices $m_1, m_2, \dots$. However, we must limit ourselves to sequences $m_1, m_2, \dots$ in which only a finite number of elements are different from zero, if for no other reason than to ensure the finiteness of the sum

$$\sum_{n=1}^{\infty} h\rho_n m_n$$

appearing in H. From now on, therefore, the Hilbert space of all sequences

$$a_{km_1m_2\dots} \text{ with finite } \sum_{k=1}^{\infty}\sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty}\cdots|a_{km_1m_2\dots}|^2$$

will be used in which the indices $k, m_1, m_2, \dots$ range on

$$k = 1, 2, \dots; \quad m_1, m_2, \dots = 0, 1, 2, \dots$$

with only a finite (but arbitrary) number of $m_n \neq 0$.[144] The final form of H is then

$$\begin{aligned}\mathsf{H}\, a_{km_1m_2\dots} &= a'_{km_1m_2\dots} \\ &= \Big(w_k + \sum_{n=1}^{\infty} h\rho_n m_n\Big)\cdot a_{km_1m_2\dots} \\ &\quad + \sum_{j,n=1}^{\infty} W_{kj}^n \Big(\sqrt{m_n+1}\, a_{km_1m_2\dots m_n+1\dots} \\ &\qquad + \sqrt{m_n}\, a_{km_1m_2\dots m_n-1\dots}\Big)\end{aligned}$$

in which W_{kj}^n is defined

$$W_{kj}^n = \sqrt{\tfrac{h}{2\rho_n}} \sum_{\nu=1}^{\ell} \frac{e_\nu}{2\pi c M_\nu} \Big(\mathsf{P}_\nu^x\, \overline{A}_{n,\nu}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^x, \mathsf{Q}_\nu^x) + \cdots\Big)_{kj}$$

Before we draw from this result the physical conclusions that interest us, we should recall that it was obtained on the basis of the electrodynamic theory of radiation. We now want to determine whether or not the standard quantum mechanical transformation which we performed suffices to account for the deviations of radiation from the wave model—for its discrete-corpuscular nature. (Note that it would be quite reasonable to expect that in order to achieve this one would have to start directly from a corpuscular model for light, instead of quantizing the electromagnetic field, as we did here.)

It can immediately be seen in our expression for H that something like the corpuscular light quantum is included in it. Suppose that we neglect the second term, which produces a sort of perturbation, and which—as we shall see later—gives rise to the quantum jumps of the system **S** from one "stationary state" to another. (This latter is the phenomenon which is actually of interest to us, but is nevertheless less striking than attributes of the material system **S** itself, which are already in evidence. As we shall see, those attributes arise from the leading term in H.) After deletion of the second term, we have

$$\mathsf{H}\, a_{km_1m_2\dots} = \Big(w_k + \sum_{n=1}^{\infty} h\rho_n m_n\Big)\cdot a_{km_1m_2\dots}$$

But this expression for the energy can be interpreted as follows: It is the energy

[144] That the totality of these index systems $k, m_1, m_2, \dots$ actually forms a sequence can be shown most simply as follows: Let $\pi_1, \pi_2, \pi_3, \dots$ be the series of prime numbers $2, 3, 5, \dots$. The products $\pi_1^{k-1}\pi_2^{m_1}\pi_3^{m_2}\cdots$ are in reality finite, because all $m_n = 0$ with only a finite number of exceptions, and (except in those exceptional cases) $\pi_{n+1}^{m_n} = 1$. Then if $k, m_1, m_2, \dots$ run through our entire set of allowed possibilities the $\pi_1^{k-1}\pi_2^{m_1}\pi_3^{m_2}\cdots$ run through all numbers $1, 2, 3, \dots$ and assume each value once. We can therefore use the $\pi_1^{k-1}\pi_2^{m_1}\pi_3^{m_2}\cdots$ to obtain a simple running index for the $a_{km_1m_2\dots}$.

w_k of the system **S**, increased by the amounts $h\rho_n m_n$ $(n = 1, 2, \ldots)$. Hence it is plausible to interpret the numbers $m_n = 0, 1, 2, \ldots$ as the numbers of particles with respective energies $h\rho_n$. But $h\rho_n$ is precisely the energy which, according to Einstein, has to be assigned to a light quantum of frequency ρ_n (see Note 134). Consequently the structure of H_1 justifies the view that the electromagnetic field existing in $\boldsymbol{\mathcal{H}}$ (less its electrostatic part)—*i.e.*, **L**—actually consists of light quanta with frequencies $\rho_1, \rho_2, \ldots$ and energies $h\rho_1, h\rho_2, \ldots$. Furthermore, the numbers of such particles are given by the indices $m_1, m_2, \ldots (= 0, 1, 2, \ldots)$. The fact that no other frequencies than $\rho_1, \rho_2, \ldots$ occur is made plausible by the observation that these are the eigenfrequencies of the cavity $\boldsymbol{\mathcal{H}}$. Indeed the vector potentials

$$\overline{\boldsymbol{A}}_n(x, y, z) \cdot \gamma \cos 2\pi\rho_n(t - \tau)$$

represent the only stationary electromagnetic oscillations possible in $\boldsymbol{\mathcal{H}}$.

While these speculations and interpretations are of only heuristic value, a fully satisfactory and final answer to our question can be obtained only if it proves possible for us to arrive at the energy expression H by an argument that proceeds from the light quantum model for the radiation **L**. That we first proceeded from the classical theory of radiation is due to the fact that the pre-quantum mechanical light quantum hypothesis supplied no expression for the interaction energy of a light quantum with matter (the reinterpretation of classical electrodynamics never succeeded in this respect). Now, however, we will be able to determine this interaction term by comparison of coefficients if our result (to be derived by use of a non-specialized expression for the interaction energy) coincides in form with H.

What is the state space of **L** (Question 1, page 161) on the basis of the light quantum hypothesis? A single light quantum (in the space $\boldsymbol{\mathcal{H}}$) may be characterized by certain coordinates whose totality we shall represent by the symbol u.[145] Its stationary states may have the wave functions $\psi_1(u), \psi_2(u), \ldots$

[145] As coordinates of the light quantum we may want to use, for example, its momenta p_x, p_y, p_z as well as a coordinate π describing its state of polarization. The momenta determine the direction of the light quantum —*i.e.*, its direction cosines $\alpha_x, \alpha_y, \alpha_z$ $(\alpha_x^2 + \alpha_y^2 + \alpha_z^2 = 1)$—as well as its frequency ν, its wavelength λ and its energy, because according to Einstein the momentum vector has magnitude $h\nu/c$ (see Note 134). Therefore

$$p_x = \tfrac{h\nu}{c}\alpha_x, \quad p_y = \tfrac{h\nu}{c}\alpha_y, \quad p_z = \tfrac{h\nu}{c}\alpha_z$$

i.e.,

$$\nu = \tfrac{c}{h}\sqrt{p_x^2 + p_y^2 + p_z^2}, \quad \lambda = \tfrac{c}{\nu}, \quad \text{Energy} = h\nu$$

$$\alpha_x = \tfrac{c}{h\nu}\,p_x, \quad \alpha_y = \tfrac{c}{h\nu}\,p_y, \quad \alpha_z = \tfrac{c}{h\nu}\,p_z$$

It is disturbing to observe that our eigen-oscillations $\overline{\boldsymbol{A}}_n(x, y, z) \cdot \gamma \cos 2\pi\rho_n(t - \tau)$ here are standing waves, as could not otherwise be possible in the cavity $\boldsymbol{\mathcal{H}}$ because of its reflecting walls, so that $\overline{\boldsymbol{A}}_n$ can be related to no unique "ray

(which form an orthonormal set) and the energies $E_1, E_2, \dots$. These correspond to the electromagnetic eigen-oscillations $\overline{\boldsymbol{A}}_1, \overline{\boldsymbol{A}}_2, \dots$ with frequencies $\rho_1, \rho_2, \dots$ (in the sense of the Einstein concept $E_n = h\rho_n$, which we shall also prove). In this regard, the following point must be noted: In the electromagnetic discussion we so normalized the energy of the light that its minimum value was 0, which corresponded to the indices $m_1 = m_2 = \cdots = 0$. In effect, we have recognized non-existence as a possible state of the light, which is in fact justified. Yet to quantum mechanics in general such a concept is entirely foreign: each particle contributes coordinates to the state space of the system, and therefore enters so intimately into the formal description of the total system that it appears to be effectively indestructible. After its annihilation, then, we must ascribe to the particle a sort of latent existence, in which its coordinates are still part of the description of the configuration space. Consequently, one of the states

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direction" $\alpha_x, \alpha_y, \alpha_z$. We can see immediately that, along with $\alpha_x, \alpha_y, \alpha_z$, at least the opposite direction $-\alpha_x, -\alpha_y, -\alpha_z$ is also present, and the same holds for the momentum. As a consequence, we must use other coordinates in $\boldsymbol{\mathcal{H}}$ than p_z, p_y, p_z, π. In some recent expositions of this subject this inconvenience has been overcome by the following artifice: Let $\boldsymbol{\mathcal{H}}$ be a parallelepiped

$$-A < x < A, \quad -B < y < B, \quad -C < z < C$$

whose boundary surfaces $x = \pm A$, $y = \pm B$, $z = \pm C$ are not treated as reflecting walls. Rather $x = +A$ is identified with $x = -A$; $y = +B$ with $y = -B$; $z = +C$ with $z = -C$. That is, radiation that impinges at A, y, z resumes at $-A, y, z$ its progress in the same direction (back again into $\boldsymbol{\mathcal{H}}$) as if nothing had happened, etc. (see, for example, the treatment of L. Landau and R. Peierls, Z. Physik **62** (1930)). We can also say that the space is taken to be periodic in the x, y, z directions with respective periods $2A, 2B, 2C$. The analytical treatment remains the same, but the boundary condition is now

$$\begin{aligned} \boldsymbol{A}(A, y, z) &= \boldsymbol{A}(-A, y, z) \\ \boldsymbol{A}(x, B, z) &= \boldsymbol{A}(x, -B, z) \\ \boldsymbol{A}(x, y, C) &= \boldsymbol{A}(x, y, -C) \end{aligned}$$

(instead of $\frac{\partial}{\partial n}\boldsymbol{A} = \boldsymbol{0}$ at the boundary) and the "elementary solutions" with which we perform the expansions are the functions

$$\begin{matrix}\cos \\ \sin\end{matrix}\left[2\pi\nu\big(t - c(\alpha_x x + \alpha_y y + \alpha_z z)\big)\right]$$

(instead of $\overline{\boldsymbol{A}}(x, y, z) \cdot \tilde{q}(t)$). We can easily determine the

$$\nu = \rho_n, \quad \alpha_x = \alpha_{n,x}, \quad \alpha_y = \alpha_{n,y}, \quad \alpha_z = \alpha_{n,z}$$

belonging to the eigen-solutions, and the further development of the theory coincides with that of the text.

$\psi_n(u)$, with energy $E_n = 0$, must correspond to the non-existence of the light quantum. We will write $\psi_0(u)$ to denote that state, so that $\psi_1(u), \psi_2(u), \ldots$ refer to the state of a light quantum that actually exists. But we must include the former to form the complete orthogonal set $\psi_0(u), \psi_1(u), \psi_2(u), \ldots$.

We proceed now to the consideration of **L**; *i.e.*, the system of all light quanta. We include all the light quanta that can ever be represented in **L** —including non-existent light quanta—which are infinite in number. But since it is inconvenient to operate with infinitely many constituents in **L**, we first contemplate the existence of only S light quanta, and at the end pass to the limit $S \to \infty$.[146] We designate these light quanta by the numbers $1, 2, \ldots, S$ and call their coordinates $u_1, \ldots, u_S$. The configuration space of **L** is therefore described by $u_1, \ldots, u_S$, and that of **S**+**L** by $\xi, u_1, \ldots, u_S$. The most general wave function for **S**+**L** is then $f(\xi, u_1, \ldots, u_S)$ and the $\phi_k(\xi) \cdot \psi_{n_1}(u_1) \cdots \psi_{n_S}(u_S)$ form (as k ranges on $1, 2, \ldots$ and the $n_1, \ldots, n_S$ range on $0, 1, 2, \ldots$) a complete orthonormal set.

Light quanta have now the fundamental property of being exactly identical; *i.e.*, there is no conceivable way to distinguish between two light quanta that have the same coordinate u. Put another way: a state in which the light quanta m and n have the corresponding u-values u' and u'' is not distinguishable from the state in which $u_m = u''$ and $u_n = u'$. But this is a classical—not a quantum mechanical—description of the point at issue, since we speak of the value of u, not of the wave function $\phi(u)$: quantum mechanically, this means that the states belonging to the wave functions

$$f(\xi, u_1, \ldots, u_m, \ldots, u_n, \ldots u_S) \quad \text{and} \quad f(\xi, u_1, \ldots, u_n, \ldots, u_m, \ldots u_S)$$

are indistinguishable. That is, each physical quantity $\mathcal{R}$ has the same expectation value in both (therefore, since this also holds for $F(\mathcal{R})$, each physical quantity has also the same statistics; see the discussion of $\mathbf{E}_1$ and $\mathbf{E}_2$ in **III.3**). If we denote the functional operation which permutes u_m, u_n by O_{mn} (O_{mn} is simultaneously Hermitian and unitary, $\mathsf{O}_{mn}^2 = \mathsf{I}$, as is immediately evident), then this means that $\mathcal{R}$ has the same value for f as for $\mathsf{O}_{mn} f$; *i.e.*,

$$(\mathsf{R}f, f) = (\mathsf{R}\mathsf{O}_{mn} f, \mathsf{O}_{mn} f) = (\mathsf{O}_{mn}\mathsf{R}\mathsf{O}_{mn} f, f)$$

Therefore

$$\mathsf{R} = \mathsf{O}_{mn}\mathsf{R}\,\mathsf{O}_{mn} \quad \text{equivalently} \quad \mathsf{O}_{mn}\mathsf{R} = \mathsf{R}\,\mathsf{O}_{mn}$$

This means that in the present context only such operators R are admissible which commute with all O_{mn} ($m, n = 1, 2, \ldots, S$); *i.e.*, (with reference to the definition of the O_{mn}) into which all the coordinates $u_1, \ldots, u_S$ enter symmetrically.

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[146] This transition to the limit $S \to \infty$ is different from the limit transition $N \to \infty$ taken in the electromagnetic theory. For if we interpret the $m_1, m_2, \ldots$ there as numbers of light quanta then N is a limit for the number of incoherent light quanta (*i.e.*, of light quanta not of the same frequency and direction —these together make up its momentum—and polarization; see Note 143), while S is a limit for the total number of light quanta.

A wave function f which is symmetrical in all variables $u_1, \ldots, u_S$, *i.e.*, for which $\mathsf{O}_{mn} f = f$ holds $(m, n = 1, \ldots, S;\ m \neq n)$, is transformed by such an operator R into one of the same kind: $\mathsf{O}_{mn}\mathsf{R}f = \mathsf{R}\,\mathsf{O}_{mn} f = \mathsf{R}f$. These f form a closed manifold, a Hilbert subspace $\overline{\mathfrak{R}}_\infty^{(S)}$ in the Hilbert space $\mathfrak{R}_\infty^{(S)}$ of all f, and the R map elements of $\overline{\mathfrak{R}}_\infty^{(S)}$ onto that same space; *i.e.*, they can be regarded as operators in the Hilbert space $\overline{\mathfrak{R}}_\infty^{(S)}$. Consequently $\overline{\mathfrak{R}}_\infty^{(S)}$ is just as useful for the purposes of quantum mechanics as the space $\mathfrak{R}_\infty^{(S)}$ originally considered, and in view of the symmetry of L with respect to exchanges of light quanta the question arises as to whether one cannot limit oneself to symmetric wave functions; *i.e.*, whether $\mathfrak{R}_\infty^{(S)}$ should be replaced by $\overline{\mathfrak{R}}_\infty^{(S)}$. We shall do this, and the end result—*i.e.*, the complete agreement which will be achieved with the H-expression derived electromagnetically—will ultimately justify our decision to do so.[147]

The $\phi_k(\xi) \cdot \psi_{n_1}(u_1) \cdots \psi_{n_S}(u_S)$ formed a complete orthonormal set in $\mathfrak{R}_\infty^{(S)}$. Making use of this fact, we shall now form one in $\overline{\mathfrak{R}}_\infty^{(S)}$. Let $m_0, m_1, \ldots$ be any numbers (drawn from $\{0, 1, 2, \ldots\}$) with $m_0 + m_1 + \cdots = S$ (therefore only a finite number of them differ from zero). We denote by $[m_1, m_2, \ldots]$ the totality of all index systems $n_1, n_2, \ldots$ in which

$$\begin{gathered} 0 \text{ appears } m_0 \text{ times} \\ 1 \text{ appears } m_1 \text{ times} \\ \vdots \\ k \text{ appears } m_k \text{ times} \\ \vdots \end{gathered}$$

There are exactly $m_0! \cdot m_1! \cdot m_2! \cdots$ such systems. We set

$$\Phi_{m_0 m_1 \ldots}(u_1, \ldots, u_S) = \sum_{n_1 \ldots n_S \text{ in } [m_0, m_1, \ldots]} \psi_{n_1}(u_1) \cdots \psi_{n_S}(u_S)$$

Since $\Phi_{m_0 m_1 \ldots}$ is the sum of $m_0! \cdot m_1! \cdot m_2! \cdots$ pairwise orthogonal summands of magnitude 1, its square is the sum of $m_0! \cdot m_1! \cdots m_2! \cdots$ terms of unit magnitude, and the magnitude of $\Phi_{m_0 m_1 \ldots}$ is therefore $\sqrt{m_0! \cdot m_1! \cdots m_2! \cdots}$. Two different $\Phi_{m_0 m_1 \ldots}$ have pairwise orthogonal summands, and are therefore orthogonal. The functions

$$\psi_{m_0 m_1 \ldots}(u_1, \ldots, u_S) = \frac{1}{\sqrt{m_0! \cdot m_1! \cdots m_2! \cdots}}\, \Phi_{m_0 m_1 \ldots}(u_1, \ldots, u_S)$$

therefore form an orthonormal set. An $f(\xi, u_1, \ldots u_S)$ symmetric in $u_1, \ldots u_S$

[147] This introduction of $\overline{\mathfrak{R}}_\infty^{(S)}$ in place of $\mathfrak{R}_\infty^{(S)}$ is equivalent to replacing ordinary statistics by so-called Bose-Einstein statistics, if we consider its consequences without reference to quantum mechanics. See Dirac in the reference cited in Note 138.

has the same inner product with all sums of $\phi_k(\xi)\Phi_{m_0 m_1 \ldots}(u_1, \ldots u_S)$ functions, hence it is orthogonal to every such sum if it is orthogonal to those functions individually; *i.e.*, to $\phi_k(\xi)\psi_{m_0 m_1 \ldots}(u_1, \ldots u_S)$. And if it is orthogonal to each of the latter it is orthogonal also to all $\phi_k(\xi) \cdot \psi_{n_1}(u_1) \cdots \psi_{n_S}(u_S)$, and therefore it is 0. Consequently the $\phi_k(\xi)\psi_{m_0 m_1 \ldots}(u_1, \ldots u_S)$ (which themselves belong to $\overline{\mathcal{R}}_\infty^{(S)}$) form a complete orthonormal set in $\overline{\mathcal{R}}_\infty^{(S)}$.

Let us now consider the three components of the energy of $\mathbf{S} + \mathbf{L}$. First, there is the energy of $\mathbf{S}$ [$2\boldsymbol{\alpha}$, page 165], whose operator for $\mathbf{S}$ is defined by $\mathsf{H}_0\phi_k(\xi) = w_k\phi_k(\xi)$, and therefore for $\mathbf{S} + \mathbf{L}$ by

$$\mathsf{H}_0\, \phi_k(\xi)\psi_{m_0 m_1 \ldots}(u_1, \ldots u_S) = w_k\, \phi_k(\xi)\psi_{m_0 m_1 \ldots}(u_1, \ldots u_S)$$

Second [$2\boldsymbol{\beta}$], each light quantum ℓ' has energy $\mathsf{H}_{\ell'}\psi_n(u) = E_n\psi_n(u)$. Therefore the m^{th} quantum in $\mathbf{S} + \mathbf{L}$ has energy

$$\begin{aligned}\mathsf{H}_{\ell_m}&\phi_k(\xi) \cdot \psi_{n_1}(u_1) \cdots \psi_{n_m}(u_m) \cdots \psi_{n_S}(u_S) \\ &= E_{n_m}\phi_k(\xi) \cdot \psi_{n_1}(u_1) \cdots \psi_{n_m}(u_m) \cdots \psi_{n_S}(u_S)\end{aligned}$$

from which we form

$$\mathsf{H}_\ell = \mathsf{H}_{\ell_1} + \cdots + \mathsf{H}_{\ell_S}$$

Finally [$2\boldsymbol{\gamma}$], let the interaction energy of a light quantum ℓ' with $\mathbf{S}$ be described by an operator V—at present not known exactly—which we identify by its matrix elements

$$\mathsf{V}_{\ell'}\, \phi_k(\xi)\psi_n(u) = \sum_{j=1}^{\infty}\sum_{p=0}^{\infty} V_{kn|jp}\, \phi_j(\xi)\psi_p(u)$$

In $\mathbf{S} + \mathbf{L}$, for the m^{th} light quantum, we then have

$$\begin{aligned}\mathsf{V}_{\ell_m}&\phi_k(\xi) \cdot \psi_{n_1}(u_1) \cdots \psi_{n_m}(u_m) \cdots \psi_{n_S}(u_S) \\ &= \sum_{j=1}^{\infty}\sum_{p=0}^{\infty} V_{kn_m|jp}\, \phi_j(\xi) \cdot \psi_{n_1}(u_1) \cdots \psi_p(u_m) \cdots \psi_{n_S}(u_S) \\ &= \sum_{j=1}^{\infty} \sum_{p_1 \ldots p_m \ldots p_S=0}^{\infty} \delta(n_1 - p_1) \cdots V_{kn_m|jp_m} \cdots \delta(n_S - p_S) \\ &\qquad\qquad \times \phi_j(\xi) \cdot \psi_{p_1}(u_1) \cdots \psi_{p_m}(u_m) \cdots \psi_{p_S}(u_S)\end{aligned}$$

—here $\delta(n) = \left\{ \begin{array}{l} 1 \text{ for } n = 0 \\ 0 \text{ for } n \neq 0 \end{array} \right\}$—and must form

$$\mathsf{H}_i = \mathsf{V}_{\ell_1} + \cdots + \mathsf{V}_{\ell_S}$$

Altogether, we now have

$$\begin{aligned}
&\mathsf{H}\,\phi_k(\xi)\cdot\psi_{n_1}(u_1)\cdots\psi_{n_S}(u_S)\\
&\quad=(w_k+E_{n_1}+\cdots+E_{n_S})\,\phi_k(\xi)\cdot\psi_{n_1}(u_1)\cdots\psi_{n_S}(u_S)\\
&\qquad+\sum_{j=1}^{\infty}\sum_{p_1\ldots p_m\ldots p_S=0}^{\infty}\sum_{m=1}^{S}\delta(n_1-p_1)\cdots V_{kn_m|jp_m}\cdots\delta(n_S-p_S)\\
&\qquad\qquad\times\phi_j(\xi)\cdot\psi_{p_1}(u_1)\cdots\psi_{p_S}(u_S)
\end{aligned}$$

By a simple transformation this becomes

$$\begin{aligned}
&\mathsf{H}\,\phi_k(\xi)\Phi_{m_0m_1\ldots}(u_1,\ldots,u_S)\\
&\quad=\Big(w_k+\sum_{n=0}^{\infty}m_nE_n\Big)\phi_k(\xi)\Phi_{m_0m_1\ldots}(u_1,\ldots,u_S)\\
&\qquad+\sum_{j=1}^{\infty}\sum_{n,p=0}^{\infty}m_nV_{kn|jp}\,\phi_j(\xi)\Phi_{m_0m_1\ldots m_n-1\ldots m_p+1\ldots}(u_1,\ldots,u_S)
\end{aligned}$$

where in the case $n=p$ the subscript $_{m_0m_1\ldots m_n-1\ldots m_p+1\ldots}$ is to be replaced by $_{m_0m_1\ldots\ldots m_n\ldots\ldots}$. When expressed in terms of the orthonormal functions this result becomes

$$\begin{aligned}
&\mathsf{H}\,\phi_k(\xi)\psi_{m_0m_1\ldots}(u_1,\ldots,u_S)\\
&\quad=\Big(w_k+\sum_{n=0}^{\infty}m_nE_n\Big)\phi_k(\xi)\psi_{m_0m_1\ldots}(u_1,\ldots,u_S)\\
&\qquad+\sum_{j=1}^{\infty}\sum_{n,p=0}^{\infty}\sqrt{m_n(m_p+1-\delta(n-p))}\,V_{kn|jp}\\
&\qquad\qquad\times\phi_j(\xi)\,\psi_{m_0m_1\ldots m_n-1\ldots m_p+1\ldots}(u_1,\ldots,u_S)
\end{aligned}$$

We can expand the general $f(\xi,u_1,\ldots,u_S)$ of $\overline{\mathfrak{R}}_\infty^{(S)}$ in terms of these orthonormal functions:

$$f(\xi,u_1,\ldots,u_S)=\sum_{k=1}^{\infty}\sum_{\substack{m_0m_1\ldots=0\\ m_1+m_2+\cdots=S}}^{\infty}a_{k\,m_0m_1\ldots}\phi_k(\xi)\psi_{m_0m_1\ldots}(u_1,\ldots,u_S)$$

Therefore $\overline{\mathfrak{R}}_\infty^{(S)}$ can be conceived as the Hilbert space of sequences $a_{k\,m_0m_1\ldots}$ with $k=1,2,\ldots;\ m_0,m_1,\ldots=0,1,2,\ldots;\ m_1+m_2+\ldots=S$ and with finite

$$\sum_{k\,m_0m_1\ldots}|a_{k\,m_0m_1\ldots}|^2$$

In that language, the defining action of H reads $\mathsf{H}a_{k\,m_0m_1\ldots}=a'_{k\,m_0m_1\ldots}$ which

when spelled out in detail means

$$\mathsf{H}\sum_{k=1}^{\infty}\sum_{\substack{m_0m_1\ldots=0\\ m_1+m_2+\cdots=S}}^{\infty} a_{k\,m_0m_1\ldots}\phi_k(\xi)\,\psi_{m_0m_1\ldots}(u_1,\ldots,u_S)$$
$$=\sum_{k=1}^{\infty}\sum_{\substack{m_0m_1\ldots=0\\ m_1+m_2+\cdots=S}}^{\infty} a'_{k\,m_0m_1\ldots}\phi_k(\xi)\,\psi_{m_0m_1\ldots}(u_1,\ldots,u_S)$$

where results now in hand supply

$$a'_{k\,m_0m_1\ldots}=\Big(w_k+\sum_{n=0}^{\infty}m_nE_n\Big)a_{k\,m_0m_1\ldots}$$
$$+\sum_{j=1}^{\infty}\sum_{n,p=0}^{\infty}\sqrt{m_n(m_p+1-\delta(n-p))}\,\overline{V_{kn|jp}}$$
$$\times\, a_{j\,m_0m_1\ldots m_n-1\ldots m_p+1\ldots}$$

(Here the subscripts k,j and n,p have exchanged roles relative to those in the $\phi_k(\xi)\psi_{m_0m_1\ldots}(u_1,\ldots,u_S)$ formula; in place of $V_{jp|kn}$ we have written $\overline{V_{kn|jp}}$, keeping in mind the Hermitian nature of V.)

We proceed now to prepare for the transition to the limit $S\to\infty$. Since m_0 is determined by $m_1,m_2,\ldots$ (use $m_0=S-m_1-m_2-\cdots$) we can write $a_{k\,m_1m_2\ldots}$ in place of $a_{k\,m_0m_1m_2\ldots}$. In this way the ranges of the indices become

$$k=1,2,\ldots;\quad m_1,m_2,\ldots=0,1,2,\ldots;\quad m_1+m_2+\cdots\leqslant S$$

If we consider $E_0=0$ and introduce the notation

$$SV_{k0|j0}=V_{k|j}$$
$$\sqrt{S}V_{k0|jn}=V_{k|jn}$$
$$\sqrt{S}V_{kn|j0}=\overline{V}_{j|kn}\quad:\quad V_{kn|jp}\text{ is Hermitian!}$$

then $\mathsf{H}a_{k\,m_1m_2\ldots}=a'_{k\,m_1m_2\ldots}$ with

$$a'_{k\,m_1m_2\ldots}=\Big(w_k+\sum_{n=1}^{\infty}m_nE_n\Big)a_{k\,m_1m_2\ldots}$$
$$+\sum_{j=1}^{\infty}V_{k|j}\,a_{j\,m_1m_2\ldots}$$
$$+\sum_{j=1}^{\infty}\sum_{n=1}^{\infty}\sqrt{m_n}\frac{\sqrt{1+S-m_1-m_2-\cdots}}{\sqrt{S}}V_{j|kn}\,a_{j\,m_1m_2\ldots m_n-1\ldots}$$
$$+\sum_{j=1}^{\infty}\sum_{n=1}^{\infty}\sqrt{m_n+1}\frac{\sqrt{S-m_1-m_2-\cdots}}{\sqrt{S}}\overline{V_{k|jn}}\,a_{j\,m_1m_2\ldots m_n+1\ldots}$$
$$+\sum_{j=1}^{\infty}\sum_{n,p=1}^{\infty}\sqrt{m_n(m_p+1)}\,\overline{V_{kn|jp}}\,a_{j\,m_1m_2\ldots m_n-1\ldots m_p+1\ldots}$$

Now let $S \to \infty$. The $a_{k\,m_1 m_{2\ldots}}$ are again defined over all sequences $k\,m_1 m_2 \ldots$ with $k = 1, 2, \ldots$; $m_1, m_2, \ldots = 0, 1, 2, \ldots$ with only a finite (but arbitrary) number of $m_n \neq 0$ (see Note 144). For H we obtain in the limit

$$\mathsf{H} a_{k\,m_1 m_{2\ldots}} = a'_{k\,m_1 m_{2\ldots}}$$

with

$$\begin{aligned} a'_{k\,m_1 m_{2\ldots}} = &\Big(w_k + \sum_{n=1}^{\infty} m_n E_n\Big) a_{k\,m_1 m_{2\ldots}} \\ &+ \sum_{j=1}^{\infty} V_{k|j}\, a_{j\,m_1 m_{2\ldots}} \\ &+ \sum_{j=1}^{\infty}\sum_{n=1}^{\infty} \sqrt{m_n + 1}\, V_{j|kn}\, a_{j\,m_1 m_2 \ldots m_n{+}1\ldots} \\ &+ \sum_{j=1}^{\infty}\sum_{n=1}^{\infty} \sqrt{m_n}\, \overline{V_{k|jn}}\, a_{j\,m_1 m_2 \ldots m_n{-}1\ldots} \\ &+ \sum_{j=1}^{\infty}\sum_{n,p=1}^{\infty} \sqrt{m_n(m_p+1)}\, \overline{V_{kn|jp}}\, a_{j\,m_1 m_2 \ldots m_n{-}1\ldots m_p{+}1\ldots} \end{aligned}$$

The similarity with the equation derived from the electromagnetic theory of radiation is now apparent. To make the two identical (compare page 171) we need only set

$$E_n = h\rho_n, \quad V_{k|j} = 0, \quad V_{k|jn} = W^n_{jk} = \overline{W}^n_{kj}, \quad V_{kn|jp} = 0$$

We then see that the light quanta concept proves to be identical to the classical electromagnetic concept if we observe these rules:

1. The latter is rewritten according to the general quantum mechanical scheme.
2. The energy of each light quantum is given by the Einstein rule: $E_n = h\rho_n$
3. The interaction energy of light quanta with matter is appropriately defined (see the above expressions for V).

In this way one of the most difficult paradoxes of the earlier form of the quantum theory—dual nature of light (electromagnetic waves on the one hand, discrete corpuscules or light quanta on the other)—is brilliantly resolved.[148] To be sure, it is difficult to find a direct, clear-cut interpretation of the interaction energy V which has just been calculated. This is made even more difficult by the

[148] The reader will find further discussion of how this "dual nature" was conceived, and how paradoxical it was considered to be, in the contemporary literature. See, for example, the works listed in Note 6.

It has often been said that quantum mechanics involves the same dual nature, since discrete particles (electrons, protons) are also described by wave

circumstance that those individual matrix elements $V_{kn|jp}$ which differ from zero (those with $n \neq 0, p = 0$ or $n = 0, p \neq 0$) depend upon the number S of all possible light quanta (they are proportional to $1/\sqrt{S}$), yet in the end one has to effect $S \to +\infty$. Nevertheless , we can accept this on the ground that each model-dependent description is only an approximation, while the exact content of the theory is furnished solely by the expression for the H operator.

We now return to our actual task: the determination of the transition probabilities. In the sense of the time-dependent Schrödinger theory, the changes in the $a_{k\,m_1 m_2 \ldots} = a_{k\,m_1 m_2 \ldots}(t)$ are determined by

$$\begin{aligned}\tfrac{\hbar}{i}\tfrac{\partial}{\partial t} a_{k\,m_1 m_2 \ldots} &= -\mathsf{H}\, a_{k\,m_1 m_2 \ldots} \\ &= -\Big(w_k + \sum_{n=1}^{\infty} h\rho_n m_n\Big) a_{k\,m_1 m_2 \ldots} \\ &\qquad - \sum_{j=1}^{\infty}\sum_{n=1}^{\infty} W_{kj}^{n} \cdot \big(\sqrt{m_n + 1}\, a_{j\,m_1 m_2 \ldots m_n+1 \ldots} \\ &\qquad\qquad + \sqrt{m_n}\, a_{j\,m_1 m_2 \ldots m_n - 1 \ldots}\big)\end{aligned}$$

Since the chief change of the $a_{k\,m_1 m_2 \ldots}$ is caused by the first term in this expression, it is appropriate to separate this out by the substitution

$$a_{k\,m_1 m_2 \ldots}(t) = \exp\Big\{-\tfrac{i}{\hbar}\Big(w_k + \sum_{n=1}^{\infty} h\rho_n m_n\Big)t\Big\} \cdot b_{k\,m_1 m_2 \ldots}(t)$$

Then

$$\begin{aligned}\tfrac{\partial}{\partial t} b_{k\,m_1 m_2 \ldots} = \tfrac{i}{\hbar} \sum_{j=1}^{\infty}\sum_{n=1}^{\infty} W_{kj}^{n} \cdot \Big(&e^{-\frac{i}{\hbar}(w_j - w_k + h\rho_n)t} \sqrt{m_n + 1}\, b_{j\,m_1 m_2 \ldots m_n+1 \ldots} \\ &- e^{-\frac{i}{\hbar}(w_j - w_k - h\rho_n)t} \sqrt{m_n}\, b_{j\,m_1 m_2 \ldots m_n - 1 \ldots}\Big)\end{aligned}$$

The physical meaning of the $a_{k\,m_1 m_2 \ldots}$ and $b_{k\,m_1 m_2 \ldots}$ may be seen from their origin: for finite $\bar{m}_0 + \bar{m}_1 + \bar{m}_2 + \cdots = S$, $\phi_{\bar{k}}(\xi)\psi_{\bar{m}_0 \bar{m}_1 \ldots}(u_1, \ldots, u_S)$ was the state in which $\mathbf{S}$ is in the $\bar{k}^{\text{th}}$ quantum orbit and $\bar{m}_0, \bar{m}_1, \bar{m}_2, \ldots$ light quanta in the respective states $\psi_0, \psi_1, \psi_2, \ldots$ are present; *i.e.*, $\bar{m}_0$ in the state of "non-existence" and $\bar{m}_1, \bar{m}_2, \ldots$ in the states belonging to the corresponding characteristic oscillations $\overline{\boldsymbol{A}}_1, \overline{\boldsymbol{A}}_2, \ldots$. The $a_{k\,m_1 m_2 \ldots}$ belonging to this wave

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functions, and exhibit typical wave properties. (See the experiments of Davison-Germer, Phys. Rev. **50** (1927), PNAS **15**, (1928); also C. F. Thomson, Proc. Roy. Soc. **117** (1928) and Rupp, Ann.Physik **85** (1928).) In contrast with this, however, it is to be noted that quantum mechanics derives both "natures" from a single unified theory of elementary phenomena. The paradox of the earlier theory lay in the circumstance that one had to draw alternately on two contradictory theories (the electromagnetic radiation theory of Maxwell-Hertz, the light quantum theory of Einstein) for the explanation of experience.

function are then

$$a_{k\,m_1 m_2\ldots} = \delta(k-\bar{k})\cdot\delta(m_1-\bar{m}_1)\cdot\delta(m_2-\bar{m}_2)\cdots$$

(Only a finite number of those numbers differ from 1 since $m_n = \bar{m}_n = 0$ with only a finite number of exceptions.) This, of course, remains valid also as $S \to +\infty$. For an arbitrary state $a_{k\,m_1 m_2\ldots}$ of **S** + **L**, therefore, the configuration mentioned above (if it is measured: see the comments in **III.3** on the non-degenerate pure discrete spectrum) has the probability

$$\Big|\sum_{k\,m_1 m_2\ldots} a_{k\,m_1 m_2\ldots}\delta(k-\bar{k})\cdot\delta(m_1-\bar{m}_1)\cdot\delta(m_2-\bar{m}_2)\cdots\Big|^2 = |a_{\bar{k}\,\bar{m}_1\bar{m}_2\ldots}|^2$$
$$= |b_{\bar{k}\,\bar{m}_1\bar{m}_2\ldots}|^2$$

In particular, the total probability that **S** will be found in the $\bar{k}^{\text{th}}$ quantum orbit is

$$\theta_{\bar{k}} = \sum_{\bar{m}_1\bar{m}_2\ldots} |b_{\bar{k}\,\bar{m}_1\bar{m}_2\ldots}|^2$$

Let an atom be initially ($t = 0$) in the $\bar{k}^{\text{th}}$ state, and let $\bar{m}_1, \bar{m}_2, \ldots$ identify the light quanta in the respective states $\overline{\boldsymbol{A}}_1, \overline{\boldsymbol{A}}_2, \ldots$ that are assumed to be initially present; *i.e.*,

$$b_{k\,m_1 m_2\ldots}(0) = a_{k\,m_1 m_2\ldots}(0) = \delta(k-\bar{k})\cdot\delta(m_1-\bar{m}_1)\cdot\delta(m_2-\bar{m}_2)\cdots$$

In the sense of the above differential equation, and as a first approximation (*i.e.*, for such short times that the right sides can still be considered constant), only those $\frac{\partial}{\partial t} b_{k\,m_1 m_2\ldots}$ will differ from zero for which an $m_1, m_2, \ldots, m_n + 1, \ldots$ or an $m_1, m_2, \ldots, m_n - 1, \ldots$ coincides with $\bar{m}_1, \bar{m}_2, \ldots$; *i.e.*, with all $k, \bar{m}_1, \bar{m}_2, \ldots, \bar{m}_n \pm 1, \ldots$. If we integrate in this case, we find

$$b_{k\bar{m}_1\bar{m}_2\ldots\bar{m}_n+1\ldots}(t) = W^n_{k\bar{k}}\,\frac{1-e^{-\frac{i}{\hbar}(w_{\bar{k}}-w_k-h\rho_n)t}}{w_{\bar{k}}-w_k-h\rho_n}\,\sqrt{\bar{m}_n+1}$$
$$b_{k\bar{m}_1\bar{m}_2\ldots\bar{m}_n-1\ldots}(t) = W^n_{k\bar{k}}\,\frac{1-e^{-\frac{i}{\hbar}(w_{\bar{k}}-w_k+h\rho_n)t}}{w_{\bar{k}}-w_k-h\rho_n}\,\sqrt{\bar{m}_n}$$

All other $b_{k\,m_1 m_2\ldots}$ vanish in this approximation. (Except for $b_{\bar{k}\,\bar{m}_1\bar{m}_2\ldots}$, which would equal 1 in this approximation; *i.e.*, except for terms of order t^2. Yet the conclusion $\frac{\partial}{\partial t} b_{k\,\bar{m}_1\bar{m}_2\ldots} = 0$ is made doubtful in this case by the fact that the right side of our differential equation contains an infinite number of terms $b_{k\bar{m}_1\bar{m}_2\ldots\bar{m}_n\pm 1\ldots}$ which do not vanish in our approximation. Hence we cannot argue from the smallness (for small t) of each of these terms to the smallness of their sum. Actually, the calculation in the next order of approximation would show that the deviation of $b_{\bar{k}\bar{m}_1\bar{m}_2\ldots}$ from 1 is proportional not to t^2 but to t.[149]

[149] The exact solution of this differential equation was given by Weisskopf and Wigner (Z. Physik **63** (1930)), and establishes the validity of these statements.

However, since

$$\sum_{k\,m_1 m_2 \ldots} |b_{k\,m_1 m_2 \ldots}|^2 = \sum_{k\,m_1 m_2 \ldots} |a_{k\,m_1 m_2 \ldots}|^2 = 1$$

$$\sum_{k\,m_1 m_2 \ldots} |b_{\bar{k}\,\bar{m}_1 \bar{m}_2 \ldots}|^2 = 1 - \sum_{k\,m_1 m_2 \ldots \neq \bar{k}\,\bar{m}_1 \bar{m}_2 \ldots} |b_{k\,m_1 m_2 \ldots}|^2$$

the direct determination of this $b_{k\,m_1 m_2 \ldots}$ is not actually necessary.)

The qualitative significance of the preceding results is clearly evident: $b_{k\bar{m}_1 \bar{m}_2 \ldots \bar{m}_n + 1 \ldots}$—which refers to the emission of an $\overline{\boldsymbol{A}}_n$ light quantum (of frequency ρ_n)—becomes larger as the denominator $w_{\bar{k}} - w_k - h\rho_n$ becomes smaller; *i.e.*, the closer the light frequency ρ_n lies to the "Bohr frequency" $(w_{\bar{k}} - w_k)/h$.[150] In the same way, $b_{k\bar{m}_1 \bar{m}_2 \ldots \bar{m}_n - 1 \ldots}$—which refers to absorption—increases as ρ_n becomes closer to $(w_k - w_{\bar{k}})/h$. We see that the Bohr frequency relation does not hold exactly (of course, not all frequencies are placed at one's disposal by the ρ_n) but only with high probability if the time t is short and the ρ_n are very dense (which will be the case if the cavity $\boldsymbol{\mathcal{H}}$ is large). In addition, the $W^n_{k\bar{k}}$ affect the frequency of occurence of such processes. We shall soon identify them with the transition probabilities.

From our $b_{k\bar{m}_1 \bar{m}_2 \ldots \bar{m}_n \pm 1 \ldots}$-formulae it follows[151] that (for sufficiently small values of t)

$$|b_{k\,\bar{m}_1 \bar{m}_2 \ldots \bar{m}_n + 1 \ldots}(t)|^2 = \frac{2}{h^2}\,(\bar{m}_n + 1)\,|W^n_{k\bar{k}}|^2\,\frac{1 - \cos 2\pi\Big(\rho_n - \dfrac{w_{\bar{k}} - w_k}{h}\Big)t}{\Big(\rho_n - \dfrac{w_{\bar{k}} - w_k}{h}\Big)^2}$$

$$|b_{k\,\bar{m}_1 \bar{m}_2 \ldots \bar{m}_n - 1 \ldots}(t)|^2 = \frac{2}{h^2}\,\bar{m}_n\,|W^n_{k\bar{k}}|^2\,\frac{1 - \cos 2\pi\Big(\rho_n - \dfrac{w_k - w_{\bar{k}}}{h}\Big)t}{\Big(\rho_n - \dfrac{w_k - w_{\bar{k}}}{h}\Big)^2}$$

$$|b_{k\,m_1 m_2 \ldots}(t)|^2 = 0 \qquad \text{for} \quad k m_1 m_2 \ldots \neq \begin{cases} \bar{k}\bar{m}_1 \bar{m}_2 \ldots & \text{or} \\ k\bar{m}_1 \bar{m}_2 \ldots \bar{m}_n \pm 1 \ldots \end{cases}$$

From this we get for $\theta_k(t)$ $(k \neq \bar{k})$

[150] N. Bohr, as is well known, stated the fundamental principle in 1913 (see the reference cited in Note 5) that in transitions from a stationary state of energy $W^{(1)}$ to a stationary state of energy $W^{(2)} < W^{(1)}$ an atom emits radiation of frequency $(W^{(1)} - W^{(2)})/h$. In our case, this corresponds to $(w_{\bar{k}} - w_k)/h$.

[151] We have

$$|e^{ix} - 1|^2 = (e^{ix} - 1)(e^{-ix} - 1) = 2 - (e^{ix} + e^{-ix}) = 2(1 - \cos x)$$

$$\theta_k(t) = \sum_{n=1}^{\infty} \frac{2}{h^2}\,(\bar{m}_n + 1)\,|W^n_{k\bar{k}}|^2\,\frac{1-\cos 2\pi\Big(\rho_n - \dfrac{w_{\bar{k}} - w_k}{h}\Big)t}{\Big(\rho_n - \dfrac{w_{\bar{k}} - w_k}{h}\Big)^2}$$
$$+ \sum_{n=1}^{\infty} \frac{2}{h^2}\,\bar{m}_n\,|W^n_{k\bar{k}}|^2\,\frac{1-\cos 2\pi\Big(\rho_n - \dfrac{w_k - w_{\bar{k}}}{h}\Big)t}{\Big(\rho_n - \dfrac{w_k - w_{\bar{k}}}{h}\Big)^2}$$

where the first $\sum_{n=1}^{\infty}$ refers to emission, the second $\sum_{n=1}^{\infty}$ to absorption. In order to be able to give these θ_k in closed form we must make simplifying assumptions: we will, on the one hand, assume the volume of the enclosure $\boldsymbol{\mathcal{H}}$ to be very large ($\mathcal{V} \to \infty$) and will, on the other hand, consider the characteristic oscillations $\overline{\boldsymbol{A}}_n$ in $\boldsymbol{\mathcal{H}}$ statistically. For this purpose, we combine all terms in the above summations which belong to ρ_n between ρ and $\rho + d\rho$ (for $W^n_{k\bar{k}}$ we introduce its value and assume $d\rho \ll \rho$):

$$\frac{1}{4\pi^2 c^2 h\rho}\Bigg[\sum_{\substack{n\\ \rho \leqslant \rho_n < \rho + d\rho}} \Big|\sum_{\nu=1}^{\ell} \frac{e_\nu}{M_\nu}\big(\mathsf{P}^x_\nu \overline{\boldsymbol{A}}_{n,x}(\mathsf{Q}^x_\nu, \mathsf{Q}^y_\nu, \mathsf{Q}^z_\nu) + \cdots\big)_{k\bar{k}}\Big|^2 (\bar{m}_n + 1)\Bigg]$$
$$\times \frac{1-\cos 2\pi\Big(\rho - \dfrac{w_{\bar{k}} - w_k}{h}\Big)t}{\Big(\rho - \dfrac{w_{\bar{k}} - w_k}{h}\Big)^2}$$

We then repeat this procedure, but with $\bar{m}_n$ in place of $\bar{m}_n + 1$ and $(w_k - w_{\bar{k}})/h$ in place of $(w_{\bar{k}} - w_k)/h$. The expressions in brackets $[\cdots]$ are now to be evaluated.

The customary method of describing the $m_1, m_2, \ldots$ is not by enumeration of their values but much less—namely, the listing of their intensities; *i.e.*, the radiation energy $I(\rho)d\rho$ that lies in the spectral interval from ρ to $\rho + d\rho$ and in unit volume. This means that

$$\sum_{\substack{n\\ \rho \leqslant \rho_n < \rho + d\rho}} h\rho_n \cdot \bar{m}_n \quad \approx \quad h\rho \sum_{\substack{n\\ \rho \leqslant \rho_n < \rho + d\rho}} \bar{m}_n = \mathcal{V} \cdot I(\rho)d\rho$$

i.e.,

$$\sum_{\substack{n\\ \rho \leqslant \rho_n < \rho + d\rho}} \bar{m}_n = \frac{\mathcal{V} \cdot I(\rho)d\rho}{h\rho}$$

The number of ρ_n in the interval $\rho \leqslant \rho_n < \rho + d\rho$ is

$$\frac{8\pi\mathcal{V}\rho^2}{c^2}d\rho$$

according to an asymptotic formula of Weyl (see the reference in Note 140) which is valid generally, and therefore

$$\sum_{\substack{n\\ \rho \leqslant \rho_n < \rho + d\rho}} (\bar{m} + 1) \approx \frac{\mathcal{V}\Big(I(\rho) + \dfrac{8\pi h\rho^3}{c^3}\Big)}{h\rho}d\rho$$

If

$$\Big|\sum_{\nu=1}^{\ell}\frac{e_\nu}{M_\nu}\big(\mathsf{P}_\nu^x\overline{\boldsymbol{A}}_{n,x}(\mathsf{Q}_\nu^x,\mathsf{Q}_\nu^y,\mathsf{Q}_\nu^z)+\cdots\big)_{k\bar{k}}\Big|^2$$

executes (sufficiently rapid) fluctuations in the interval $\rho\leqslant\rho_n<\rho+d\rho$ (about a mean value which we will call $W_{k\bar{k}}(\rho)$) then the expressions $[\ldots]$ in question become

$$W_{k\bar{k}}(\rho)\frac{\mathcal{V}\Big(I(\rho)+\dfrac{8\pi h\rho^3}{c^3}\Big)}{h\rho}d\rho\qquad\text{and}\qquad W_{k\bar{k}}(\rho)\frac{\mathcal{V}I(\rho)}{h\rho}d\rho$$

If in addition we write $\nu_{\bar{k}k}$ for $(w_{\bar{k}}-w_k)/h$, and $\nu_{k\bar{k}}$ for $(w_k-w_{\bar{k}})/h$, then our sums become

$$\theta_k(t)=\frac{\mathcal{V}}{4\pi^2c^2h^2}\int_0^\infty\left\{\Big(I(\rho)+\frac{8\pi h\rho^3}{c^3}\Big)\cdot\frac{1-\cos 2\pi(\rho-\nu_{\bar{k}k})\,t}{(\rho-\nu_{\bar{k}k})^2}\right.$$
$$\left.+I(\rho)\cdot\frac{1-\cos 2\pi(\rho-\nu_{k\bar{k}})\,t}{(\rho-\nu_{k\bar{k}})^2}\right\}\frac{W_{k\bar{k}}(\rho)}{\rho^2}d\rho$$

For small t this integral is evidently of order t^2 (because $1-\cos 2\pi ct$ is) except in that part of the integration region in which the denominators $(\rho-\nu_{\bar{k}k})$, $(\rho-\nu_{k\bar{k}})$ are small. Here contributions can arise which are large in comparison with t^2, and when this is the case the contributions in question supply asymptotic evaluations for $\theta_k(t)$. It will be shown that this is actually the case, because we shall obtain contributions of order t.

Since $\nu_{\bar{k}k}=-\nu_{k\bar{k}}=(w_{\bar{k}}-w_k)/h$, for $w_{\bar{k}}>w_k$ only the denominator of the first term can become small, while for $w_{\bar{k}}<w_k$ only the denominator of the second term, so according as $w_{\bar{k}}$ is $>$ or $<w_k$ it is the first or second term which predominates; the other term will be abandoned. Moreover, since the ρ that lie remote from $\nu_{\bar{k}k}$ and $\nu_{k\bar{k}}$ contribute only in order t^2 to the integral, we can replace some of the factors in the surviving integrand by the values which they assume at the dominant value of ρ. Thus do we obtain

$$\theta_k(t)=\frac{\mathcal{V}IW_{k\bar{k}}(\bar{\nu}_{k\bar{k}})}{4\pi^2c^2h^2\bar{\nu}_{k\bar{k}}^2}\int_0^\infty\frac{1-\cos 2\pi(\rho-\bar{\nu}_{k\bar{k}})t}{(\rho-\bar{\nu}_{k\bar{k}})^2}d\rho$$

where we have adopted the abbreviation $\bar{\nu}_{k\bar{k}}=|w_{\bar{k}}-w_k|/h$ and where

$$I=\begin{cases}I(\bar{\nu}_{k\bar{k}})+\dfrac{8\pi h}{c^3}\bar{\nu}_{k\bar{k}}^3 & \text{for}\quad w_{\bar{k}k}>w_{k\bar{k}}\ :\ \text{radiative case}\\[2ex] I(\bar{\nu}_{k\bar{k}}) & \text{for}\quad w_{\bar{k}k}<w_{k\bar{k}}\ :\ \text{absorptive case}\end{cases}$$

Since this again leads only to a t^2 contribution, we can replace $\int_0^\infty$ by $\int_{-\infty}^{+\infty}$ and

introduce the new variable $x = 2\pi(\rho - \bar{\nu}_{k\bar{k}})t$. Then[152]

$$\int_{-\infty}^{+\infty} \frac{1-\cos 2\pi(\rho-\bar{\nu}_{k\bar{k}})t}{(\rho-\bar{\nu}_{k\bar{k}})^2}\,d\rho = 2\pi t \int_{-\infty}^{+\infty} \frac{1-\cos x}{x^2}\,dx = 2\pi^2 t$$

so finally

$$\theta_k(t) = \frac{\mathcal{V} I W_{k\bar{k}}(\bar{\nu}_{k\bar{k}})}{2h^2\bar{\nu}_{k\bar{k}}^2}\,t$$

with which it is also established that $\theta_k(t)$ is of order t.

In order to evaluate $W_{k\bar{k}}(\bar{\nu}_{k\bar{k}})$ we must find an expression for

$$\Big|\sum_{\nu=1}^{\ell} \frac{e_\nu}{M_\nu}\big(\mathsf{P}_\nu^x \overline{\boldsymbol{A}}_{n,x}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z) + \cdots\big)_{k\bar{k}}\Big|^2$$

which is free of $\overline{\boldsymbol{A}}_n$. This can be obtained if we replace $\overline{\boldsymbol{A}}_n$ (considering its rapid fluctuations) by an irregularly oriented vector of constant length. Because of its spatial constancy (*i.e.*, its $\{\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z\}$-independence) such a vector is a number vector times the unit matrix I, and its constant length γ_n can be obtained from the normalization condition

$$\iiint_{\mathcal{H}} [\overline{\boldsymbol{A}}_n, \overline{\boldsymbol{A}}_n]\,dxdydz = 4\pi c^2$$

Therefore

$$\mathcal{V}\gamma_n^2 = 4\pi c^2 \quad i.e., \quad \gamma_n^2 = \frac{4\pi c^2}{\mathcal{V}}$$

On average, $\frac{1}{3}$ of $[\overline{\boldsymbol{A}}_n, \overline{\boldsymbol{A}}_n] = \overline{\boldsymbol{A}}_{n,x}^2 + \overline{\boldsymbol{A}}_{n,y}^2 + \overline{\boldsymbol{A}}_{n,z}^2 = \gamma_n^2$ contributes to the x-component $\overline{\boldsymbol{A}}_{n,x}^2$. Hence $\frac{1}{3}\gamma_n^2 = \frac{4}{3}\pi c^2/\mathcal{V}$ and similarly for $\overline{\boldsymbol{A}}_{n,y}^2$ and $\overline{\boldsymbol{A}}_{n,z}^2$. Consequently, we have

$$\begin{aligned} W_{k\bar{k}}(\rho) &= \operatorname*{mean}_{\rho \leqslant \rho_n < \rho+d\rho} \Big|\sum_{\nu=1}^{\ell} \frac{e_\nu}{M_\nu}\big(\mathsf{P}_\nu^x \overline{\boldsymbol{A}}_{n,x}(\mathsf{Q}_\nu^x, \mathsf{Q}_\nu^y, \mathsf{Q}_\nu^z) + \cdots\big)_{k\bar{k}}\Big|^2 \\ &\approx \frac{4\pi c^2}{3\mathcal{V}}\left(\Big|\Big(\sum_{\nu=1}^{\ell} \frac{e_\nu}{M_\nu}\mathsf{P}_\nu^x\Big)_{k\bar{k}}\Big|^2 + \cdots\right) \end{aligned}$$

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[152] Here we use (see Courant-Hilbert, page 49)

$$\begin{aligned} \int_{-\infty}^{+\infty} \frac{1-\cos x}{x^2}\,dx &= 2\int_0^{\infty} \frac{1-\cos x}{x^2}\,dx \\ &= \int_0^{\infty} \frac{1-\cos 2y}{y}\,dy = 2\int_0^{\infty} \frac{\sin^2 y}{y^2}\,dy = \pi \end{aligned}$$

Since H_0, the energy of the system **S** alone, is equal to the kinetic energy plus the potential energy it has therefore the form

$$\mathsf{H}_0 = \sum_{\nu=1}^{\ell} \tfrac{1}{2M_\nu}\big[(\mathsf{P}_\nu^x)^2 + (\mathsf{P}_\nu^y)^2 + (\mathsf{P}_\nu^z)^2\big] + V\big(\mathsf{Q}_1^x, \mathsf{Q}_1^y, \mathsf{Q}_1^z, \ldots, \mathsf{Q}_\ell^x, \mathsf{Q}_\ell^y, \mathsf{Q}_\ell^z\big)$$

in view of which one has[153]

$$\mathsf{H}_0\mathsf{Q}_\nu^x - \mathsf{Q}_\nu^x\mathsf{H}_0 = \tfrac{\hbar}{i}\tfrac{1}{M_\nu}\mathsf{P}_\nu^x$$

Since H_0 is a diagonal matrix with diagonal matrix elements $w_1, w_2, \ldots$ (which is to say: $(\mathsf{H}_0)_{kj} = w_k\delta_{kj}$) it follows from this that

$$\begin{aligned}(\mathsf{P}_\nu^x)_{k\bar{k}} &= \tfrac{i}{\hbar}M_\nu(\mathsf{H}_0\mathsf{Q}_\nu^x - \mathsf{Q}_\nu^x\mathsf{H}_0)_{k\bar{k}}\\ &= \tfrac{i}{\hbar}M_\nu(w_k - w_{\bar{k}})(\mathsf{Q}_\nu^x)_{k\bar{k}}\\ &= \pm i\cdot 2\pi M_\nu\bar{\nu}_{k\bar{k}}(\mathsf{Q}_\nu^x)_{k\bar{k}}\end{aligned}$$

Therefore

$$W_{k\bar{k}}(\rho) = \frac{16\pi^3c^2}{3\mathcal{V}h^2}\bar{\nu}_{k\bar{k}}^2\left(\Big|\Big(\sum_{\nu=1}^{\ell} e_\nu\mathsf{Q}_\nu^x\Big)_{k\bar{k}}\Big|^2 + \cdots\right)$$

Substitution into the previously-obtained expression for $\theta_k(t)$ results in

$$\theta_k(t) = I\,\frac{8\pi^3}{3h^2}\left(\Big|\Big(\sum_{\nu=1}^{\ell} e_\nu\mathsf{Q}_\nu^x\Big)_{k\bar{k}}\Big|^2 + \cdots\right)t$$

If we set

$$W_{k\bar{k}} = \Big|\Big(\sum_{\nu=1}^{\ell} e_\nu\mathsf{Q}_\nu^x\Big)_{k\bar{k}}\Big|^2 + \cdots$$

this result is evidently to be interpreted as follows: The atom **S** in the k^{th} state executes the following transitions (quantum jumps):

1. A transition $k \to \bar{k}$ into a higher state ($w_{\bar{k}} > w_k$) occurs

$$I\,\frac{8\pi^3}{3h^2}W_{k\bar{k}}\cdot\frac{w_{\bar{k}} - w_k}{h}$$

times per second; *i.e.*, at a rate proportional to the intensity of the radiation field at the corresponding Bohr frequency $(w_{\bar{k}} - w_k)/h$.

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[153] P_ν^x commutes with all $\mathsf{Q}_\mu^x, \mathsf{Q}_\mu^y, \mathsf{Q}_\mu^z, \mathsf{P}_\mu^x, \mathsf{P}_\mu^y, \mathsf{P}_\mu^z$ except Q_ν^x. In fact

$$\mathsf{P}_\nu^x\mathsf{Q}_\nu^x - \mathsf{Q}_\nu^x\mathsf{P}_\nu^x = \tfrac{\hbar}{i}\mathsf{I}$$

Therefore

$$\mathsf{H}_0\mathsf{Q}_\nu^x - \mathsf{Q}_\nu^x\mathsf{H}_0 = \tfrac{1}{2M_\nu}(\mathsf{P}_\nu^x)^2\mathsf{Q}_\nu^x - \mathsf{Q}_\nu^x\tfrac{1}{2M_\nu}(\mathsf{P}_\nu^x)^2 = \tfrac{\hbar}{i}\tfrac{1}{M_\nu}\mathsf{P}_\nu^x$$

See Note 143.

2. A transition $\bar{k} \leftarrow k$ into a lower state ($w_{\bar{k}} < w_k$) occurs

$$I \, \frac{8\pi^3}{3h^2} W_{k\bar{k}} \cdot \frac{w_k - w_{\bar{k}}}{h}$$

times per second; *i.e.*, at a rate proportional to the intensity of the radiation field at the corresponding Bohr frequency $(w_k - w_{\bar{k}})/h$.

3. A transition $\bar{k} \leftarrow k$ into a lower state ($w_{\bar{k}} < w_k$) also occurs

$$\frac{64\pi^4}{3hc^3} W_{k\bar{k}} \cdot \Big(\frac{w_k - w_{\bar{k}}}{h} \Big)^3$$

times per second; *i.e.*, in complete independence of the ambient radiation field.

Process **1** refers to absorption from the radiation field; **2** to emission which is induced by the radiation field. Process **3** refers, however, to spontaneous emission which the atom will always undergo, so long as it has not attained complete stability in its lowest stationary state (minimum w_k).

The three transition mechanisms **1**–**3** were already found thermodynamically by Einstein before the discovery of quantum mechanics;[154] only the value of the "transition probability" was lacking. The above value

$$W_{k\bar{k}} = \Big| \Big(\sum_{\nu=1}^{\ell} e_\nu \mathsf{Q}_\nu^x \Big)_{k\bar{k}} \Big|^2 + \Big| \Big(\sum_{\nu=1}^{\ell} e_\nu \mathsf{Q}_\nu^y \Big)_{k\bar{k}} \Big|^2 + \Big| \Big(\sum_{\nu=1}^{\ell} e_\nu \mathsf{Q}_\nu^z \Big)_{k\bar{k}} \Big|^2$$

is, as we have already mentioned, contained in the first interpretation contributed by Heisenberg. We have now obtained it again (by Dirac's method) from the general theory.

[154] Physik Z. **18** (1917).

CHAPTER IV

DEDUCTIVE DEVELOPMENT OF THE THEORY

1. THE FUNDAMENTAL BASIS OF THE STATISTICAL THEORY

In Chapter III we succeeded in reducing all assertions of quantum mechanics to the statistical formula (called there $\mathbf{E}_2$)

$$\overline{\mathbf{E}} \qquad\qquad \mathrm{Exp}(\mathcal{R}, \phi) = (\mathsf{R}\phi, \phi)$$

(Here $\mathrm{Exp}(\mathcal{R}, \phi)$ is the expectation value of the quantity $\mathcal{R}$ in the state ϕ, and R is the operator belonging to $\mathcal{R}$.) In the course of the following discussion we will see how this formula itself can be derived from a few qualitative assumptions, and simultaneously we will check the entire structure of quantum mechanics as it was developed in Chapter III. Before we do this, however, a further remark is necessary.

In the state ϕ the quantity $\mathcal{R}$ has the expectation value $\rho = (\mathsf{R}\phi, \phi)$ and has as its dispersion ϵ^2 the expectation value of the quantity $(\mathcal{R} - \rho)^2$; *i.e.*, $\epsilon^2 = ((\mathsf{R} - \rho \cdot \mathsf{I})^2\phi, \phi) = \|\mathsf{R}\phi\|^2 - (\mathsf{R}\phi, \phi)^2$ (see Note 130; all these are calculated with the aid of $\overline{\mathbf{E}}$!), which is in general > 0 (and $= 0$ only for $\mathsf{R}\phi = \rho\phi$; see **III.3**). Therefore there exists a statistical distribution of $\mathcal{R}$ even though ϕ is one individual state, as we have repeatedly noted. But such statistical considerations acquire a new aspect when we do not even know what state is actually present—for example, when states $\phi_1, \phi_2, \ldots$ might be present with respective probabilities $w_1, w_2, \ldots$ (all non-negative, and sum to unity). Then the expectation value of the quantity $\mathcal{R}$, in the sense of the generally valid rules of the calculus of probabilities, is $\rho' = \sum_n w_n \cdot (\mathsf{R}\phi_n, \phi_n)$.

Now in general $(\mathsf{R}\phi, \phi) = \mathrm{Tr}(\mathsf{P}_{[\phi]} \cdot \mathsf{R})$. Indeed, if we select a complete orthonormal set $\psi_1, \psi_2, \ldots$ with $\psi_1 = \phi$ (therefore $\psi_2, \psi_3, \ldots$ are orthogonal

to ϕ), then

$$\mathsf{P}_{[\phi]}\psi_n = \begin{cases} \phi & \text{for} \quad n = 1 \\ 0 & \text{for} \quad n \neq 1 \end{cases}$$

and therefore

$$\begin{aligned} \mathrm{Tr}(\mathsf{P}_{[\phi]} \cdot \mathsf{R}) &= \sum_{m,n} (\mathsf{P}_{[\phi]}\psi_n, \psi_m)(\mathsf{R}\psi_m, \psi_n) \\ &= \sum_{m} (\phi, \psi_m)(\mathsf{R}\psi_m, \phi) = (\mathsf{R}\phi, \phi) \end{aligned}$$

whence our $\rho' = \mathrm{Tr}\Big(\{\sum_n w_m \mathsf{P}_{[\phi_n]}\} \cdot \mathsf{R}\Big)$. The operator

$$\mathsf{U} = \sum_n w_n P_{[\phi_n]}$$

is definite because of the definiteness of all $\mathsf{P}_{[\phi_n]}$ and $w_n \geqslant 0$, and its trace is equal to $\sum_n w_n = 1$ since $\mathrm{Tr}\mathsf{P}_{[\phi_n]} = 1$. It provides a complete characterization of the mixture just described, so far as concerns its statistical properties:

$$\rho' = \mathrm{Tr}(\mathsf{UR})$$

We shall have to pay attention to such mixtures of states, in addition to the individual states themselves. We turn first, however, to more general investigations.

Let us forget the whole of quantum mechanics but retain the following: Suppose that a system $\mathbf{S}$[155] is given, which is characterized for experimenters

[155] It is important to emphasize the conceptual difference between a system as such and a system in a certain state. This is an example of a system: a hydrogen atom; *i.e.*, an electron and proton with the known forces acting between them. It is described formally by these data: the configuration space has six dimensions; the coordinates are $q_1, \ldots, q_6$; the momenta are $p_1, \ldots, p_6$; the Hamiltonian function is

$$\begin{aligned} H(q_1, \ldots, q_6, p_1, \ldots, p_6) = \frac{p_1^2 + p_2^2 + p_3^2}{2m_e} + \frac{p_4^2 + p_5^2 + p_6^2}{2m_p} \\ + \frac{e^2}{\sqrt{(q_1 - q_4)^2 + (q_2 - q_5)^2 + (q_3 - q_6)^2}} \end{aligned}$$

A state is then determined by additional data. In classical mechanics this is done by assigning numerical initial values $q_1^0, \ldots, q_6^0, p_1^0, \ldots, p_6^0$ to the coordinates and momenta; in quantum mechanics by specifying the initial wave function $\phi_0(q_1 \ldots, q_6)$. One never needs more information than this: if both system and state are known, then the theory gives unambiguous directions for answering all questions by calculation.

by the enumeration of all the effectively measurable quantities in it and their functional relations with one another. With each quantity we include directions as to how it is to be measured, and how its value is to be read or calculated from the indicator positions on the measuring instruments. If $\mathcal{R}$ is a quantity and $f(x)$ any function, then the quantity $f(\mathcal{R})$ is defined as follows: To measure $f(\mathcal{R})$ we measure $\mathcal{R}$ and find the value a (for $\mathcal{R}$). Then $f(\mathcal{R})$ has the value $f(a)$. As we see, all quantities $f(\mathcal{R})$ ($\mathcal{R}$ fixed, $f(x)$ arbitrary) are measured simultaneously with $\mathcal{R}$. This is a first example of simultaneously measurable quantities. In general, we call two (or more) quantities $\mathcal{R}, \mathcal{S}$ simultaneously measurable in the same system if there is an arrangement that measures both simultaneously in the same system—except that their respective values are to be calculated in different ways from the instrument readings. (In classical mechanics, as is well known, all quantities are simultaneously measurable, but this is not the case in quantum mechanics, as we have seen in **III.3**.) Given such quantities and a function $f(x, y)$ of two variables, we can also define the quantity $f(\mathcal{R}, \mathcal{S})$. This is measured if we measure $\mathcal{R}, \mathcal{S}$ simultaneously. If the values a, b are found for these, then the value of $f(\mathcal{R}, \mathcal{S})$ is $f(a, b)$. But it should be realized that it is completely meaningless to try to form $f(\mathcal{R}, \mathcal{S})$ if $\mathcal{R}, \mathcal{S}$ are not simultaneously measurable: there is no way to construct the corresponding experimental arrangement.

However, investigation of the physical quantities related to a single object $\mathbf{S}$ is not the only thing which can be done—especially if doubts exist concerning the simultaneous measurability of several quantities. In such cases it is possible to construct statistical ensembles which consist of many systems $\mathbf{S}_1, \ldots, \mathbf{S}_N$ (*i.e.*, N copies of $\mathbf{S}$, N large).[156] In such an ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ we do not measure the "value" of a quantity $\mathcal{R}$ but its distribution of values; *i.e.*, for each interval $a' < a \leqslant a''$ (a', a'' given, $a' \leqslant a''$) we look to the number of systems among the $\mathbf{S}_1, \ldots, \mathbf{S}_N$ for which the value of $\mathcal{R}$ lies in the interval and—dividing by N—obtain the probability function $w(a', a'') = w(a'') - w(a')$.[157]

[156] Such ensembles—sometimes called collectives—are in general necessary for establishing probability theory as a theory of frequencies. They were introduced by R. von Mises, who discovered their meaning for probability theory and who built a complete theory on this foundation (see, for example, his book *Wahrscheinlichkeit, Statistik und ihre Wahreheit*, Berlin, 1928).

[157] $w(a')$ is the probability of $a \leqslant a'$; *i.e.*, that a falls within the interval $\{-\infty, a']$. This $w(a)$—or, as we shall call it, $w_{\mathcal{R}}(a)$ in order to emphasize its dependence on $\mathcal{R}$—is easily seen to have the following properties:

$$0 \leftarrow w_{\mathcal{R}}(a) \quad \text{as} \quad -\infty \leftarrow a$$
$$w_{\mathcal{R}}(a) \to 1 \quad \text{as} \quad a \to +\infty$$
$$\text{for } a \geqslant a_0 \ : \ a_0 \leftarrow a \implies w_{\mathcal{R}}(a_0) \leftarrow w_{\mathcal{R}}(a)$$
$$a' \leqslant a'' \implies w_{\mathcal{R}}(a') \leqslant w_{\mathcal{R}}(a'')$$

(In quantum mechanics, if $\mathsf{E}(\lambda)$ is the resolution of the identity belonging to R then $w_{\mathcal{R}}(a) = \|\mathsf{E}(a)\phi\|^2 = (\mathsf{E}(a)\phi, \phi)$.) If $w_{\mathcal{R}}(a)$ is differentiable then the

The essential advantages of the observation of such ensembles are these:

> **1**. Even if the measurement of a quantity $\mathcal{R}$ should alter the measured system **S** to an important degree (in quantum mechanics this may be actually the case, and in **III.4** we saw that this is necessarily so in the physics of elementary processes, since the measurement's interference with the observed system is of the same order of magnitude as the system or its observed parts), the statistical determination of the probability distribution of $\mathcal{R}$ in the ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ will alter this ensemble arbitrarily little if N is sufficiently large.
>
> **2**. Even if two (or more) quantities $\mathcal{R}$, $\mathcal{S}$ in a single system **S** are not simultaneously measurable, their probability distributions in a given ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ can be obtained with arbitrary accuracy if N is sufficiently large.

Indeed, with an ensemble of N elements it suffices to carry out the statistical inspections not on all N elements of $\mathbf{S}_1, \ldots, \mathbf{S}_N$ but on any subset of $M \leqslant N$ elements—say, $[\mathbf{S}_1, \ldots, \mathbf{S}_M]$—provided that M, N are both large and that M is very small compared to N.[158] Then only the M/N^{th} part of the ensemble is affected by the changes which result from the measurement. The effect is an arbitrarily small one if M/N is chosen to be small enough, which is possible for sufficiently large N, even in the case of large M, as was stated in **1**. In order to measure two (or several) quantities $\mathcal{R}$, $\mathcal{S}$ simultaneously we need two ensembles—say $[\mathbf{S}_1, \ldots, \mathbf{S}_M]$ and $[\mathbf{S}_{M+1}, \ldots, \mathbf{S}_{2M}]$ $(2M \leqslant N)$—of such a type that the first is employed in obtaining the statistics of $\mathcal{R}$, and the second in obtaining those of $\mathcal{S}$. The two measurements therefore do not disturb each other, although they are performed in the same ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$, and they change this ensemble only by an arbitrarily small amount if $2M/N$ is sufficiently small, which is possible for sufficiently large N even in the case of large M, as was stated in **2**.

We see that the introduction of statistical ensembles—*i.e.*, of probability methods—is undertaken because of the possibility of affecting a single system by measurement, and the possibility that several quantities may not be measurable simultaneously. A general theory must consider these circumstances, since their appearance in elementary processes had always been suspected,[159]

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ordinary "probability density" $\frac{d}{da} w_{\mathcal{R}}(a)$ can be introduced in its place; if it is not continuous (from the left) at $a = a_0$ then the single point $a = a_0$ has the "discrete probability" $w_{\mathcal{R}}(a_0) - w_{\mathcal{R}}(a_0 - 0)$. But the general concept which is meaningful under all conditions is $w_{\mathcal{R}}(a)$: see the reference in Note 156.

[158] This follows from the so-called Law of Large Numbers, the theorem of Bernoulli.

[159] So, for example, it was considered to constitute a basic difficulty in defining the electric field that the electrical test charge to be used cannot be smaller than the charge of an electron.

and their reality is now an established certainty, as the detailed discussion of the situation makes clear (see **III.4**). The use of statistical ensembles eliminates these difficulties, and again makes possible an objective description (which is independent of chance, as well as of whether one measures—in a given state—the one or the other of two not simultaneously measurable quantities).

For such ensembles it is not surprising that a physical quantity $\mathcal{R}$ does not have a sharp value; *i.e.*, that its distribution function does not consist of a single value a_0,[160] but that several values or intervals are possible, and that a positive dispersion exists.[160] Two different reasons for this are *a priori* conceivable:

> **I**. The individual systems $\mathbf{S}_1, \ldots, \mathbf{S}_N$ of our ensemble can be in different states, so that the ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ is shaped by the relative frequencies of those states. The fact that we do not obtain sharp values for the physical quantities in this case is caused by our lack of information: we do not know in which state we are measuring, and therefore cannot predict the results.
>
> **II**. The individual systems $\mathbf{S}_1, \ldots, \mathbf{S}_N$ are in the same state, but the laws of nature are not causal. Then the cause of the dispersion is not our lack of information, but nature itself, which has disregarded the "principle of sufficient cause."

Case **I** is generally well known, while Case **II** is important and new. To be sure, we will be skeptical at first of such a possibility, but we find an objective criterion that will enable us to decide whether it is or is not possible to entertain such an idea. It appears at first that serious objections can be raised about the conceivability and meaningfulness of such a notion, but we believe that these objections are not valid, and that certain difficulties (for example, in quantum mechanics) permit no other way out but **II**. We therefore apply ourselves to discussion of the conceptual difficulties posed by **II**.

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[160] The sharp value a_0 corresponds to the probability function

$$w_{\mathcal{R}}(a) = \begin{cases} 1 & \text{for} \quad a \geqslant a_0 \\ 0 & \text{for} \quad a < a_0 \end{cases}$$

In this case—and only in this—the dispersion ϵ^2 is zero. The mean value and the dispersion are in general calculated as follows (these are Stieltjes integrals!):

$$\begin{aligned} \rho &= \textstyle\int_{-\infty}^{+\infty} a \, dw_{\mathcal{R}}(a) \\ \epsilon^2 &= \textstyle\int_{-\infty}^{+\infty} (a-\rho)^2 \, dw_{\mathcal{R}}(a) \\ &= \textstyle\int_{-\infty}^{+\infty} a^2 \, dw_{\mathcal{R}}(a) - 2\rho \int_{-\infty}^{+\infty} a \, dw_{\mathcal{R}}(a) + \rho^2 \\ &= \textstyle\int_{-\infty}^{+\infty} a^2 \, dw_{\mathcal{R}}(a) - \rho^2 \\ &= \textstyle\int_{-\infty}^{+\infty} a^2 \, dw_{\mathcal{R}}(a) - \left(\int_{-\infty}^{+\infty} a \, dw_{\mathcal{R}}(a) \right)^2 \end{aligned}$$

(See **III.4**, Note 130.)

One might raise against **II** the objection that nature cannot possibly violate the "principle of sufficient cause"—*i.e.*, causality—because this is merely a definition of identity. That is, the proposition that two identical objects $\mathbf{S}_1, \mathbf{S}_2$—*i.e.*, two replicas of the system $\mathbf{S}$ which are in the same state—will remain identical in all conceivable identical circumstances is true because it is tautological. For if $\mathbf{S}_1, \mathbf{S}_2$ could react differently to identical interactions (for example: if they responded with different values to measurement of the same quantity $\mathcal{R}$) then we would not have called them identical. Therefore, in an ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ which as dispersion relative to a quantity $\mathcal{R}$, the individual systems $\mathbf{S}_1, \ldots, \mathbf{S}_N$ cannot (by definition) all be in the same state. (The application to quantum mechanics would be: Since one can obtain different values in the measurement of the same quantity $\mathcal{R}$ in several systems all of which are in the same state ϕ—not an eigenstate of the operator R associated with $\mathcal{R}$[161]—these systems cannot be equal to one another; *i.e.*, the description of state provided by the wave function cannot be complete. Therefore other variables must exist, the "hidden parameters" mentioned in **III.2**. We will soon see what difficulties this presents.) In a large statistical ensemble, therefore, as long as any physical quantity $\mathcal{R}$ is found to exhibit dispersion the possibility must exist of resolving the ensemble into several differently constituted parts (according to the various states of their respective elements). This procedure is made all the more plausible by the observation that a simple method for achieving such a resolution seems to exist: namely, we can look to the various values which $\mathcal{R}$ has in the ensemble. After a subdivision or resolution relative to all possible quantities $\mathcal{R}$, $\mathcal{S}$, $\mathcal{T}$, ... has been carried out a truly homogeneous ensemble would then be obtained. At the end of the process these quantities would have no further dispersion in any of the sub-ensembles.

But, first of all, the statements contained in the last sentence are incorrect because we did not consider the fact that the act of measurement changes the measured system. If we measure $\mathcal{R}$ (which we will assume for simplicity can have only two values: a_1, a_2) for all objects and get perhaps a_1 on $\mathbf{S}_1', \ldots, \mathbf{S}_{N_1}'$ and a_2 on $\mathbf{S}_1'', \ldots, \mathbf{S}_{N_2}''$ ($N_1 + N_2 = N$), then there is no dispersion in $[\mathbf{S}_1', \ldots, \mathbf{S}_{N_1}']$ and none in $[\mathbf{S}_1'', \ldots, \mathbf{S}_{N_2}'']$ ($\mathcal{R}$ has always the value a_1 or a_2 respectively). Still, this is not merely a resolution of $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ into the two sets mentioned, because the individual systems would be changed by the $\mathcal{R}$ measurement. It is true that by **I** we have a method to determine the distribution $\mathcal{R}$-values in such a way that $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ is changed only slightly (we measure only in $[\mathbf{S}_1, \ldots, \mathbf{S}_M]$ with M large, M/N small). This procedure, however, does not lead to the desired resolution since for most of the $\mathbf{S}_1, \ldots, \mathbf{S}_N$ (namely $\mathbf{S}_{M+1}, \ldots, \mathbf{S}_N$) it does not make certain what value $\mathcal{R}$ has in each one of them.

We show now that the method given above fails to produce completely homogeneous ensembles. Use a second physical quantity $\mathcal{S}$ (assumed again to have only two values: b_1, b_2) to resolve $[\mathbf{S}_1', \ldots, \mathbf{S}_{N_1}']$ into sub-ensembles

[161] We contemplate independent measurements on several systems: successive measurements on the same system would always give the same result (see **III.3**).

$$[\mathbf{S}'_1,\ldots,\mathbf{S}'_{N_1}] = [\mathbf{S}'^{\circ}_1,\ldots,\mathbf{S}'^{\circ}_{N_{1,1}}] + [\mathbf{S}'^{\circ\circ}_1,\ldots,\mathbf{S}'^{\circ\circ}_{N_{1,2}}] \quad : \quad N_{1,1}+N_{1,2}=N_1$$

and similarly resolve $[\mathbf{S}''_1,\ldots,\mathbf{S}''_{N_2}]$:

$$[\mathbf{S}''_1,\ldots,\mathbf{S}''_{N_2}] = [\mathbf{S}''^{\circ}_1,\ldots,\mathbf{S}''^{\circ}_{N_{2,1}}] + [\mathbf{S}''^{\circ\circ}_1,\ldots,\mathbf{S}''^{\circ\circ}_{N_{2,2}}] \quad : \quad N_{2,1}+N_{2,2}=N_2$$

(Here $^{\circ}$ indicates that $\mathcal{S}$-measurements always yield b_1, $^{\circ\circ}$ that they always yield b_2.) The quantity $\mathcal{S}$ is dispersionless in each of the four sub-ensembles

$$[\mathbf{S}'^{\circ}_1,\ldots,\mathbf{S}'^{\circ}_{N_{1,1}}],\ [\mathbf{S}'^{\circ\circ}_1,\ldots,\mathbf{S}'^{\circ\circ}_{N_{1,2}}],\ [\mathbf{S}''^{\circ}_1,\ldots,\mathbf{S}''^{\circ}_{N_{2,1}}],\ [\mathbf{S}''^{\circ\circ}_1,\ldots,\mathbf{S}''^{\circ\circ}_{N_{2,2}}]$$

(the measured values are invariably b_1, b_2, b_1, b_2 respectively). But although the first two ensembles are parts of $[\mathbf{S}'_1,\ldots,\mathbf{S}'_{N_1}]$, and the latter two parts of $[\mathbf{S}''_1,\ldots,\mathbf{S}''_{N_2}]$ in which $\mathcal{R}$ did not have dispersion, $\mathcal{R}$ can now have dispersion in each one of them, because the $\mathcal{S}$ measurements have changed the individual systems of which they are comprised. In short, we do not get ahead: each step destroys the results of the preceding one,[162] and no further repetition of successive measurements can bring order to this confusion. In an atom we are at the boundary of the physical world, where each measurement is an interference of the same order of magnitude as the quantity being measured, and therefore affects it profoundly. It is evident that the uncertainty relations are at the root of these difficulties.

Therefore we have no method which would make it always possible to resolve further the dispersing ensembles (without a change of their elements) or to penetrate to those imagined homogeneous ensembles which no longer have dispersion—the ensembles we are accustomed to supposing are composed of individual particles, all identical, and all determined causally. Nevertheless, we might attempt to maintain the fiction that every dispersing ensemble can be divided into two (or more) parts, different from each other and from it, without a change of its elements. The imagined division would be such that superposition of the resolved ensembles would again produce the original ensemble. As we see, the attempt to interpret causality as an equality definition led to a question of fact which can and must be answered, and which might conceivably be answered negatively. This is the question: Is it really possible to represent each ensemble $[\mathbf{S}_1,\ldots,\mathbf{S}_N]$, in which there is a quantity $\mathcal{R}$ with dispersion, as a superposition of two (or more) ensembles different from one another and from it? (More than two—say, $n = 3, 4, \ldots$—can be reduced to two if we consider the first and the superposition of the $n-1$ others.)

If $[\mathbf{S}_1,\ldots,\mathbf{S}_N]$ were the mixture (sum) of $[\mathbf{S}'_1,\ldots,\mathbf{S}'_P]$ and $[\mathbf{S}''_1,\ldots,\mathbf{S}''_Q]$ the probability function $w_{\mathcal{R}}(a)$ (see Note 157) for each quantity $\mathcal{R}$ could be

[162] One should consider, for example, what happens if we substitute q and p (cartesian coordinate and momentum, which are not simultaneously measurable because of the uncertainty relations) for $\mathcal{R}$ and $\mathcal{S}$. If q has very small dispersion in an ensemble, then the p-measurement with accuracy (*i.e.*, dispersion) ϵ sets up a q dispersion of at least $\frac{1}{2}\hbar/\epsilon$ (see **III.4**): everything is ruined.

expressed with the aid of the probability functions $w'_{\mathcal{R}}(a)$ and $w''_{\mathcal{R}}(a)$ of the two sub-ensembles:

$$\mathbf{M}_1 \qquad w_{\mathcal{R}}(a) = \alpha w'_{\mathcal{R}}(a) + \beta w''_{\mathcal{R}}(a) \quad : \quad \alpha > 0, \beta > 0, \alpha + \beta = 1$$

Here $\alpha = P/N, \beta = Q/N$ $(N = P + Q)$ are independent of $\mathcal{R}$. Fundamentally, this is a purely mathematical problem: If in an ensemble with probability functions $w_{\mathcal{R}}(a)$ there exist quantities $\mathcal{R}$ with dispersion (which is a property of $w_{\mathcal{R}}(a)$, as indicated in Note 160), are there two other ensembles, with respective probability functions $w'_{\mathcal{R}}(a)$ and $w''_{\mathcal{R}}(a)$, such that—for all $\mathcal{R}$—$\mathbf{M}_1$ holds? The question can also be formulated in a somewhat different way if we characterize an ensemble not by the probability functions $w_{\mathcal{R}}(a)$ of quantities $\mathcal{R}$ but by their expectation values

$$\mathrm{Exp}(\mathcal{R}) = \int_{-\infty}^{+\infty} a\, dw_{\mathcal{R}}(a)$$

Then our question is the following: An ensemble is dispersion-free if in it, for each $\mathcal{R}$,

$$\mathrm{Exp}\big([\mathcal{R} - \mathrm{Exp}(\mathcal{R})]^2\big) = \mathrm{Exp}(\mathcal{R}^2) - [\mathrm{Exp}(\mathcal{R})]^2$$

is equal to zero (see again Note 160); *i.e.*,

$$\mathbf{Dis}_1 \qquad \mathrm{Exp}(\mathcal{R}^2) = [\mathrm{Exp}(\mathcal{R})]^2$$

If this is not the case, is it always possible to find two sub-ensembles (with expectation values denoted $\mathrm{Exp}'(\mathcal{R}), \mathrm{Exp}''(\mathcal{R}) : \mathrm{Exp}(\mathcal{R}) \not\equiv \mathrm{Exp}'(\mathcal{R}) \not\equiv \mathrm{Exp}''(\mathcal{R})$) such that

$$\mathbf{M}_2 \qquad \mathrm{Exp}(\mathcal{R}) = \alpha \mathrm{Exp}'(\mathcal{R}) + \beta \mathrm{Exp}''(\mathcal{R}) \quad : \quad \alpha > 0, \beta > 0, \alpha + \beta = 1$$

always holds (α, β independent of $\mathcal{R}$)? (It should be noted that for a single quantity $\mathcal{R}$ the number $\mathrm{Exp}(\mathcal{R})$ is not a substitute for the function $w_{\mathcal{R}}(a)$, but on the other hand: knowledge of all $\mathrm{Exp}(\mathcal{R})$ is equivalent to knowledge of all $w_{\mathcal{R}}(a)$. Indeed, if $f_a(x)$ is defined

$$f_a(x) = \begin{cases} 1 & \text{for} \quad x \leqslant a \\ 0 & \text{for} \quad x > a \end{cases}$$

then $w_{\mathcal{R}}(a) = \mathrm{Exp}\big(f_a(\mathcal{R})\big)$.)

To handle this question mathematically it is preferable not to consider the $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ themselves, but rather the corresponding $\mathrm{Exp}(\mathcal{R})$. To each such ensemble there belongs one such function which is defined for all physical quantities $\mathcal{R}$ in $\mathbf{S}$, which takes on real numbers as values and which, conversely, completely characterizes the ensemble in all its statistical properties (see the discussion above on the relation between $\mathrm{Exp}(\mathcal{R})$ and $w_{\mathcal{R}}(a)$). Of course, it remains to discover what properties an $\mathcal{R}$-function must possess if it is to be the $\mathrm{Exp}(\mathcal{R})$ of a suitable ensemble. But as soon as we have done this we will

be in position to make these definitions:

α. An $\mathcal{R}$-function, if it is an $\mathrm{Exp}(\mathcal{R})$, is said to be *dispersion-free* if it satisfies the condition $\mathbf{Dis}_1$.

β. An $\mathcal{R}$-function, if it is an $\mathrm{Exp}(\mathcal{R})$, is said to be *homogeneous* or *pure* if, for it, $\mathbf{M}_2$ implies

$$\mathrm{Exp}(\mathcal{R}) \equiv \mathrm{Exp}'(\mathcal{R}) \equiv \mathrm{Exp}''(\mathcal{R})$$

It is conceptually plausible that each dispersion-free $\mathrm{Exp}(\mathcal{R})$-function should be pure, and we shall soon prove it. But we are interested at the moment in the converse question: Is each pure $\mathrm{Exp}(\mathcal{R})$-function dispersion-free?

It is evident that each $\mathrm{Exp}(\mathcal{R})$-function must possess the following properties:

A. If the quantity $\mathcal{R}$ is identically 1 (*i.e.*, if the "directions for measurement" are: no measurement is necessary, because $\mathcal{R}$ always has the value 1), then $\mathrm{Exp}(\mathcal{R}) = 1$.

B. For each $\mathcal{R}$ and each real number a, $\mathrm{Exp}(a\mathcal{R}) = a\,\mathrm{Exp}(\mathcal{R})$.[163]

C. If the quantity $\mathcal{R}$ is by nature non-negative (if, for example, it is the square of another quantity $\mathcal{S}$[163]) then also $\mathrm{Exp}(\mathcal{R}) \geqslant 0$.

D. If the quantities $\mathcal{R}$, $\mathcal{S}$, ... are simultaneously measurable then

$$\mathrm{Exp}(\mathcal{R} + \mathcal{S} + \cdots) = \mathrm{Exp}(\mathcal{R}) + \mathrm{Exp}(\mathcal{S}) + \cdots$$

(If $\mathcal{R}$, $\mathcal{S}$, ... are not simultaneously measurable then their sum is undefined: see above.)

All this follows immediately from the definitions of the quantities under consideration (*i.e.*, from the directions for their measurement) and from the definition of expectation value as the arithmetic mean of all the results of measurement in a sufficiently large statistical ensemble. Regarding **D**, it should be noted that its correctness depends upon this theorem on probability: The expectation value of a sum is always the sum of the expectation values, independently of whether or not dependencies exist between these (in contrast, for example, to the probability of the product). That **D** embodies this basic fact only as it pertains to simultaneously measurable $\mathcal{R}$, $\mathcal{S}$, ... is natural, since otherwise $\mathcal{R} + \mathcal{S} + \cdots$ is meaningless.

But quantum mechanics exploits still another operation, which goes beyond the one just discussed: namely, the addition of two arbitrary quantities which are not necessarily simultaneously observable. This operation depends upon the

[163] $a\mathcal{R}, \mathcal{S}^2, \mathcal{R}+\mathcal{S}+\cdots$ mean that we may substitute $\mathcal{R}$, $\mathcal{S}$, ... in the functions $f(x) = ax, f(x) = x^2, f(x, y, \ldots) = x + y + \cdots$ respectively, in the sense of the definitions given above.

fact that for two Hermitian operators R, S the sum $\mathsf{R}+\mathsf{S}$ is also Hermitian, even if R and S do not commute (while, for example, the product RS is Hermitian only if the two operators commute: see **II.5**). In each state ϕ the expectation values behave additively: $(\mathsf{R}\phi,\phi)+(\mathsf{S}\phi,\phi)=((\mathsf{R}+\mathsf{S})\phi,\phi)$ (see **III.1**). The same holds for several summands. We now incorporate this fact into our general set-up (which at this point is not yet specialized to quantum mechanics):

> **E**. If $\mathcal{R}$, $\mathcal{S}$, ... are arbitrary quantities then there is an additional quantity $\mathcal{R}+\mathcal{S}+\cdots$ (which does not depend upon the choice of the $\mathrm{Exp}(\mathcal{R})$-function) such that
>
> $$\mathrm{Exp}(\mathcal{R}+\mathcal{S}+\cdots)=\mathrm{Exp}(\mathcal{R})+\mathrm{Exp}(\mathcal{S})+\cdots$$

If $\mathcal{R}$, $\mathcal{S}$, ... are simultaneously measurable then $\mathcal{R}+\mathcal{S}+\cdots$ must be the ordinary sum (by **D**). But in general the sum is characterized only in an implicit way by **E**, which provides no indication of how one is to proceed from the measurement instructions for the quantities $\mathcal{R}$, $\mathcal{S}$, ... to measurement instructions for the quantity called $\mathcal{R}+\mathcal{S}+\cdots$.[164]

In addition, it must be remarked that we shall admit not only $\mathrm{Exp}(\mathcal{R})$-functions representing expectation values, but also functions which correspond to relative values; *i.e.*, , we allow the normalization condition **A** to be dropped. If $\mathrm{Exp}(1)$ (which is $\geqslant 0$ by **C**) is finite and $\neq 0$ this is unimportant, since for $\mathrm{Exp}(R)/\mathrm{Exp}(1)$ everything is as before. But $\mathrm{Exp}(1)=\infty$ is an entirely different matter, and it is to address this issue that we undertake the following extension of the material developed above. The point at issue is best illustrated by a simple example. The fact is that there are cases in which it is better to operate with relative probabilities than with true probabilities—specifically

[164] For example, the energy operator

$$\mathsf{H}_0=\frac{(\mathsf{P}^x)^2+(\mathsf{P}^y)^2+(\mathsf{P}^z)^2}{2m}+V(\mathsf{Q}^x,\mathsf{Q}^y,\mathsf{Q}^z)$$

of a (charged) particle moving in a potential field $V(x,y,z)$ (see, for example, **III.6**) is a sum of two non-commuting operators

$$\mathsf{R}=\frac{(\mathsf{P}^x)^2+(\mathsf{P}^y)^2+(\mathsf{P}^z)^2}{2m},\qquad \mathsf{S}=V(\mathsf{Q}^x,\mathsf{Q}^y,\mathsf{Q}^z)$$

While the measurement of the quantity $\mathcal{R}$ belonging to R is a momentum measurement, and that of the $\mathcal{S}$ belonging to S is a coordinate measurement, we measure the $\mathcal{R}+\mathcal{S}$ belonging to $\mathsf{H}_0=\mathsf{R}+\mathsf{S}$ in an entirely different way: for example, by measurement of the frequencies of the spectral lines, since these lines determine (by reason of the Bohr frequency relation) the energy levels; *i.e.*, the $\mathcal{R}+\mathcal{S}$ values. Nevertheless, under all circumstances,

$$\mathrm{Exp}(\mathcal{R}+\mathcal{S})=\mathrm{Exp}(\mathcal{R})+\mathrm{Exp}(\mathcal{S})$$

the cases with an infinite total relative probability ($\mathrm{Exp}(1)$ is the total probability). The following is such an example: Let the observed system be a particle in one dimension, and let its statistical distribution be of such a kind that it lies with equal probability everywhere in the infinite interval. Then each finite interval has probability zero, but the equal probability of all places is not expressed in this way, but rather by the fact that two finite intervals have as their probability ratio the quotient of their lengths. Since $0/0$ has no meaning, this can be expressed only if we introduce their lengths as relative probabilities. The total relative probability will then of course be ∞.

Upon consideration of the foregoing, we arrive at the following adjusted form of our conditions ($\mathbf{A}'$ corresponds to **C**, $\mathbf{B}'$ corresponds to **B**, **D**, **E**):

> $\mathbf{A}'$. If the quantity $\mathcal{R}$ is by nature non-negative (if, for example, it is the square of another quantity $\mathcal{S}$) then also $\mathrm{Exp}(\mathcal{R}) \geqslant 0$.
>
> $\mathbf{B}'$. If $\mathcal{R}$, $\mathcal{S}$, ... are arbitrary quantities and $a, b, \ldots$ real numbers, then
>
> $$\mathrm{Exp}(a\mathcal{R} + b\mathcal{S} + \cdots) = a\,\mathrm{Exp}(\mathcal{R}) + b\,\mathrm{Exp}(\mathcal{S}) + \cdots$$

We emphasize:

> **1**. So far as concerns the construction of relative probabilities, $\mathrm{Exp}(\mathcal{R})$ and $c\,\mathrm{Exp}(\mathcal{R})$ (here c is any non-negative constant) are not essentially different from each other.
>
> **2**. $\mathrm{Exp}(\mathcal{R}) \equiv 0$ (for all $\mathcal{R}$) supplies no information, and therefore this function is excluded.
>
> **3**. Absolute—*i.e.*, correctly normalized expectation values—exist if $\mathrm{Exp}(1) = 1$. $\mathrm{Exp}(1)$ is in any case non-negative (by $\mathbf{A}'$), and if it is finite then **1** (with $c = 1/\mathrm{Exp}(1)$) leads to the correct normalization. The case $\mathrm{Exp}(\mathcal{R}) = 0$, as we will show, leads back again to **2**, and is therefore eliminated. For $\mathrm{Exp}(\mathcal{R}) = \infty$, however, an essentially non-normalized (*i.e.*, relative) statistic exists.

We must still return to our definitions $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$. By **1**, $\mathbf{M}_2$ can be replaced by the following simpler condition

$\mathbf{M}_3$ $$\mathrm{Exp}(\mathcal{R}) = \mathrm{Exp}'(\mathcal{R}) + \mathrm{Exp}''(\mathcal{R})$$

And in the case of $\mathbf{Dis}_1$ it is to be observed that the calculation there presupposes $\mathrm{Exp}(\mathcal{R}) = 1$. For $\mathrm{Exp}(\mathcal{R}) = \infty$ the dispersion-free condition cannot be defined, since it means $\mathrm{Exp}((\mathcal{R} - \rho)^2) = 0$, where ρ is the absolute expectation value of $\mathcal{R}$; *i.e.*, $\mathrm{Exp}(\mathcal{R})/\mathrm{Exp}(1)$, which in this case becomes ∞/∞ and is therefore meaningless.[165] Therefore $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ are rephrased as follows:

[165] For dispersion-free ensembles there is, however, no reason for not introducing the correct expectation values.

$\boldsymbol{\alpha}'$. An $\mathcal{R}$-function which is an $\mathrm{Exp}(\mathcal{R})$ is said to be *dispersion-free* if $\mathrm{Exp}(\mathcal{R}) \neq 0$ and is finite, so that we can assume $\mathrm{Exp}(\mathcal{R}) = 1$ by **1**. Then $\mathbf{Dis}_1$ is characteristic.

$\boldsymbol{\beta}'$. An $\mathcal{R}$-function which is an $\mathrm{Exp}(\mathcal{R})$ is said to be *homogeneous* or *pure* if for it $\mathbf{M}_3$ has

$$\mathrm{Exp}'(\mathcal{R}) = c' \mathrm{Exp}(\mathcal{R}), \quad \mathrm{Exp}''(\mathcal{R}) = c'' \mathrm{Exp}(\mathcal{R})$$

as a consequence (here c', c'' are constants with $c' + c'' = 1$ and—because of $\mathbf{A}'$ and **1**, **2**—also $c' > 0$, $c'' > 0$).

By reason of $\mathbf{A}'$, $\mathbf{B}'$ and $\boldsymbol{\alpha}'$, $\boldsymbol{\beta}'$ we are now in position to make a decision on the question of causality, as soon as we know the physical quantities in **S** as well as the functional relationships between them. In the following section this will be carried out for the relations of quantum mechanics.

As a conclusion to this section, two remarks should be added.

First: one which concerns the case $\mathrm{Exp}(1) = 0$. It follows from $\mathbf{B}'$ that $\mathrm{Exp}(c) = 0$. Therefore if a quantity $\mathcal{R}$ is always $\geqslant c'$ but $\leqslant c''$ then (by $\mathbf{A}'$) $\mathrm{Exp}(c'' - \mathcal{R}) \geqslant 0$, $\mathrm{Exp}(\mathcal{R} - c') \geqslant 0$ and hence (by $\mathbf{B}'$)

$$\mathrm{Exp}(c') \leqslant \mathrm{Exp}(\mathcal{R}) \leqslant \mathrm{Exp}(c'')$$

i.e., $\mathrm{Exp}(\mathcal{R}) = 0$. Now let $\mathcal{R}$ be arbitrary and $f_1(x), f_2(x), \ldots$ a sequence of bounded functions with

$$f_1(x) + f_2(x) + \cdots = 1$$

(An example:

$$f_1(x) = \frac{\sin x}{x}, \qquad f_n(x) = \frac{\sin nx}{nx} - \frac{\sin(n-1)x}{(n-1)x}$$

with $n = 2, 3, \ldots$.) Then $\mathrm{Exp}(f_n(\mathcal{R})) = 0$ for $n = 1, 2, \ldots$, and therefore (by $\mathbf{B}'$) we also have $\mathrm{Exp}(\mathcal{R}) = 0$. Consequently, $\mathrm{Exp}(1) = 0$ is excluded by **2**, according to the proposition stated previously.

Second: it is remarkable that, by $\mathbf{Dis}_1$,

$$\mathrm{Exp}(\mathcal{R}^2) = [\mathrm{Exp}(\mathcal{R})]^2$$

is characteristic for the dispersion-free case, although in this case

$\mathbf{Dis}_2$ $$\mathrm{Exp}(f(\mathcal{R})) = f(\mathrm{Exp}(\mathcal{R}))$$

must hold for each function $f(x)$, since $\mathrm{Exp}(\mathcal{R})$ is simply the value of $\mathcal{R}$, and $\mathrm{Exp}(f(\mathcal{R}))$ the value of $f(\mathcal{R})$. $\mathbf{Dis}_1$ is a special case of $\mathbf{Dis}_2$: $f(x) = x^2$, but how is it that this suffices? The answer is the following: If $\mathbf{Dis}_2$ holds for $f(x) = x^2$ it holds of itself for all $f(x)$. One would even be able to replace x^2 by any other continuous and convex function of x (*i.e.*, one for which $f(\frac{x+y}{2}) < \frac{1}{2}[f(x)+f(y)]$ for all $x \neq y$). We do not enter into the proof.

2. PROOF OF THE STATISTICAL FORMULAS

There corresponds to every physical quantity of a quantum mechanical system a unique hypermaximal Hermitian operator, as we know (see, for example, the discussion in **III.5**), and it is convenient to assume that this correspondence is one-to-one; *i.e.*, that actually every hypermaximal operator corresponds to a physical quantity. (We made occasional use of this presumption in **III.3**). Granted the validity of that assumption, the following rules are valid (see **F**, **L** in **III.5**, as well as the discussion at the end of **IV.1**):

> **I**. If the quantity $\mathcal{R}$ has the operator R then the quantity $f(\mathcal{R})$ has the operator $f(\mathsf{R})$.
>
> **II**. If the quantities $\mathcal{R}$, $\mathcal{S}$, ... have the operators $\mathsf{R}, \mathsf{S}, \ldots$ then the quantity $\mathcal{R}+\mathcal{S}+\cdots$ has the operator $\mathsf{R}+\mathsf{S}+\cdots$. (The simultaneous measurability of $\mathcal{R}$, $\mathcal{S}$, ... is not assumed: see previous discussion of this point.)

A′, **B′**, **α′**, **β′**, **I** and **II** provide the mathematical basis of our analysis.

Let $\phi_1, \phi_2, \ldots$ be a complete orthonormal basis. We look—instead of to operators R themselves—to their matrix elements $a_{\mu\nu} = (\mathsf{R}\phi_\mu, \phi_\nu)$ with respect to that basis. We define Hermitian operators $\mathsf{U}^{(n)}, \mathsf{V}^{(mn)}, \mathsf{W}^{(mn)}$ in terms of their matrix elements:

$$e_{\mu\nu}^{(n)} = \begin{cases} 1 & \text{for} \quad \mu = \nu = n \\ 0 & \text{otherwise} \end{cases}$$

$$f_{\mu\nu}^{(mn)} = \begin{cases} 1 & \text{for} \quad \mu = m, \ \nu = n \\ 1 & \text{for} \quad \mu = n \ , \ \nu = m \\ 0 & \text{otherwise} \end{cases}$$

$$g_{\mu\nu}^{(mn)} = \begin{cases} +i & \text{for} \quad \mu = m, \ \nu = n \\ -i & \text{for} \quad \mu = n \ , \ \nu = m \\ 0 & \text{otherwise} \end{cases}$$

which entail

$$\mathsf{U}^{(n)} = \mathsf{P}_{[\phi_n]}$$

$$\mathsf{V}^{(mn)} = \mathsf{P}_{\left[\frac{\phi_m+\phi_n}{\sqrt{2}}\right]} - \mathsf{P}_{\left[\frac{\phi_m-\phi_n}{\sqrt{2}}\right]}$$

$$\mathsf{W}^{(mn)} = \mathsf{P}_{\left[\frac{\phi_m+i\phi_n}{\sqrt{2}}\right]} - \mathsf{P}_{\left[\frac{\phi_m-i\phi_n}{\sqrt{2}}\right]}$$

The corresponding quantities will be denoted $\mathcal{U}^{(n)}$, $\mathcal{W}^{(mn)}$, $\mathcal{U}^{(mn)}$. Evidently (because $a_{nm} = \bar{a}_{mn}$)

$$a_{\mu\nu} = \sum_n a_{nn} e_{\mu\nu}^{(n)} + \sum_{\substack{m,n \\ m<n}} \mathrm{Re}(a_{mn}) f_{\mu\nu}^{(mn)} + \sum_{\substack{m,n \\ m<n}} \mathrm{Im}(a_{mn})\, g_{\mu\nu}^{(mn)}$$

Therefore

$$\mathcal{R} = \sum_n a_{nn} \mathcal{U}^{(n)} + \sum_{\substack{m,n \\ m<n}} \mathrm{Re}(a_{mn}) \mathcal{V}^{(mn)} + \sum_{\substack{m,n \\ m<n}} \mathrm{Im}(a_{mn})\, \mathcal{W}^{(mn)}$$

and because of **II**, **B′**

$$\mathrm{Exp}(\mathcal{R}) = \sum_n a_{nn}\,\mathrm{Exp}(\mathcal{U}^{(n)}) + \sum_{\substack{m,n\\ m<n}} \mathrm{Re}(a_{mn})\mathrm{Exp}(\mathcal{V}^{(mn)}) + \sum_{\substack{m,n\\ m<n}} \mathrm{Im}(a_{mn})\,\mathrm{Exp}(\mathcal{W}^{(mn)})$$

Therefore if we set

$$\left.\begin{aligned} \mu_{nn} &= \mathrm{Exp}(\mathcal{U}^{(n)}) \\ \mu_{mn} &= \tfrac{1}{2}\mathrm{Exp}(\mathcal{V}^{(mn)}) + i\,\tfrac{1}{2}\mathrm{Exp}(\mathcal{W}^{(mn)}) \\ \mu_{nm} &= \tfrac{1}{2}\mathrm{Exp}(\mathcal{V}^{(mn)}) - i\,\tfrac{1}{2}\mathrm{Exp}(\mathcal{W}^{(mn)}) \end{aligned}\right\} \quad : \quad m < n$$

we obtain

$$\mathrm{Exp}(\mathcal{R}) = \sum_{m,n} \mu_{nm} a_{mn}$$

Since $\mu_{mn} = \bar{\mu}_{nm}$ we can define a Hermitian operator U by $(\mathsf{U}\phi_m, \phi_n) = \mu_{mn}$,[166] and the right side of the preceding equation becomes $\mathrm{Tr}(\mathsf{UR})$ (see **II.11**). We are

[166] That is,

$$\mathsf{U}\phi_m = \sum_n \mu_{mn}\phi_n$$

where the finiteness of $\sum_n |\mu_{mn}|^2$ is of course necessary. This can be established in the following way: If $\sum_n |x_n|^2 = 1$ then $\mathsf{R} = \mathsf{P}_{[\phi]}$ has the matrix $\bar{x}_\mu x_\nu$ for $\phi = \sum_n x_n\phi$, and its $\mathcal{R}$ has the expectation value $\sum_{m,n} \mu_{nm}\bar{x}_m x_n$. Because of

$$\mathsf{P}_{[\phi]} = \mathsf{P}_{[\phi]}^2, \qquad \mathsf{I} - \mathsf{P}_{[\phi]} = (\mathsf{I} - \mathsf{P}_{[\phi]})^2$$

this is $\geqslant 0$ and $\leqslant \mathrm{Exp}(1)$, therefore $\geqslant 0$ and $\leqslant 1$ at least for normalized $\mathrm{Exp}(\mathcal{R})$. If $x_{N+1} = x_{N+2} = \cdots = 0$, this means that the N-dimensional Hermitian form

$$\sum_{m,n=1}^{N} \mu_{nm}\bar{x}_m x_n$$

has values $\geqslant 0$ but $\leqslant 1$ for $\sum_{n=1}^{N} |x_n|^2 = 1$; *i.e.*, that the eigenvalues of the matrix $\mu_{\rho\sigma}$ $(\rho, \sigma = 1, 2, \ldots, N)$ are $\geqslant 0$ but $\leqslant 1$. Therefore the length of the vector

$$y_m = \sum_{n=1}^{N} \mu_{mn} x_n$$

is always $\leqslant$ that of the vector x_m. For

$$x_m = \begin{cases} 1 & \text{for} \quad m = \bar{m} \\ 0 & \text{otherwise} \end{cases}$$

led thus to the formula

Tr $$\mathrm{Exp}(\mathcal{R}) = \mathrm{Tr}(\mathsf{UR})$$

U is a Hermitian operator[167] independent of R, and is therefore determined by the ensemble itself.

With regard to **II**, **Tr** satisfies $\mathbf{B}'$ for every choice of U: therefore we have only to determine what limitation $\mathbf{A}'$ imposes upon U.

If $\|\phi\| = 1$ but is otherwise arbitrary, then $\mathcal{R}^2 = \mathcal{R}$ for the quantity $\mathcal{R}$ belonging to $\mathsf{P}_{[\phi]}$ because of $\mathsf{P}_{[\phi]}^2 = \mathsf{P}_{[\phi]}$ and **I**. Therefore, by $\mathbf{A}'$, $\mathrm{Exp}(\mathcal{R}) \geqslant 0$. Consequently $\mathrm{Tr}(\mathsf{UP}_{[\phi]}) = (\mathsf{U}\phi, \phi) \geqslant 0$. If f is arbitrary then, for $f \neq 0$, ϕ can be written $f/\|f\|$, giving $(\mathsf{U}\phi, \phi) = (\mathsf{U}f, f)/\|f\|^2$. Hence $(\mathsf{U}f, f) \geqslant 0$; for $f = 0$ this holds automatically. Consequently U is definite. But the definiteness of U, which thus follows from $\mathbf{A}'$, is also sufficient for the validity of $\mathbf{A}'$.

Indeed, $\mathbf{A}'$ asserts that each $\mathrm{Exp}(\mathcal{S}^2) \geqslant 0$ and no more. Because if $\mathcal{R}$ admits only of non-negative values then for $f(x) = |x|$ one has $f(\mathcal{R}) = \mathcal{R}$. And since $(g(x))^2 = f(x)$ identically for $g(x) = \sqrt{|x|}$ one has $(g(\mathcal{R}))^2 = f(\mathcal{R})$, $\mathcal{R} = \mathcal{S}^2$, $\mathcal{S} = g(\mathcal{R})$.[168] Hence we must prove only this: If S is the operator belonging to $\mathcal{S}$ then $\mathrm{Tr}(\mathsf{US}^2) \geqslant 0$. Now S^2 is definite ($(\mathsf{S}^2 f, f) = (\mathsf{S}f, \mathsf{S}f) \geqslant 0$). Therefore if we write A, B in place of U, S^2 the problem reduces to proof of the following theorem: If A, B are Hermitian and definite then $\mathrm{Tr}(\mathsf{AB}) \geqslant 0$. But we

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we have $y_m = \mu_{m\bar{m}}$ and therefore

$$\sum_{m=1}^{N} |x_m|^2 \geqslant \sum_{m=1}^{N} |y_m|^2, \qquad 1 \geqslant \sum_{m=1}^{N} |\mu_{m\bar{m}}|^2$$

Since this holds for each N, $\sum_n |\mu_{\bar{m}n}|^2 \leqslant 1$.

[167] The whole argument is rigorous only if all $\phi_1, \phi_2, \ldots$ belong to the domain of R. Now for each R one can find such a complete orthonormal set $\phi_1, \phi_2, \ldots$ (see **II.11**), but if R does not have meaning everywhere then this set depends upon R. Actually, therefore, for each complete orthonormal set $\phi_1, \phi_2, \ldots$ we have a U dependent upon this set, such that $\mathrm{Exp}(\mathcal{R}) = \mathrm{Tr}(\mathsf{UR})$ need be valid only for those R to whose domain the $\phi_1, \phi_2, \ldots$ belong.

However, all these U are equal to one another. Because if U' and U'' are two such then the above formula holds for both, provided that R has meaning everywhere, for in that case $\mathrm{Tr}(\mathsf{U}'\mathsf{R}) = \mathrm{Tr}(\mathsf{U}''\mathsf{R})$. For $\mathsf{R} = \mathsf{P}_{[\phi]}$ therefore $(\mathsf{U}'\phi, \phi) = (\mathsf{U}''\phi, \phi)$, $((\mathsf{U}' - \mathsf{U}'')\phi, \phi) = 0$. Since this holds for all ϕ with $\|\phi\| = 1$, and therefore for all elements of the Hilbert space, $\mathsf{U}' - \mathsf{U}'' = \mathsf{O}$, and therefore $\mathsf{U}' = \mathsf{U}''$.

[168] We cannot substitute $\mathcal{S} = \sqrt{\mathcal{R}}$ directly (*i.e.*, $\mathcal{S} = h(\mathcal{R})$, $h(x) = \sqrt{x}$) because we only consider real-valued functions defined for all real x, and $\sqrt{x}$ is not such a thing, since it is imaginary for negative x.

have proved this in **II.11** by use of a general theorem on definite operators (see Note 114).[169]

Thus have we determined the functions $\mathrm{Exp}(\mathcal{R})$ completely; they correspond to the definite Hermitian operator U, and the connection is given by **Tr**. We shall call U the *statistical operator* of the ensemble under consideration.

The points **1**, **2**, **3** in **IV.1** are now easy to discuss. These are the results:

1. From the standpoint of relative probabilities and expectation values, U and $c\mathsf{U}$ (c any positive constant) are not essentially different from each other.

2. $\mathsf{U} = \mathsf{O}$ supplies no information, and is therefore to be excluded.

3. Absolute (which is to say: correctly normalized) probabilities and expectation values are obtained if $\mathrm{Tr}\mathsf{U} = 1$. So long as $\mathrm{Tr}\mathsf{U}$ is finite we can normalize by multiplication with $c = 1/\mathrm{Tr}\mathsf{U}$, according to **1**. (Because of the definiteness of U, $\mathrm{Tr}\mathsf{U} \geqslant 0$. But actually $\mathrm{Tr}\mathsf{U} > 0$, since it follows from $\mathrm{Tr}\mathsf{U} = 0$ that $\mathsf{U} = \mathsf{O}$, as was shown at the end of **IV.1** in the general case; in our case this also follows from **II.11**; this is the case excluded by **2**.) It is only when $\mathrm{Tr}\mathsf{U}$ is infinite that relative probabilities and expectation values become essential.

Finally we must investigate $\boldsymbol{\alpha}, \boldsymbol{\beta}$ from **IV.1**; *i.e.*, we must identify the dispersion-free and homogeneous ensembles among the U.

First we consider the dispersion-free ensembles. For them we are obliged to assume that U is correctly normalized (see **IV.1**) and that it is invariably true that $\mathrm{Exp}(\mathcal{R}^2) = [\mathrm{Exp}(\mathcal{R})]^2$; *i.e.*, $\mathrm{Tr}(\mathsf{U}\mathsf{R}^2) = [\mathrm{Tr}(\mathsf{U}\mathsf{R})]^2$. For $\mathsf{R} = \mathsf{P}_{[\phi]}$ one has

[169] It is also possible to give a simple direct proof. Let $\phi_1, \phi_2, \ldots$ be a complete orthonormal set, $a_{\mu\nu} = (\mathsf{A}\phi_\mu, \phi_\nu)$, $b_{\mu\nu} = (\mathsf{B}\phi_\mu, \phi_\nu)$, $\mathrm{Tr}(\mathsf{A}\mathsf{B}) = \sum_{\mu,\nu} a_{\mu\nu} b_{\nu\mu}$. The trace $\mathrm{Tr}(\mathsf{A}\mathsf{B})$ is $\geqslant 0$ if $\sum_{\mu,\nu=1}^{N} a_{\mu\nu} b_{\nu\mu} \geqslant 0$. If $f = \sum_{\mu=1}^{N} x_\mu \phi_\mu$ then

$$(\mathsf{A}f, f) = \sum_{\mu,\nu=1}^{N} a_{\mu\nu} x_\mu \bar{x}_\nu \geqslant 0, \qquad (\mathsf{B}f, f) = \sum_{\mu,\nu=1}^{N} b_{\mu\nu} x_\mu \bar{x}_\nu \geqslant 0$$

and therefore the finite matrices $a_{\mu\nu}, b_{\mu\nu}$ $(\mu, \nu = 1, 2, \ldots, N)$ are also definite. Now both the definiteness and the value of $\sum_{\mu,\nu=1}^{N} a_{\mu\nu} b_{\nu\mu}$ are orthogonally invariant in N-dimensional space; since $b_{\mu\nu}$ is Hermitian it can (in N-space) be brought to diagonal form by an orthogonal transformation. We may therefore assume it to be diagonal in the first place; *i.e.*, $b_{\mu\nu} = 0$ for $\mu \neq \nu$. Then

$$\sum_{\mu,\nu=1}^{N} a_{\mu\nu} b_{\nu\mu} = \sum_{\mu=1}^{N} a_{\mu\mu} b_{\mu\mu}$$

Because of the definiteness of both matrices $a_{\mu\mu} \geqslant 0$ and $b_{\mu\mu} \geqslant 0$ (we set $x_\nu = \begin{cases} 1 & \text{for} \quad \nu = \mu \\ 0 & \text{for} \quad \nu \neq \mu \end{cases}$) and this implies that the above sum is $\geqslant 0$.

$\mathsf{R}^2 = \mathsf{R} = \mathsf{P}_{[\phi]}$, $\mathrm{Tr}(\mathsf{U}\mathsf{P}_{[\phi]}) = (\mathsf{U}\phi, \phi)$ and therefore $(\mathsf{U}\phi, \phi) = (\mathsf{U}\phi, \phi)^2$, so $(\mathsf{U}\phi, \phi) = 0$ or $(\mathsf{U}\phi, \phi) = 1$. If $\|\phi'\| = \|\phi''\| = 1$ then we can vary ϕ continuously so that it begins at ϕ', ends at ϕ'', and at all intermediate points satisfies $\|\phi\| = 1$.[170] Clearly, $(\mathsf{U}\phi, \phi)$ also varies continuously, and—since it can be only 0 or 1—it is constant. Therefore $(\mathsf{U}\phi', \phi') = (\mathsf{U}\phi'', \phi'')$. Consequently, $(\mathsf{U}\phi, \phi)$ is either always 0 or always 1, from which we obtain $\mathsf{U} = \mathsf{O}$ or $\mathsf{U} = \mathsf{I}$, respectively. $\mathsf{U} = \mathsf{O}$ is excluded by **2**, while $\mathsf{U} = \mathsf{I}$ cannot be normalized:

$$\mathrm{Tr}(\mathsf{I}) = \text{dimension of the space} = \infty$$

So (as we can also see directly) $\mathsf{U} = \mathsf{I}$ is not dispersion-free. Consequently there can exist no dispersion-free ensembles.

Let us now look to the homogeneous (or pure) case. By ***β*** and **Tr**, U is homogeneous if from

$$\mathsf{U} = \mathsf{V} + \mathsf{W}$$

(here V and W are, like U, Hermitian and definite) it follows that $\mathsf{V} = c'\mathsf{U}$ and $\mathsf{W} = c''\mathsf{U}$.[171] We assert that this property holds for $\mathsf{U} = \mathsf{P}_{[\phi]}$ ($\|\phi\| = 1$) and only for these.

First, let U have the property mentioned. Because $\mathsf{U} \neq \mathsf{O}$ there is an f_0 with $\mathsf{U}f_0 \neq 0$; therefore $f_0 \neq 0$ and consequently $(\mathsf{U}f_0, f_0) > 0$ (see **II.5**, THEOREM 19). We introduce Hermitian operators V, W by describing their defining action:

$$\mathsf{V}f = \frac{(f, \mathsf{U}f_0)}{(\mathsf{U}f_0, f_0)} \cdot \mathsf{U}f_0, \qquad \mathsf{W}f = \mathsf{U}f - \mathsf{V}f$$

Then

$$(\mathsf{V}f, f) = \frac{|(f, \mathsf{U}f_0)|^2}{(\mathsf{U}f_0, f_0)} \geqslant 0$$

$$(\mathsf{W}f, f) = \frac{(\mathsf{U}f, f)(\mathsf{U}f_0, f_0) - |(f,\ Uf_0)|^2}{(\mathsf{U}f_0, f_0)} \geqslant 0$$

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[170] This is clear for $\phi' = \phi''$ so let us suppose that $\phi' \neq \phi''$. "Orthogonalization" of ϕ', ϕ'' leads to a $\phi_\perp$ which is orthogonal to ϕ' and such that ϕ'' can be developed as a linear combination of $\phi', \phi_\perp$:

$$\phi'' = a\,\phi' + b\phi_\perp, \qquad \|\phi''\|^2 = |a|^2 + |b|^2 = 1$$

Let $|a| = \cos\theta$, $|b| = \sin\theta$. Then $a = e^{i\alpha}\cos\theta$, $b = e^{i\beta}\sin\theta$ and if we now define

$$a^{(x)} = e^{ix\alpha}\cos(x\theta), \qquad b^{(x)} = e^{ix\beta}\sin(x\theta), \qquad \phi^{(x)} = a^{(x)}\phi' + b^{(x)}\phi_\perp$$

we have $|a^{(x)}|^2 + |b^{(x)}|^2 = 1$, $\|\phi^{(x)}\| = 1$ and observe that $\phi^{(x)}$ varies continuously from ϕ' (at $x = 0$) to ϕ'' (at $x = 1$).

[171] Actually, because of **2**, we should require that $\mathsf{V} \neq \mathsf{O}$, $\mathsf{W} \neq \mathsf{O}$. The cases $\mathsf{V} = \mathsf{O}$ or $\mathsf{W} = \mathsf{O}$ are, however, included with $c' = 0, c'' = 1$ or $c' = 1, c'' = 0$ respectively.

(see again **II.5**, THEOREM 19); *i.e.*, V, W are definite, and furthermore $\mathsf{U} = \mathsf{V}+\mathsf{W}$. Therefore $\mathsf{V} = c'\mathsf{U}$ and, because $\mathsf{V}f_0 = \mathsf{U}f_0 \neq 0$, $c' = 1$; *i.e.*, $\mathsf{U} = \mathsf{V}$. If we now set

$$\phi = \frac{1}{\|\mathsf{U}f_0\|} \cdot \mathsf{U}f_0$$

(which entails $\|\phi\| = 1$) and

$$c = \frac{\|\mathsf{U}f_0\|^2}{(\mathsf{U}f_0, f_0)}$$

(which entails $c > 0$) we obtain $\mathsf{U}f = \mathsf{V}f = c(f,\phi)\phi = c\mathsf{P}_{[\phi]}f$, which (by **1**) gives $\mathsf{U} = c\mathsf{P}_{[\phi]}$: U is essentially $\mathsf{P}_{[\phi]}$.

Conversely, let it be assumed that $\mathsf{U} = c\mathsf{P}_{[\phi]}$ with $\|\phi\| = 1$. If $\mathsf{U} = \mathsf{V} + \mathsf{W}$ and V, W are definite then it follows from $\mathsf{U}f = 0$ that

$$0 \leqslant (\mathsf{V}f, f) \leqslant (\mathsf{V}f, f) + (\mathsf{W}f, f) = (\mathsf{U}f, f) = 0$$

whence $(\mathsf{V}f, f) = 0$ and therefore that $\mathsf{V}f = 0$ (see above). But $\mathsf{U}f = c\mathsf{P}_{[\phi]}f = 0$ follows from and implies $(f,\phi) = 0$ which—as we have just seen—implies also $\mathsf{V}f = 0$. Therefore for each g, $(f, \mathsf{V}g) = (\mathsf{V}f, g) = 0$. That is: everything which is orthogonal to ϕ is orthogonal also to $\mathsf{V}g$, and consequently $\mathsf{V}g = c_g \cdot \phi$ (where c_g is a number dependent upon g). But of this general fact we will use only the case $g = \phi$; *i.e.*, $\mathsf{V}\phi = c'\phi$. Each f has the form $(f,\phi)\cdot\phi + f_\perp$, where $f_\perp$ is orthogonal to ϕ. Therefore

$$\mathsf{V}f = (f,\phi)\cdot\mathsf{V}\phi + \mathsf{V}f_\perp = (f,\phi)\cdot c'\phi = c'\mathsf{P}_{[\phi]}f = c'\mathsf{U}f$$

Consequently $\mathsf{V} = c'\mathsf{U}$, $\mathsf{W} = \mathsf{U} - \mathsf{V} = (1-c')\mathsf{U}$, and the proof is complete.

So homogeneous ensembles correspond to cases of the type $\mathsf{U} = \mathsf{P}_{[\phi]}$ with $\|\phi\| = 1$, and for such ensembles **Tr** gives back the formula $\mathbf{E}_2$ of **III.1**:

$\mathbf{E}_2$ $$\mathrm{Exp}(\mathcal{R}) = \mathrm{Tr}(\mathsf{P}_{[\phi]}\mathsf{R}) = (\mathsf{R}\phi, \phi)$$

It should be observed that $\mathrm{Exp}(1) = \mathrm{Tr}(\mathsf{P}_{[\phi]}) = 1$ (because $\mathsf{P}_{[\phi]}$ belongs to the one-dimensional space $[\phi]$, or by $\mathbf{E}_2$); *i.e.*, the present form of U is correctly normalized. Finally, we inquire into when $\mathsf{P}_{[\phi]}$ and $\mathsf{P}_{[\psi]}$ have the same statistics; *i.e.*, when $\mathsf{P}_{[\phi]} = c\mathsf{P}_{[\psi]}$ (c a positive constant: see **1**). From $\mathrm{Tr}(\mathsf{P}_{[\phi]}) = \mathrm{Tr}(\mathsf{P}_{[\psi]}) = 1$ we have $c = 1$ whence $\mathsf{P}_{[\phi]} = \mathsf{P}_{[\psi]}$. So the spaces $[\phi]$ and $[\psi]$ are identical, and therefore $\phi = a\psi$. It follows from $\|\phi\| = \|\psi\| = 1$ that the constant a has $|a| = 1$. This is also clearly sufficient.

Assembling these results, we can say: There are no ensembles which are free from dispersion. There are homogeneous ensembles, and these correspond to $\mathsf{U} = \mathsf{P}_{[\phi]}$, $\|\phi\| = 1$ and only to these. For these U, **Tr** goes over into $\mathbf{E}_2$, the normalization is correct and U does not change if ϕ is replaced by $a\phi$ (a constant with $|a| = 1$), but every other change of ϕ changes U in an essential way (see **1**). The homogeneous ensembles therefore correspond to the states of quantum mechanics as these were characterized earlier: the ϕ of Hilbert space,

with $\|\phi\| = 1$, in which a constant factor of absolute value 1 is unimportant (see, for example, **II.2**), and the statistical assertions are made by E_2.[172]

We have arrived at all these results from the purely qualitative conditions A', B', $\boldsymbol{\alpha}'$, $\boldsymbol{\beta}'$, **I** and **II**.

Hence, within the limits defined by our conditions, the decision is made, and it is against causality, because all ensembles—even homogeneous ensembles—have dispersion.

Still be discussed is the question of "hidden parameters," brought up in **III.2**; *i.e.*, the question as to whether the dispersions of the homogeneous ensembles characterized by the wave functions ϕ (*i.e.*, by E_2) may be due to the circumstance that these are not the real states, but only mixtures of several states, and that to describe the actual state additional data—besides the data supplied by the wave function ϕ—is necessary (these would be the "hidden parameters"), and that all that data together would determine everything causally; *i.e.*, would lead to dispersion-free ensembles. The statistics of the homogeneous ensemble ($\mathsf{U} = \mathsf{P}_{[\phi]}$, $\|\phi\| = 1$) would then have resulted from averaging over all the actual states of which it is composed; *i.e.*, by averaging over the values of the "hidden parameters" which are involved in those states. But this is impossible for two reasons: First, because then the homogeneous ensemble in question could be represented as a mixture of two different ensembles,[173] contrary to its definition. Second, because the dispersion-free ensembles, which would have to correspond to the "actual" states (*i.e.*, which consist only of systems in their own "actual" states) do not exist. It should be noted that we need not go any further into the mechanism of the "hidden parameters," since we now know that the established results of quantum mechanics can never be re-derived with their help. In fact, we have even established that it is impossible for the same physical quantities to exist with the same functional connections (*i.e.*, for **I** and **II** to hold) if other variables (*i.e.*, "hidden parameters") exist in addition to the wave functions.

Nor would it help if there existed other, as yet undiscovered, physical

[172] The deductions given in the last two sections, which lead to the concept of the homogeneous ensemble, were given by the author, Gött. Nachr. 1927. The existence of homogeneous ensembles and their relation to general ensembles was discovered independently by H. Weyl, Z. Phys. **47** (1927) and the author (reference cited above). A special case of the more general ensembles (namely, for two coupled systems: see the discussion in **VI.2**) was produced by L. Landau, Z. Physik **45**, (1927).

[173] If the "hidden parameters"—the totality of which we shall denote by π—take on only discrete values $\pi_1, \pi_2, \ldots, \pi_n$ ($n > 1$) we obtain two ensembles, whose superposition is the original one, by assuming the systems with $\pi = \pi_1$ are in one, and the systems with $\pi \neq \pi_1$ in the other. If π varies continuously over a region Π, then let Π' be a sub-region of Π; the first sub-ensemble would then contain systems with π from Π', and the other those systems whose π does not belong to Π'.

quantities in addition to those represented by the operators in quantum mechanics because the relations assumed by quantum mechanics (*i.e.*, **I** and **II**) would have to fail already for the by-now-known quantities—those that we discussed above. It is therefore not, as is often assumed, a question of the reinterpretation of quantum mechanics—the present system of quantum mechanics would have to be objectively false for a description other than the statistical description of elementary processes to be possible.

The following circumstance is also worthy of mention. The indeterminacy relations have at first glance a certain similarity to the basic postulate of relativity theory. There it is maintained that it is impossible in principle to determine the simultaneity of two events occurring at points a distance r apart more precisely than within a time interval of magnitude r/c (c is the velocity of light), while the indeterminacy relations assert that it is impossible in principle to give the position of a material point in phase space more precisely than with a region of volume $(\frac{1}{2}\hbar)^3$.[174] Nevertheless there exists a fundamental difference. Relativity theory denies the possibility of an objective, precise measurement of distant simultaneity. But in spite of this, with the introduction into the world of a Galilean reference frame it does become possible to construct a simultaneity definition that is in reasonable accord with our normal concepts on this subject. An objective meaning will not be attributed to such a definition of distant simultaneity only because such coordinate systems can be chosen in an infinite number of different ways, so that infinitely many distant simultaneity definitions can be obtained, all of which are equally good. So the impossibility of measurement hinges in this instance on the existence of an infinite multiplicity of possible theoretical definitions. It is otherwise in quantum mechanics, where it is in general not possible to describe the wave function ϕ by points in phase space, not even if we introduce new (hypothetical, unobserved) coordinates—the "hidden parameters"—since this would lead to dispersion-free ensembles. That is: not only is the measurement impossible, so also is any reasonable theoretical definition; *i.e.*, any definition which, although not susceptible to experimental proof, lies beyond the reach also of experimental refutation. The principle of impossibility of measurement thus arises in one case from the fact that there are an infinite number of ways in which the relevant concepts can be defined without conflicting with experience (or with the general, basic assumptions of the theory)—while in the other case no way exists at all.

To summarize, the position of causality in modern physics can therefore be characterized as follows: In the macroscopic case there is no experimental

[174] The phase space is 6-dimensional: its six coordinates are the three cartesian coordinates q_1, q_2, q_3 of the mass particle and the three corresponding momenta p_1, p_2, p_3. By **III.4** we have for the relative dispersions $\epsilon_1, \epsilon_2, \epsilon_3, \eta_1, \eta_2, \eta_3$

$$\epsilon_1\eta_1 \geqslant \tfrac{1}{2}\hbar, \qquad \epsilon_2\eta_2 \geqslant \tfrac{1}{2}\hbar, \qquad \epsilon_3\eta_3 \geqslant \tfrac{1}{2}\hbar$$

i.e., $\epsilon_1\epsilon_2\epsilon_3\eta_1\eta_2\eta_3 \geqslant (\frac{1}{2}\hbar)^3$, which sets a universal limit on the precision with which position in the phase space of classical mechanics can be known.

evidence which supports it, and none can be devised because the apparent causal order of the world at large (*i.e.*, for objects visible to the naked eye) has certainly no other cause than the "law of large numbers" and is completely independent of whether the natural laws governing elementary processes are causal or not.[175] That macroscopically identical objects exhibit identical behavior has little to do with causality: they are in fact not equal at all, since the coordinates that determine the states of their atoms almost never coincide exactly, and the macroscopic method of observation averages over these coordinates (here they are the "hidden parameters"). The number of these coordinates is, however, very large (for one gram of matter, about 10^{25}), and therefore the above-mentioned averaging process entails an extensive diminution of all dispersions, according to the well-known laws of the calculus of probability. (Naturally, this is true only in typical cases; in suitable special cases—such as Brownian motion, systems in unstable states, among others—this apparent macroscopic causality fails.) The question of causality could be put to a true test only in the atom, in the elementary processes themselves, and here everything in the present state of our knowledge militates against it. The only formal theory existing at the present time which orders and summarizes our experiences in this area in a half-way satisfactory manner—*i.e.*, quantum mechanics—is in compelling logical contradiction with causality. Of course, it would be an exaggeration to maintain that causality has thereby been done away with: quantum mechanics has, in its present form, several serious lacunae, and it may even be that it is false, although this latter possibility is highly unlikely in view of the theory's startling capacity in the qualitative explanation of general problems, and the quantitative success of calculations relating to special problems. In spite of the fact that quantum mechanics agrees well with experiment, and that it has opened up for us a qualitatively new side of the world, one can never say of the theory that it has been proved by experience, but only that it the best known summarization of experience. However, mindful of such precautions, we may still say that there is at present no occasion and no reason to speak of causality in nature. Because no experiment indicates its presence: the macroscopic are unsuitable in principle, while the only known theory which is compatible with our experiences relative to elementary processes—quantum mechanics—contradicts it.

To be sure, we are dealing with an age-old way of thinking that has been embraced by all mankind. But that way of thinking does not arise from logical necessity (else it would not have been possible to build a statistical theory), and anyone who enters the subject without preconceived notions has no reason to adhere to that way of thinking. Under such circumstances, is it reasonable to sacrifice a reasonable physical theory for the sake of an unsupported idea?

[175] See the extremely lucid discussions of Schrödinger on this subject: Naturwiss. **17** (1929), page 37.

3. CONCLUSIONS FROM EXPERIMENTS

The last section taught us that the most general statistical ensemble which is compatible with our qualitative basic assumptions is characterized, according to **Tr**, by a definite operator U. Those particular ensembles which we have called "homogeneous" were characterized by $\mathsf{U} = \mathsf{P}_{[\phi]}$ ($\|\phi\| = 1$), and since these are the actual states of the systems **S** (*i.e.*, not capable of further resolution) we also call them *states* (specifically, $\mathsf{U} = \mathsf{P}_{[\phi]}$ is the state ϕ).

If U has a pure discrete spectrum, perhaps with eigenvalues $w_1, w_2, \ldots$ and eigenfunctions $\phi_1, \phi_2, \ldots$ (which form a complete orthonormal set) then (see **II.8**)

$$\mathsf{U} = \sum_n w_n \mathsf{P}_{[\phi_n]}$$

Because of the definiteness of U, all $w_n \geqslant 0$ (indeed $\mathsf{U}\phi_n = w\phi_n$, therefore $(\mathsf{U}\phi_n, \phi_n) = w_n$ and therefore $(\mathsf{U}\phi_n, \phi_n) \geqslant 0$) and $\sum_n w_n = \sum_n (\mathsf{U}\phi_n, \phi_n) = \mathrm{Tr}\mathsf{U}$ (see also the beginning of **IV.1**); that is, $\sum_n w_n = 1$ if U is correctly normalized. By the remarks at the beginning of **IV.1**, U can be interpreted as a superposition of the states $\phi_1, \phi_2, \ldots$ with the respective relative weights $w_1, w_2, \ldots$ and if U is correctly normalized then these are also the absolute weights.

But a correctly normalized U (*i.e.*, one with $\mathrm{Tr}\mathsf{U} = 1$) is totally continuous (by **II.11**; see in particular Note 115), and therefore has a pure discrete spectrum. The same is true if $\mathrm{Tr}\mathsf{U}$ is finite. (An infinite $\mathrm{Tr}\mathsf{U}$ can be regarded as a limiting case which we shall not go into here.) In the really interesting case, therefore, the observed ensemble can be represented as a superposition of states, which we have actually chosen to be pair-wise orthogonal. We are led thus to call general ensembles *mixtures* (in contrast to the homogeneous ensembles, which are states).

If all the eigenvalues of U are simple (*i.e.*, if all the $w_1, w_2, \ldots$ are different from each other) then, as we know, the $\phi_1, \phi_2, \ldots$ are uniquely determined except for constant factors of absolute value 1. The corresponding states (and the $\mathsf{P}_{[\phi_1]}, \mathsf{P}_{[\phi_2]}, \ldots$) are then uniquely determined. Likewise, the weights $w_1, w_2, \ldots$ are uniquely determined, except for a permutation of the sequence. In this case, therefore, we can state uniquely from which (pair-wise orthogonal) states the mixture U is formed. If U has multiple eigenvalues ("degeneracies"), however, the situation is quite different. Exactly how the $\phi_1, \phi_2, \ldots$ can be chosen was discussed in **II.8**. This can be done in infinitely many ways, all essentially different (while the $w_1, w_2, \ldots$ are still uniquely determined). We must write down those among the $w_1, w_2, \ldots$ which are different from one another and then form the closed linear manifolds $\mathfrak{M}_{w'}, \mathfrak{M}_{w''}, \ldots$ associated with each of the distinct weights $w', w'', \ldots$ (thus $\mathfrak{M}_{w'}$ contains all solutions of $\mathsf{U}f = w'f$). After this we proceed in the following manner: From each $\mathfrak{M}_{w'}, \mathfrak{M}_{w''}, \ldots$ choose an arbitrary orthonormal set spanning that manifold: $\chi_1', \chi_2', \ldots$; $\chi_1'', \chi_2'', \ldots$; ... respectively. The $\chi_1', \chi_2', \ldots$; $\chi_1'', \chi_2'', \ldots$; ... are

the $\phi_1, \phi_2, \ldots$ and the corresponding eigenvalues $w', w', \ldots ; w'', w'', \ldots ; \ldots$ are the $w_1, w_2, \ldots$. When $\mathfrak{M}_w$ has more than one dimension (*i.e.*, when w is degenerate) the corresponding $\chi_1, \chi_2, \ldots$ are no longer determined to within a constant factor of unit absolute value (χ_1, for example, can be any normalized element of $\mathfrak{M}_w$); *i.e.*, the states themselves are also multivalued.

This phenomenon can also be formulated as follows: If the states $\chi_1, \chi_2, \ldots$ are pair-wise orthogonal (*i.e.*, the $\chi_1, \chi_2, \ldots$ form an orthogonal set, which may be finite or infinite), and if we mix them in such a way that all get the same weight (*i.e.*, the relative weights are $1 : 1 : \cdots$), then the resulting mixture depends only upon the closed manifold $\mathfrak{M}$ which is spanned by the $\chi_1, \chi_2, \ldots$. In fact,

$$\mathsf{U} = \mathsf{P}_{[\chi_1]} + \mathsf{P}_{[\chi_2]} + \cdots = \mathsf{P}_{\mathfrak{M}}$$

If the number of the $\chi_1, \chi_2, \ldots$ is finite (say $s : \chi_1, \ldots, \chi_s$) then this U can be considered to be a mixture of all the normalized elements of $\mathfrak{M}$; *i.e.*, of all the states in $\mathfrak{M}$. These are the states

$$\chi = x_1\chi_1 + x_2\chi_2 + \cdots + x_s\chi_s \quad : \quad |x_1|^2 + |x_2|^2 + \cdots + |x_s|^2 = 1$$

Actually, if we write $x_1 = u_1 + iv_1, \ \ldots \ , x_s = u_s + iv_s$ then

$$|x_1|^2 + \cdots + |x_s|^2 = u_1^2 + v_1^2 + \cdots + u_s^2 + v_s^2 = 1$$

describes the $(2s-1)$-dimensional surface K of a unit sphere in $2s$-space, and for

$$\mathsf{U}' = \iint\cdots\iint_K \mathsf{P}_{[\chi]}\, d\Omega \quad : \quad d\Omega \text{ denotes the differential surface element}$$

we have

$$\begin{aligned}
(\mathsf{U}'f, g) &= \iint\cdots\iint_K (\mathsf{P}_{[\chi]}f, g)\, d\Omega \\
&= \iint\cdots\iint_K (f, \chi)\overline{(g, \chi)}\, d\Omega \\
&= \iint\cdots\iint_K \big(f, \textstyle\sum_{\mu=1}^{s}(u_\mu + iv_\mu)\chi_\mu\big)\overline{\big(g, \sum_{\nu=1}^{s}(u_\nu + iv_\nu)\chi_\nu\big)}\, d\Omega \\
&= \iint\cdots\iint_K \sum_{\mu,\nu=1}^{s} (f, \chi_\mu)\overline{(g, \chi_\nu)}(u_\mu - iv_\mu)(u_\nu + iv_\nu)\, d\Omega \\
&= \sum_{\mu,\nu=1}^{s} (f, \chi_\mu)\overline{(g, \chi_\nu)} \cdot \iint\cdots\iint_K \big[(u_\mu u_\nu + v_\mu v_\nu) + i(u_\mu v_\nu - u_\nu v_\mu)\big]\, d\Omega
\end{aligned}$$

All the $u_\mu v_\nu$ and $u_\nu v_\mu$-integrals, as well as all $u_\mu u_\nu$ and $v_\mu v_\nu$-integrals with

$\mu \neq \nu$, vanish by symmetry,[176] while in the cases $\mu = \nu$ all of the latter integrals have value $C/2s$ $(C > 0)$.[176] Therefore

$$(\mathsf{U}'f, g) = \frac{C}{s}\sum_{\mu=1}^{s}(f, \chi_\mu)\overline{(g, \chi_\mu)}$$
$$= \frac{C}{s}\sum_{\mu=1}^{s}(\mathsf{P}_{[\chi_\mu]}f, g) = \left(\left\{\frac{C}{s}\sum_{\mu=1}^{s}\mathsf{P}_{[\chi_\mu]}\right\}f, g\right)$$

Consequently

$$\mathsf{U}' = \frac{C}{s}\sum_{\mu=1}^{s}\mathsf{P}_{[\chi_\mu]} = \frac{C}{s}\cdot\mathsf{U}$$

i.e., U' and U are not essentially different.

These results are of such great significance to the nature of quantum statistics that we shall repeat them:

> **1**. If a mixture is made up of mutually orthogonal states with exactly equal weights, then it can no longer be determined what these states were. Or—equivalently—we can produce the same mixture from different (mutually orthogonal) components by again mixing in exactly equal proportions.
>
> **2**. The mixture so obtained is—if the number of states is finite—identical to the mixture of all states which are linear combinations of these components.

The simplest example of this type is the following: If we mix ϕ, ψ (orthogonal) in the proportion $1:1$ then we obtain the same result as if we were to mix (for example)

$$\frac{\phi+\psi}{\sqrt{2}}, \quad \frac{\phi-\psi}{\sqrt{2}}$$

in the proportion $1:1$ or even all $x\phi + y\psi$ $(|x|^2 + |y|^2 = 1)$. If we mix two non-orthogonal ϕ, ψ (in a proportion possibly different from $1:1$) then we are still less able to determine the composition of the final mixture, since this

[176] $u_\mu \to -u_\mu$ (similarly $u_\nu \to -u_\nu$ and $v_\mu \to -v_\mu$) is a symmetry operation of K in which the former integrands change their signs, and their integrals are therefore equal to zero. On the other hand, $u_\mu \leftrightarrow v_\mu$ and $u_\mu \leftrightarrow u_\nu$ are symmetry operations of K in which the latter integrals are interchanged; their integrals are therefore equal and hence equal to $\frac{1}{2s}$ times their sum:

$$\iint\cdots\iint_K \left(u_1^2 + v_1^2 + \cdots + u_s^2 + v_s^2\right)d\Omega = \iint\cdots\iint_K d\Omega$$
$$= \text{surface area of K}$$

which we will agree to call C.

mixture certainly could have been obtained also by mixing orthogonal states.

We postpone further investigation into the nature of mixtures until the thermodynamic discussions in **V.2** and thereafter.

The formula **Tr** in **IV.2** states how the expectation value of the quantity $\mathcal{R}$ with the operator R is to be calculated in a mixture with the statistical operator U: it is $\mathrm{Tr}(\mathsf{UR})$. The probability therefore that the value a of R lies in the interval $a' < a \leqslant a''$ (a', a'' given, $a' < a''$) is to be found as in **III.1** or **III.5**: If the quantity $F(\mathcal{R})$ is formed with the function

$$F(x) = \begin{cases} 1 & \text{for} \quad a' < x \leqslant a'' \\ 0 & \text{otherwise} \end{cases}$$

then its expectation value is the probability mentioned. Now $F(\mathcal{R})$ has (by **I** in **IV.2**) the operator $F(\mathsf{R})$, and if $\mathsf{E}(\lambda)$ is the resolution of the identity belonging to R, then—as we have calculated more than once—$F(\mathsf{R}) = \mathsf{E}(a'') - \mathsf{E}(a')$ and the desired probability is $w(a', a'') = \mathrm{Tr}\mathsf{U}[\mathsf{E}(a'') - \mathsf{E}(a')]$. Consequently the probability function which describes the statistics of $\mathcal{R}$ is $w(a) = \mathrm{Tr}\mathsf{UE}(a)$ (see **IV.1**, Note 175; for states, *i.e.*, for $\mathsf{U} = \mathsf{P}_{[\phi]}$, we again have $w(a) = \mathrm{Tr}\mathsf{P}_{[\phi]}\mathsf{E}(a) = (\mathsf{E}(a)\phi, \phi)$). Naturally these probabilities are only relative if U is not correctly normalized.

The question as to when the quantity $\mathcal{R}$ with operator R, in a mixture with the statistical operator U, takes on the value λ^* with certainty can be answered directly with the aid of $w(a)$: for $a < \lambda^*$ we must require $w(a) = 0$, and for $a \geqslant \lambda^*$ we must require $w(a) = 1$ or—if U is not correctly normalized—$w(a) = \mathrm{Exp}(1) = \mathrm{Tr}\mathsf{U}$. That is, $\mathrm{Tr}\mathsf{UE}(a) = 0$ for $a < \lambda^*$, $\mathrm{Tr}\mathsf{U}[\mathsf{I} - \mathsf{E}(a)] = 0$ for $a \geqslant \lambda^*$.[177] Now for definite operators A, B the equation $\mathrm{Tr}\mathsf{AB} = 0$ has $\mathsf{AB} = \mathsf{O}$ as a consequence (see **II.11**), and therefore

$$\mathsf{UE}(a) = \begin{cases} \mathsf{O} & \text{for} \quad a < \lambda^* \\ \mathsf{U} & \text{for} \quad a \geqslant \lambda^* \end{cases}$$

or, what is equivalent, $\mathsf{E}(a)\mathsf{U} = \mathsf{O}$ or U respectively, since the factors must commute because of the Hermitian nature of the product. That is, for $f = \mathsf{U}g$

$$\mathsf{E}(a)f = \begin{cases} 0 & \text{for} \quad a < \lambda^* \\ f & \text{for} \quad a \geqslant \lambda^* \end{cases}$$

and by the discussion presented in **II.8** this means that $\mathsf{R}f = \lambda^* f$; *i.e.*, $\mathsf{RU}g = \lambda^*\mathsf{U}$ identically in g. Consequently, the ultimate condition is $\mathsf{RU} = \lambda^*\mathsf{U}$. Or, if we

[177] If $\mathrm{Tr}\mathsf{U}$ is infinite the latter formulas, obtained by subtractions, may appear doubtful. They can, however, be established as follows: That $\mathcal{R}$ has the value λ^* means that $w(a', a'') = 0$; *i.e.*, $\mathrm{Tr}\mathsf{U}[\mathsf{E}(a'') - \mathsf{E}(a')] = 0$ for $a'' < \lambda^*$ or $a' \geqslant \lambda^*$. Since this trace is always $\geqslant 0$, and since it is monotone increasing with a'' as well as monotone decreasing with a' it suffices to consider the $\lim_{-\infty \leftarrow a''}$ for $a'' < \lambda^*$ and the $\lim_{a' \to +\infty}$ for $a' \geqslant \lambda^*$. That is, $\mathrm{Tr}\mathsf{U}[\mathsf{I} - \mathsf{E}(a')] = 0$ for $a' \geqslant \lambda^*$ and $\mathrm{Tr}\mathsf{UE}(a'') = 0$ for $a'' < \lambda^*$.

denote by $\mathcal{M}$ the closed linear manifold formed by all solutions h of $\mathsf{R}h = \lambda^* h$: $\mathsf{U}f$ always lies in $\mathcal{M}$.

This same result could also have been obtained from the vanishing of the dispersion; *i.e.*, the (possibly relative) expectation value of $(\mathcal{R} - \lambda^*)^2$.

In **III.3** we answered the following questions (let $\mathcal{R}, \mathcal{S}, \ldots$ be physical quantities, $\mathsf{R}, \mathsf{S}, \ldots$ their respective operators):

> **1**. When is $\mathcal{R}$ measurable with absolute precision? ANSWER: Whenever R has only a discrete spectrum.
>
> **2**. When are $\mathcal{R}$, $\mathcal{S}$ measurable simultaneously with absolute precision? ANSWER: Whenever R, S have only a discrete spectra and commute.
>
> **3**. When are several quantities $\mathcal{R}, \mathcal{S}, \ldots$ measurable simultaneously with absolute precision? ANSWER: Whenever $\mathsf{R}, \mathsf{S}, \ldots$ have only a discrete spectra and all commute.
>
> **4**. When are several quantities $\mathcal{R}, \mathcal{S}, \ldots$ measurable simultaneously with arbitrary precision? ANSWER: Whenever $\mathsf{R}, \mathsf{S}, \ldots$ all commute.

In the latter case we used the following principle, abstracted from the result of the Compton-Simons experiment:

> **M**. If the physical quantity $\mathcal{R}$ is measured twice in prompt succession in a system **S** then we get the same value each time. This is the case even though $\mathcal{R}$ may have non-zero dispersion in the original state of **S**, and even though the $\mathcal{R}$-measurement can change the state of **S**.

We have discussed the physical meaning of **M** in detail in **III.3**. Further assumptions drawn upon in constructing answers to **1**–**4** were: the statistical formula $\mathbf{E}_2$ of **III.3** for states; the assumption **F** of **III.3**, according to which $F(\mathcal{R})$ has the operator $F(\mathsf{R})$ if $\mathcal{R}$ has the operator R; the assumption according to which $\mathcal{R}+\mathcal{S}$ has the operator $\mathsf{R}+\mathsf{S}$ if the (simultaneously measurable) quantities $\mathcal{R}$, $\mathcal{S}$ have the respective operators R, S.

Since these three assumptions are again at our disposal (the first follows from the formula **Tr** in **IV.2**, the other two correspond to **I**, **II** in **IV.2**) and **M** must also be assumed to correct—because we have perceived that it is indispensable to the conceptual structure of quantum mechanics—the proofs given in **III.3** for **1**–**4** also hold here. The answers given are therefore again correct.

In **III.5** we investigated physical quantities which take only two values: 0, 1. Those quantities stood in unique correspondence with the "properties" $\mathfrak{E}$. Indeed, if $\mathfrak{E}$ is given then the quantity could be defined like this: it is measured by distinguishing whether the property $\mathfrak{E}$ is present or not, and its value is 1 or 0 respectively. Conversely, if the quantity was given, then $\mathfrak{E}$ was this property: the quantity in question has the value 1 (*i.e.*, not 0). From **F** in **III.5** (*i.e.*, from **I** in **IV.2**) it followed that the corresponding operators E are actually and invariably projections. The probability therefore that $\mathfrak{E}$ be present was equal to

the expectation value of the quantity defined above. In **III.5** it was calculated only for states (*i.e.*, for cases of the type $\mathsf{U} = \mathsf{P}_{[\phi]}$, $\|\phi\| = 1$), but we can determine it in general from **Tr**: it is $\operatorname{Tr} \mathsf{UE}$. (Relative! The absolute value is obtained only if U is correctly normalized; *i.e.*, if $\operatorname{Tr} \mathsf{U} = 1$.)

Since we have made certain of **1**–**4**, the statements derived from them—namely $\boldsymbol{\alpha}$–$\boldsymbol{\zeta}$ in **III.5**—are likewise valid. Of course, it should be observed that in the former case $\boldsymbol{\alpha}$ gave information only for states, but here we state the extension that pertains to all mixtures:

> $\boldsymbol{\alpha}'$) The property $\mathfrak{E}$ is present or not present in the mixture with the statistical operator U with the respective probabilities
>
> $$\operatorname{Tr}(\mathsf{UE}) \quad \text{and} \quad \operatorname{Tr}(\mathsf{U}(\mathsf{I} - \mathsf{E}]))$$
>
> (Relative probabilities! These are absolute only if U is correctly normalized: $\operatorname{Tr} \mathsf{U} = 1$.)

If several quantities $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$ are investigated, and if they correspond respectively to operators $\mathsf{R}_1, \ldots, \mathsf{R}_\ell$ that have the respective resolutions of the identity $\mathsf{E}_1(\lambda), \ldots, \mathsf{E}_\ell(\lambda)$; if, moreover, ℓ intervals

$$\begin{aligned} I_1 \quad &: \quad \lambda_1' < \lambda \leqslant \lambda_1'' \\ &\vdots \\ I_\ell \quad &: \quad \lambda_\ell' < \lambda \leqslant \lambda_\ell'' \end{aligned}$$

are given and if

$$\begin{aligned} \mathsf{E}_1(I_1) &= \mathsf{E}_1(\lambda_1'') - \mathsf{E}_1(\lambda_1') \\ &\vdots \\ \mathsf{E}_\ell(I_\ell) &= \mathsf{E}_\ell(\lambda_\ell'') - \mathsf{E}_\ell(\lambda_\ell') \end{aligned}$$

then the projections $\mathsf{E}_1(I_1), \mathsf{E}_2(I_2), \ldots, \mathsf{E}_\ell(I_\ell)$ belong (see $\boldsymbol{\zeta}$) to the respective properties

$$\begin{gathered} \text{“}\mathcal{R}_1 \text{ lies in } I_1\text{”} \\ \text{“}\mathcal{R}_2 \text{ lies in } I_2\text{”} \\ \vdots \\ \text{“}\mathcal{R}_\ell \text{ lies in } I_\ell\text{”} \end{gathered}$$

The commutativity of the $\mathsf{E}_1(I_1), \mathsf{E}_2(I_2), \ldots, \mathsf{E}_\ell(I_\ell)$ is then characteristic (see $\boldsymbol{\gamma}$) for these to be simultaneously decidable, and (see $\boldsymbol{\epsilon}$) the projection for their simultaneous validity is $\mathsf{E} = \mathsf{E}_1(I_1)\mathsf{E}_2(I_2) \cdots \mathsf{E}_\ell(I_\ell)$. The probability of that composite event is given therefore by $\operatorname{Tr}(\mathsf{UE})$ (see $\boldsymbol{\alpha}'$).

Let us now follow the converse path: Let us assume that we do not know the state of the system **S**, but that we have made certain measurements on **S** and know the results. In reality, it always happens this way, because we can learn something about the state of **S** only from the results of measurements. The states are only a theoretical construction: only the results of measurements

are actually available, and the problem of physics is to discover relations between the results of past and future measurements. To be sure, this is always accomplished through the introduction of the auxiliary concept of "state," but the physical theory must tell us on the one hand how from past measurements to make inferences about the present state and, on the other hand, how to go from the present state to the predicted results of future measurements. Up to now, we have dealt only with the latter question, and we must now apply ourselves to the former.

If anterior measurements do not suffice to determine the present state uniquely we may still be able to infer from those measurements—under certain circumstances—with what probabilities particular states are present. (This holds in causal theories—for example, in classical mechanics—as well as in quantum mechanics.) The proper problem is then this: Given certain results of measurements, find a mixture whose statistics are the same as those which we would expect for a system **S** of which we know only that these measurements were carried out on it and that they had the results mentioned. Of course, we must actually be more precise: we must indicate what it means to say that "we know only this, and no more" about **S**, and how this can lead to a set of statistics.

In any case, the connection with statistics must be the following: If for many systems $\mathbf{S}_1', \ldots, \mathbf{S}_M'$ (replicas of **S**) these measurements give the results mentioned, then this ensemble $[\mathbf{S}_1', \ldots, \mathbf{S}_M']$ coincides in all its statistical properties with the results of the measurements. That the results of the measurements are the same for all $\mathbf{S}_1', \ldots, \mathbf{S}_M'$ can be attributed—by **M**—to the circumstance that originally a large ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ was given in which the measurements were carried out, and then those elements for which the desired results occurred were collected into a new ensemble: this is then $[\mathbf{S}_1', \ldots, \mathbf{S}_M']$. Of course, everything depends upon how $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ was chosen. This initial ensemble gives, so to speak, the *a priori* probabilities of the individual states of the system **S**. The whole state of affairs is well known from general probability theory: to be able to proceed from the results of measurements to the states; *i.e.*, from effect to cause—*i.e.*, to be able to calculate *a posteriori* probabilities—we must know the *a priori* probabilities. In general these can be chosen in many different ways, and accordingly our problem cannot be solved uniquely. However, we shall see that under the special conditions presented by quantum mechanics, a certain determination of the initial ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$ (*i.e.*, of the *a priori* probabilities) is particularly satisfactory.

The results are quite different if the results of measurements at our disposal suffice for us to determine the state of **S** completely. Then the answer to every question must be unique. We will soon see how this circumstance makes itself felt.

Finally, let us mention the following: Instead of saying that several results of measurements (on **S**) are known we can say that **S** was examined in relation to a certain property $\mathfrak{E}$ and its presence was ascertained. From $\boldsymbol{\alpha}$–$\boldsymbol{\zeta}$ we know

how these things are related: if, for example, the results of (simultaneous) measurements are available, according to which the values of the quantities $\mathcal{R}_1, \ldots, \mathcal{R}_\ell$ lie in the respective intervals $I_1, \ldots, I_\ell$, then (with the symbols used earlier) the projection operator belonging to the proposition (or property) $\mathfrak{E}$ is $\mathsf{E} = \mathsf{E}_1(I_1)\mathsf{E}_2(I_2)\cdots\mathsf{E}_\ell(I_\ell)$.

The information about $\mathbf{S}$ always amounts, therefore, to the presence of a certain property $\mathfrak{E}$ which is formally characterized by presentation of the associated projection operator E. Let us investigate the statistical operator U of the equivalent ensemble $[\mathbf{S}'_1, \ldots, \mathbf{S}'_M]$, as well as the statistical operator U_0 of the general initial ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$. What are the mathematical relations among E, U and U_0?

Because of $\mathbf{M}$, $\mathfrak{E}$ is certainly present in $[\mathbf{S}'_1, \ldots, \mathbf{S}'_M]$; *i.e.*, the quantity corresponding to $\mathfrak{E}$ has the value 1. This means that $\mathsf{EU} = \mathsf{U}$, as we saw at the beginning of this section; *i.e.*, $\mathsf{U}f$ always lies in $\mathcal{M}$, where $\mathcal{M}$ is the set of all f with $\mathsf{E}f = f$; *i.e.*, the closed linear manifold belonging to E.

Instead of $\mathsf{EU} = \mathsf{U}$ we can also write $\mathsf{UE} = \mathsf{U}$ or $\mathsf{U}(\mathsf{I} - \mathsf{E}) = \mathsf{O}$; *i.e.*, $\mathsf{U}g = 0$ for all $g = (\mathsf{I} - \mathsf{E})f$; *i.e.*, for all g of the closed linear manifold belonging to $\mathsf{I} - \mathsf{E}$; *i.e.*, for all g of $\mathcal{R} - \mathcal{M}$. Therefore $\mathsf{U}f$ is equal to 0 for all f of $\mathcal{R} - \mathcal{M}$. And for the f of $\mathcal{M}$, $\mathsf{U}f$ also lies in $\mathcal{M}$. Nothing further can be said about U in this way.

This (essentially, *i.e.*, except for a constant factor) determines U if and only if $\mathcal{M}$ is 0- or 1-dimensional. In fact, for $\mathcal{M} = [0]$ we have $\mathsf{U} = \mathsf{O}$, which is impossible (by **IV.2**, Remark 1). For $\mathcal{M} = [\phi]$ ($\phi \neq 0$, so we may assume $\|\phi\| = 1$) we have $\mathsf{U}\phi = c\phi$, and therefore for all f of $\mathcal{M}$ (since these are all equal to $a\phi$) $\mathsf{U}f = cf$. Hence, in general, $\mathsf{U}f = \mathsf{UE}f = c\mathsf{E}f$ which give $\mathsf{U} = c\mathsf{E} = c\mathsf{P}_{[\phi]}$. Since $c > 0$ (because U is definite and $\neq \mathsf{O}$) we have essentially $\mathsf{U} = \mathsf{E} = \mathsf{P}_{[\phi]}$. For $\dim(\mathcal{M}) \geqslant 2$ we can choose two orthonormal ϕ, ψ from $\mathcal{M}$. Then $\mathsf{P}_{[\phi]}, \mathsf{P}_{[\psi]}$ are two essentially different U which satisfy our condition. Therefore $\mathsf{E} = \mathsf{O}$ is impossible; for $\mathsf{E} = \mathsf{P}_{[\phi]}$ ($\|\phi\| = 1$) we have $\mathsf{U} = \mathsf{E} = \mathsf{P}_{[\phi]}$; otherwise U is many-valued.

The fact that $\mathsf{E} = \mathsf{O}$ is incompatible with finding any U at all would be disastrous if it were possible for an $\mathbf{S}$ to possess such a property $\mathfrak{E}$. This, however, is excluded by $\boldsymbol{\eta}$: such an $\mathfrak{E}$ can never exist; its probability is always 0. A one-dimensional $\mathcal{M}$—*i.e.*, an $\mathsf{E} = \mathsf{P}_{[\phi]}$ ($\|\phi\| = 1$)—determines U uniquely and fixes the state ϕ. Therefore this is the kind of measurement which—if it turns out in the affirmative—determines the state of $\mathbf{S}$ completely, and in fact determines it to be ϕ.[178] All other measurements are incomplete, and do not determine a unique state.

[178] That is, if $\mathfrak{E}$ is present, the state is ϕ. If it is not present, then "not $\mathfrak{E}$" is present: $\mathsf{I} - \mathsf{E} = \mathsf{I} - \mathsf{P}_{[\phi]}$ and $\mathcal{R} - \mathcal{M} = \mathcal{R} - [\phi]$ appear in place of $\mathsf{E} = \mathsf{P}_{[\phi]}$, $\mathcal{M} = [\phi]$. This does not determine U uniquely. (E corresponds to the question "Is the state ϕ?") A measurement for which each process determines the state uniquely is a measurement of a quantity $\mathcal{R}$ whose operator R has a discrete spectrum with simple eigenvalues (**III.3**). After the measurement, one of the states $\phi_1, \phi_2, \ldots$ (the eigenfunctions of R) is present; *i.e.*, the state of $\mathbf{S}$ is in

In the general case we proceed as follows: Let the quantity corresponding to the proposition $\mathfrak{E}$ also be called $\mathfrak{E}$. Then U obtains like this: $\mathfrak{E}$ is measured on the whole ensemble $([\mathbf{S}_1, \ldots, \mathbf{S}_N])$ of U_0, and all the elements for which the measurement gave 1 are collected, forming the ensemble $([\mathbf{S}'_1, \ldots, \mathbf{S}'_M])$ of U. The measurement of $\mathfrak{E}$ might be effected in many different ways: for example, another quantity $\mathcal{R}$, of which $\mathfrak{E}$ is a known function, $\mathfrak{E} = f(\mathcal{R})$, could be measured. To be more specific, let $\phi_1, \phi_2, \ldots$ be an orthonormal set which spans $\mathcal{M}$, and let $\psi_1, \psi_2, \ldots$ be a corresponding set for $\mathcal{R} - \mathcal{M}$. Then

$$\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots \quad \text{spans} \quad \mathcal{M} + (\mathcal{R} - \mathcal{M}) = \mathcal{R}$$

i.e., it is complete. Let $\lambda_1, \lambda_2, \ldots, \mu_1, \mu_2, \ldots$ be distinct real numbers, and define the operator R by

$$\mathsf{R}\Big(\textstyle\sum_n x_n\phi_n + \sum_m y_m\phi_m\Big) = \displaystyle\sum_n \lambda_n x_n\phi_n + \sum_m \mu_m y_m\psi_m$$

R clearly has the pure discrete spectrum $\lambda_1, \lambda_2, \ldots, \mu_1, \mu_2, \ldots$ with respective eigenfunctions $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$, and all the eigenvalues are simple. Let $F(x)$ be any function with

$$F(\lambda_n) = 1 \text{ (all } \lambda_n) \quad : \quad F(\mu_m) = 0 \text{ (all } \mu_m)$$

Then $F(\mathsf{R})$ has eigenvalue 1 for $\phi_1, \phi_2, \ldots$ and therefore for each f of $\mathcal{M}$, while $F(\mathsf{R})$ has eigenvalue 0 for $\psi_1, \psi_2, \ldots$ and therefore for each f of $\mathcal{R} - \mathcal{M}$. Consequently $\mathsf{E} = F(\mathsf{R})$. If R belongs to $\mathcal{R}$ then $\mathfrak{E} = F(\mathcal{R})$. The $\mathfrak{E}$-measurement can therefore be interpreted as an $\mathcal{R}$-measurement.

In this case we can calculate how U_0, U are related. According to the $\mathcal{R}$-measurement each system is in one of the states $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$, the particular one depending on which of the values $\lambda_1, \lambda_2, \ldots, \mu_1, \mu_2, \ldots$ was found. The respective probabilities are

$$\begin{aligned} &\mathrm{Tr}(\mathsf{U}_0\mathsf{P}_{[\phi_1]}) = (\mathsf{U}_0\phi_1, \phi_1), \quad \mathrm{Tr}(\mathsf{U}_0\mathsf{P}_{[\phi_2]}) = (\mathsf{U}_0\phi_2, \phi_2), \quad \ldots \\ &\mathrm{Tr}(\mathsf{U}_0\mathsf{P}_{[\psi_1]}) = (\mathsf{U}_0\psi_1, \psi_1), \quad \mathrm{Tr}(\mathsf{U}_0\mathsf{P}_{[\psi_2]}) = (\mathsf{U}_0\psi_2, \psi_2), \quad \ldots \end{aligned}$$

(see the observations of **III.3**, the validity of which we have established). That is, these fractions of the U_0-ensemble go over into the ensembles

$$\mathsf{P}_{[\phi_1]}, \mathsf{P}_{[\phi_2]}, \ldots, \mathsf{P}_{[\psi_1]}, \mathsf{P}_{[\psi_2]} \ldots$$

Since $\mathfrak{E} = \mathsf{I}$ corresponds to $\mathcal{R} = \lambda_1, \lambda_2, \ldots$ the U ensemble arises by inclusion of that first group. Consequently

$$\mathsf{U} = \sum_n (\mathsf{U}_0\phi_n, \phi_n)\mathsf{P}_{[\phi_n]}$$

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general changed by the measurement. By analogy, the $\mathfrak{E}$-measurement also changes the state, since afterwards, for a positive result, $\mathsf{U} = \mathsf{P}_{[\phi]}$, while for a negative result $\mathsf{U}(\mathsf{I} - \mathsf{P}_{[\phi]}) = \mathsf{U}$, $\mathsf{U}\mathsf{P}_{[\phi]} = \mathsf{O}$ (*i.e.*, $\mathsf{U}\phi = 0$), while previously neither was necessarily the case. This quantum mechanical "determination" of the state thus alters it, as was to be expected.

Now each $\mathsf{P}_{[\phi_n]}$ commutes with R,[179] and therefore it must also commute with U. That is, if U does not commute with each R arising in the manner described above then certain measurement processes (namely, those depending on the corresponding $\mathcal{R}$) are eliminated from U_0 in the production of U. Then we know more about U than that it was created by an $\mathfrak{E}$-measurement. But since U should represent just this state of our knowledge, we try to adhere to the following condition: If there exists a U for which no measurement process of $\mathfrak{E}$ need be excluded, then we shall make use of such a U. Therefore, let us investigate whether there are such U, and what they are!

As we saw, U must commute with all R produced in the manner described. From this it follows that $\mathsf{RU}\phi_n = \mathsf{UR}\phi = \mathsf{U}(\lambda_n\phi_n) = \lambda_n\mathsf{U}\phi_n$; *i.e.*, $\mathsf{U}\phi_n$ is an eigenfunction of R with eigenvalue λ_n: therefore $\mathsf{U}\phi_n = a_n\phi_n$. In particular, $\mathsf{U}\phi_1 = a_1\phi_1$. If any ϕ of $\mathcal{M}$ is given, then we can so choose $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$ that $\phi_1 = \phi$, and therefore each such ϕ is an eigenfunction of U. All these ϕ must belong to the same eigenvalue; indeed, if ϕ, ψ belong to different eigenvalues then they must be orthogonal. Observe next that $\frac{1}{\sqrt{2}}(\phi + \psi)$ is also an eigenfunction, and since

$$\Big(\frac{\phi+\psi}{\sqrt{2}}, \phi\Big) = \frac{(\phi,\phi)}{\sqrt{2}} = \tfrac{1}{\sqrt{2}}$$
$$\Big(\frac{\phi+\psi}{\sqrt{2}}, \psi\Big) = \frac{(\psi,\psi)}{\sqrt{2}} = \tfrac{1}{\sqrt{2}}$$

it is orthogonal to neither ϕ nor ψ, and hence belongs to the same eigenvalue as both ϕ and ψ, which is impossible since these belong to different eigenvalues. Consequently, $\mathsf{U}\phi = a\phi$ with constant a. The restriction $\|\phi\| = 1$, to which this result is subject, can clearly be omitted. So for all f of $\mathcal{M}$, $\mathsf{U}f = af$. Therefore $\mathsf{UE}g = a\mathsf{E}g$ for all g, by which we have $\mathsf{UE} = a\mathsf{E}$. But $\mathsf{U} = \mathsf{UE}$ so $\mathsf{U} = a\mathsf{E}$. U, E are both definite and $\neq \mathsf{O}$. Therefore $a > 0$, and so we can set $\mathsf{U} = \mathsf{E}$ without changing it essentially.

Conversely, this U fulfills the requirement for each R; *i.e.*, for each set $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$ if U_0 is appropriately chosen. For $\mathsf{U}_0 = \mathsf{I}$

$$\sum_n (\mathsf{U}_0\phi_n, \phi_n)\mathsf{P}_{[\phi_n]} = \sum_n (\phi_n, \phi_n)\mathsf{P}_{[\phi_n]}$$
$$= \sum_n \mathsf{P}_{[\phi_n]} = \mathsf{P}_{\mathcal{M}} = \mathsf{E} = \mathsf{U}$$

Hence $\mathsf{E} = \mathsf{U}$ is established in the sense of the outline sketched above. Also, U_0 can be determined if we assume it to be universal; *i.e.*, independent of E and R.

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[179] Because, for example,

$$\mathsf{RP}_{[\phi_n]}f = \mathsf{R}\big((f,\phi_n)\cdot\phi_n\big) = (f,\phi_n)\cdot\mathsf{R}\phi_n = \lambda_n(f,\phi_n)\cdot\phi_n$$
$$\mathsf{P}_{[\phi_n]}\mathsf{R}f = \ (\mathsf{R}f,\phi_n)\cdot\phi_n \ = (f,\mathsf{R}\phi_n)\cdot\phi_n = \lambda_n(f,\phi_n)\cdot\phi_n$$

$\mathsf{U}_0 = \mathsf{I}$ then yields the desired result, and only this. Indeed

$$\begin{aligned}(\mathsf{U}\phi_m, \phi_m) &= (\mathsf{E}\phi_m, \phi_m) = (\phi_m, \phi_m) = 1\\ (\mathsf{U}\phi_m, \phi_m) &= \sum_n (\mathsf{U}_0\phi_n, \phi_n)(\mathsf{P}_{[\phi_n]}\phi_m, \phi_m)\\ &= \sum_n (\mathsf{U}_0\phi_n, \phi_n)|(\phi_n, \phi_m)|^2 = (\mathsf{U}_0\phi_m, \phi_m)\end{aligned}$$

Therefore $(\mathsf{U}_0\phi_m, \phi_m) = 1$. Since each ϕ of $\mathfrak{M}$ with $\|\phi\| = 1$ can be made a ϕ_1 we have $(\mathsf{U}_0\phi, \phi) = 1$, and from this it follows for all f of $\mathfrak{M}$ that $(\mathsf{U}_0 f, f) = (f, f)$. Since $\mathfrak{M}$ is arbitrary, this holds for all f in general, and consequently $\mathsf{U}_0 = \mathsf{I}$.

Consider two properties $\mathfrak{E}$ and $\mathfrak{F}$, not necessarily simultaneously decidable. What is the probability that a system **S** in which the property $\mathfrak{E}$ has just been found to hold will, in an immediately following observation, also be found to possess the property $\mathfrak{F}$? By the above, this probability is $\mathrm{Tr}(\mathsf{EF}) = \sum(\mathsf{EF})$. ($\mathsf{E}, \mathsf{F}$ are the operators of $\mathfrak{E}$, $\mathfrak{F}$; the expression on the left arises from $\mathsf{U} = \mathsf{E}$, that on the right from $\mathsf{E}^2 = \mathsf{E}, \mathsf{F}^2 = \mathsf{F}$, by **II.11**). Moreover, these probabilities are relative, so that $\mathfrak{E}$ should be considered fixed and $\mathfrak{F}$ variable; if

$$\mathrm{Tr}(\mathsf{E}) = \sum(\mathsf{E}) = \dim \mathfrak{M}$$

is finite we can normalize by dividing by $\dim \mathfrak{M}$.

In place of the properties $\mathfrak{E}$, $\mathfrak{F}$ we can consider physical quantities: Let $\mathcal{R}_1, \ldots, \mathcal{R}_j$ and $\mathcal{S}_1, \ldots, \mathcal{S}_k$ be two separate sets of simultaneously measurable quantities (they need not, however, form such a set when taken conjointly); let their respective operators be $\mathsf{R}_1, \ldots, \mathsf{R}_j, \mathsf{S}_1, \ldots, \mathsf{S}_k$ and their resolutions of the identity be $\mathsf{E}_1(\lambda), \ldots, \mathsf{E}_j(\lambda), \mathsf{F}_1(\lambda), \ldots, \mathsf{F}_k(\lambda)$. Let intervals

$$\begin{aligned} I_1 &: \quad \lambda_1' < \lambda \leqslant \lambda_1''\\ &\vdots\\ I_j &: \quad \lambda_j' < \lambda \leqslant \lambda_j''\\ J_1 &: \quad \mu_1' < \lambda \leqslant \mu_1''\\ &\vdots\\ J_k &: \quad \mu_k' < \lambda \leqslant \mu_k'' \end{aligned}$$

and let

$$\begin{aligned} \mathsf{E}_1(I_1) &= \mathsf{E}_1(\lambda_1'') - \mathsf{E}_1(\lambda_1')\\ &\vdots\\ \mathsf{E}_j(I_j) &= \mathsf{E}_j(\lambda_j'') - \mathsf{E}_j(\lambda_j')\\ \mathsf{F}_1(J_1) &= \mathsf{F}_1(\mu_1'') - \mathsf{F}_1(\mu_1')\\ &\vdots\\ \mathsf{F}_k(J_k) &= \mathsf{F}_k(\mu_k'') - \mathsf{F}_k(\mu_k') \end{aligned}$$

Suppose now that $\mathcal{R}_1, \ldots, \mathcal{R}_j$ were measured on $\mathbf{S}$ and their values found to lie in $I_1, \ldots, I_j$, respectively. The question is: What is the probability that prompt measurement will show the values of $\mathcal{S}_1, \ldots, \mathcal{S}_k$ to lie in $J_1, \ldots, J_k$, respectively? Clearly, we must set $\mathsf{E} = \mathsf{E}_1(I_1) \cdots \mathsf{E}_j(I_j)$ and $\mathsf{F} = \mathsf{F}_1(J_1) \cdots \mathsf{F}_k(J_k)$. Then the desired probability is (see $\boldsymbol{\epsilon}$, $\boldsymbol{\zeta}$)

$$\begin{aligned}\operatorname{Tr}\big(\mathsf{E}_1(I_1) \cdots \mathsf{E}_j(I_j) \cdot \mathsf{F}_1(J_1) \cdots \mathsf{F}_k(J_k)\big) \\ = \sum \big(\mathsf{E}_1(I_1) \cdots \mathsf{E}_j(I_j) \cdot \mathsf{F}_1(J_1) \cdots \mathsf{F}_k(J_k)\big)\end{aligned}$$

In conclusion, let us refer once again to the meaning of the general initial ensemble $\mathsf{U}_0 = \mathsf{I}$. We obtained U from it by resolving it, in the case of the $\mathcal{R}$ measurement, into two parts. If we had not so resolved it, *i.e.*, had we measured $\mathcal{R}$ on all its elements and joined all these together again to form an ensemble, then we would again have obtained $\mathsf{U}_0 = \mathsf{I}$. This can easily be calculated directly, or can be proved by choosing $\mathsf{E} = \mathsf{I}$. Then the $\mu_1, \mu_2, \ldots$ and the $\psi_1, \psi_2, \ldots$ are absent, and the $\lambda_1, \lambda_2, \ldots$ and $\phi_1, \phi_2, \ldots$ for a complete set. Therefore, although the measurement of $\mathcal{R}$ changes the individual elements under certain circumstances, all these changes must exactly compensate each other, because the entire ensemble does not change. Furthermore, this property is characteristic for $\mathsf{U}_0 = \mathsf{I}$. Because if for all complete orthonormal sets $\phi_1, \phi_2, \ldots$

$$\mathsf{U}_0 = \sum_{n=1}^{\infty} (\mathsf{U}_0 \phi_n, \phi_n) \mathsf{P}_{[\phi_n]}$$

then U_0 commutes with $\mathsf{P}_{[\phi_1]}$ since it does with each $\mathsf{P}_{[\phi_n]}$. That is, U_0 commutes with each $\mathsf{P}_{[\phi]}$, $\|\phi\| = 1$. Therefore

$$\mathsf{U}_0 \phi = \mathsf{U}_0 \mathsf{P}_{[\phi]} \phi = P_{[\phi]} \mathsf{U}_0 \phi = (\mathsf{U}_0 \phi, \phi) \cdot \phi$$

i.e., ϕ is an eigenfunction of U_0. From this it follows that $\mathsf{U}_0 = \mathsf{I}$, exactly as $\mathsf{U} = \mathsf{E}$ was obtained earlier from the corresponding relation (with $\mathcal{M}$, E in place of $\mathcal{R}$, I).

In $\mathsf{U}_0 = \mathsf{I}$, therefore, all possible states are in the highest possible degree of equilibrium, which no measuring process can alter. For each complete orthonormal set $\phi_1, \phi_2, \ldots$

$$\mathsf{U}_0 = \mathsf{I} = \sum_{n=1}^{\infty} \mathsf{P}_{[\phi_n]}$$

From this we learn that $\mathsf{U}_0 = \mathsf{I}$ corresponds in the older quantum theory to the ordinary thermodynamic assumption of the "*a priori* equal probability of all simple quantum orbits." It will also play an important role in our thermodynamic considerations, to which the next sections are devoted.

CHAPTER V

GENERAL CONSIDERATIONS

1. MEASUREMENT AND REVERSIBILITY

What happens to a mixture with the statistical operator U if a quantity $\mathcal{R}$ with operator R is measured in it? This operator must be thought of as measuring $\mathcal{R}$ in each element of the ensemble and collecting the thus-processed elements together into a new ensemble. We will answer the question—to the extent that it admits of an unambiguous answer.

First, let R have a pure discrete simple spectrum, let $\phi_1, \phi_2, \ldots$ be the complete orthonormal set of eigenfunctions and $\lambda_1, \lambda_2, \ldots$ the corresponding eigenvalues (by assumption all different from each other). After the measurement, the state of affairs is the following: In a fraction $(\mathsf{U}\phi_n, \phi_n)$ of their original ensemble, $\mathcal{R}$ has the value λ_n $(n = 1, 2, \ldots)$. This fraction then forms an ensemble (sub-ensemble) in which $\mathcal{R}$ has the value λ_n with certainty (by **M** in **IV.3**); it is therefore in the state ϕ_n with the (correctly normalized) statistical operator $\mathsf{P}_{[\phi_n]}$. Upon collecting these sub-ensembles, therefore, we obtain a mixture with the statistical operator

$$\mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n) \mathsf{P}_{[\phi_n]}$$

Second, let us abandon the assumption that the pure discrete spectrum of R is simple; *i.e.*, let us admit the possibility that among the λ_n there are coincidences. Then the $\mathcal{R}$-measurement process is not uniquely defined (the same was the case, for example, with $\mathfrak{E}$ in **IV.3**). Indeed, let $\mu_1, \mu_2, \ldots$ be distinct real numbers, and S the operator corresponding to the $\phi_1, \phi_2, \ldots$ and $\mu_1, \mu_2, \ldots$ Let $\mathcal{S}$ be the corresponding quantity. If $F(x)$ is a function with

$$F(\mu_n) = \lambda_n \quad : \quad n = 1, 2, \ldots$$

then $F(\mathsf{S}) = \mathsf{R}$ and therefore $F(\mathcal{S}) = \mathcal{R}$. Hence the $\mathcal{S}$-measurement can also be regarded as an $\mathcal{R}$-measurement. This now changes U into the U' given

above, and U' is independent of the (entirely arbitrary) $\mu_1, \mu_2, \ldots$ but not of the $\phi_1, \phi_2, \ldots$. But the $\phi_1, \phi_2, \ldots$ are not uniquely determined, because of the multiplicities of the eigenvalues of R. In **IV.2**—following **II.8**—we indicated what can be said regarding the $\phi_1, \phi_2, \ldots$: Let $\lambda', \lambda'', \ldots$ be the different values assumed by the eigenvalues $\lambda_1, \lambda_2, \ldots$ and let $\mathfrak{M}_{\lambda'}, \mathfrak{M}_{\lambda''}, \ldots$ be the sets of the f which satisfy $\mathsf{R}f = \lambda' f$, $\mathsf{R}f = \lambda'' f$, ... respectively. Finally, let

$$\chi_1', \chi_2', \ldots; \quad \chi_1'', \chi_2'', \ldots; \quad \ldots$$

respectively be arbitrary orthonormal sets that span $\mathfrak{M}_{\lambda'}, \mathfrak{M}_{\lambda''}, \ldots$. Then $\chi_1', \chi_2', \ldots, \chi_1'', \chi_2'', \ldots, \ldots$ is the most general $\phi_1, \phi_2, \ldots$ set. Hence U' —depending upon the choice of $\mathcal{S}$; depending, that is, upon the actual measuring arrangement—may be any expression of the form

$$\mathsf{U}' = \sum_n (\mathsf{U}\chi_n', \chi_n')\mathsf{P}_{[\chi_n']} + \sum_n (\mathsf{U}\chi_n'', \chi_n'')\mathsf{P}_{[\chi_n'']} + \cdots$$

This construction is, however, unambiguous only in special cases.

We determine this special case. Each individual term must be unambiguous. That is, for each eigenvalue λ, if $\mathfrak{M}_\lambda$ is the set of f with $\mathsf{R}f = \lambda f$, the sum

$$\sum_n (\mathsf{U}\chi_n, \chi_n)\mathsf{P}_{[\chi_n]}$$

must have the same value for every choice of the orthogonal set $\chi_1, \chi_2, \ldots$ spanning the manifold $\mathfrak{M}_\lambda$. If we call this sum V then verbatim repetition of the observations in **IV.3** (in which U_0, U, $\mathfrak{M}$ are to be replaced now by U, V, $\mathfrak{M}_\lambda$) shows that we must have $\mathsf{V} = c_\lambda \mathsf{P}_{\mathfrak{M}}$ (c_λ a positive constant), and that this is equivalent to the validity of $(\mathsf{U}f, f) = c_\lambda(f, f)$ for all f of $\mathfrak{M}_\lambda$. Since these f are the same as $\mathsf{P}_{\mathfrak{M}_\lambda} g$ for all g, we require

$$(\mathsf{U}\mathsf{P}_{\mathfrak{M}_\lambda} g, \mathsf{P}_{\mathfrak{M}_\lambda} g) = c_\lambda (\mathsf{P}_{\mathfrak{M}_\lambda} g, \mathsf{P}_{\mathfrak{M}_\lambda} g) \quad : \quad \text{all } g$$

i.e.,
$$(\mathsf{P}_{\mathfrak{M}_\lambda}\mathsf{U}\mathsf{P}_{\mathfrak{M}_\lambda} g, g) = c_\lambda (\mathsf{P}_{\mathfrak{M}_\lambda} g, g) \quad : \quad \text{all } g$$

i.e.,
$$\mathsf{P}_{\mathfrak{M}_\lambda}\mathsf{U}\mathsf{P}_{\mathfrak{M}_\lambda} = c_\lambda \mathsf{P}_{\mathfrak{M}_\lambda}$$

for all the eigenvalues λ of R. But if this condition—which clearly imposes a sharp restriction upon U—is not satisfied then different arrangements for measuring $\mathcal{R}$ can actually transform U into different statistical operators U'. (Nevertheless, we will succeed in **V.4** in making some statements about the result of a general $\mathcal{R}$-measurement, on a thermodynamic basis.)

Third, let R have no pure discrete spectrum. Then by **III.3** (or by **IV.3**, criterion **I**) it is not measurable with absolute precision, and $\mathcal{R}$-measurements of limited precision (as we discussed in the case referred to) are equivalent to measurements of quantities with pure discrete spectra.

Another type of intervention in material systems—in contrast to discontinuous, non-causal and instantaneously acting experiments or measurements—is given by the time-dependent Schrödinger differential equation. This describes how the system changes continuously and causally in the course of time, if its total energy is known. For states ϕ these equations are

$\mathbf{T}_1$ $$\frac{\partial}{\partial t}\phi_t = -\frac{i}{\hbar}\mathsf{H}\phi_t$$

where H is the energy operator.

For $\mathsf{U}_t = \mathsf{P}_{[\phi_t]}$, the statistical operator of the state ϕ_t, this means

$$\begin{aligned}\big(\tfrac{\partial}{\partial t}\mathsf{U}_t\big)f &= \tfrac{\partial}{\partial t}\big(\mathsf{U}_t f\big)\\ &= \tfrac{\partial}{\partial t}\big((f,\phi_t)\cdot\phi_t\big)\\ &= (f,\tfrac{\partial}{\partial t}\phi_t)\cdot\phi_t + (f,\phi_t)\cdot\tfrac{\partial}{\partial t}\phi_t\\ &= -(f,\tfrac{i}{\hbar}\mathsf{H}\phi_t)\cdot\phi_t - (f,\phi_t)\cdot\tfrac{i}{\hbar}\mathsf{H}\phi_t\\ &= \tfrac{i}{\hbar}\Big((\mathsf{H}f,\phi_t)\cdot\phi_t - (f,\phi_t)\cdot\mathsf{H}\phi_t\Big)\\ &= \tfrac{i}{\hbar}\big(\mathsf{U}_t\mathsf{H} - \mathsf{H}\mathsf{U}_t\big)f\end{aligned}$$

which is to say:

$\mathbf{T}_2$ $$\frac{\partial}{\partial t}\mathsf{U}_t = \frac{i}{\hbar}\big(\mathsf{U}_t\mathsf{H} - \mathsf{H}\mathsf{U}_t\big)$$

But if U_t refers not to a state but to a mixture of several states—say

$$\mathsf{P}_{[\phi_t^{(1)}]}, \mathsf{P}_{[\phi_t^{(2)}]}, \dots \quad \text{with respective weights} \quad w_1, w_2, \dots$$

—the motion of U_t must reflect the motion of the individual terms

$$\mathsf{P}_{[\phi_t^{(1)}]}, \mathsf{P}_{[\phi_t^{(2)}]}, \dots$$

By weighted addition of the corresponding instances of $\mathbf{T}_2$ we find that $\mathbf{T}_2$ pertains also to such mixtures. Since all U refer to such mixtures, or limiting cases of them (for example, each U with finite $\mathrm{Tr}\mathsf{U}$ refers to such a mixture), we can claim the general validity of $\mathbf{T}_2$.

It is, moreover, the case that in $\mathbf{T}_2$ the operator H may depend on t, just as it may in the Schrödinger differential equation. If H is not t-dependent we can even give explicit solutions: For $\mathbf{T}_1$, as we already know,

$\mathbf{T}_1'$ $$\phi_t = e^{-\frac{i}{\hbar}t\mathsf{H}}\phi_0$$

and for $\mathbf{T}_2$

$\mathbf{T}_2'$ $$\mathsf{U}_t = e^{-\frac{i}{\hbar}t\mathsf{H}}\mathsf{U}_0\, e^{+\frac{i}{\hbar}t\mathsf{H}}$$

(It is easily verified that these are solutions, and also that they follow from each other. It is clear also that there is only one solution for each given value of ϕ_0 or U_0: the differential equations $\mathbf{T}_1$ and $\mathbf{T}_2$ are of first order in t.)

We therefore have two fundamentally different types of interventions which can occur in a system **S** or in an ensemble $[\mathbf{S}_1, \ldots, \mathbf{S}_N]$. We allude here first to the abrupt changes

1 $$\mathsf{U} \longrightarrow \mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n)\mathsf{P}_{[\phi_n]}$$

that are brought about by measurement ($\phi_1, \phi_2, \ldots$ is a complete orthonormal set), and second to the temporally graded dynamical transformations

2 $$\mathsf{U} \longrightarrow \mathsf{U}_t = e^{-\frac{i}{\hbar}t\mathsf{H}}\mathsf{U}_0\, e^{+\frac{i}{\hbar}t\mathsf{H}}$$

that are generated by the energy operator (Hamiltonian) H, here assumed to be time-independent. If H does depend upon time, we may divide the time interval under consideration into brief sub-intervals during each of which H is, in sufficient approximation, constant; we apply **2** to these individual intervals, and construct the final result by iteration.

We must now analyze in greater detail these two types of intervention—their nature, and their relation to one another.

First of all, it is noteworthy that **2** admits (in the manner described above) of the possibility that H is time-dependent, so that one might expect that **2** would suffice to describe interventions caused by measurement: indeed, a physical intervention can be nothing other than the temporary insertion of a certain energy coupling into the observed system; *i.e.*, the introduction into H of a certain time dependency (prescribed by the observer). Why then have we need—for measurements—of the special process **1**? The reason is this: In a measurement we cannot observe the system **S** by itself, but must rather investigate the system $\mathbf{S} + \mathbf{M}$ in order to obtain (numerically) its interaction with the measuring apparatus **M**. The theory of measurement is a statement concerning $\mathbf{S} + \mathbf{M}$, and should describe how the state of **S** is related to certain properties of the state of **M** (namely, the positions of a certain pointer, since the observer reads these). Moreover, it is rather arbitrary whether one includes the observer in **M**, and replaces the relation between the **S** state and the pointer positions in **M** by relations between this state and chemical changes in his eye or even in his brain (*i.e.*, to that which he has "seen" or "perceived"). We shall investigate this more precisely in **VI.1**. In any case, the application of **2** is of importance only for $\mathbf{S} + \mathbf{M}$. Of course, we must show that this gives the same result for **S** as does the direct application of **1** to **S**. If this is proves successful, then we will have achieved a unified way of looking at the physical world on a quantum mechanical basis. We postpone discussion of this question until **VI.3**.

Second, it has to be noted with regard to **1** that we have repeatedly shown that a measurement in the sense of **1** must be instantaneous; *i.e.*, must be carried out in so brief a time that the change of U given by **2** is not noticeable. (If we wanted to correct this by calculating the changed U_t by **2** we would still gain nothing because to apply any U_t we must first know t—the moment of

measurement—exactly; *i.e.*, the duration of the measurement must be short.) But this now is questionable in principle, because it is well known that there is a quantity which, in classical mechanics, is conjugate to time: the energy.[180] Therefore it is to be expected that for the canonically conjugate pair time-energy there must exist indeterminacy relations similar to those of the conjugate pair cartesian coordinate-momentum.[181] Note that the theory of special relativity shows that a far-reaching analogy must exist: the three space coordinates and time form a "four vector" as do the momentum coordinates and energy. Such an indeterminacy relation would mean that it is not possible to carry out a very precise measurement of energy in a very short time. In fact, one would expect the error ϵ of the energy measurement and the duration τ of the measurement to stand in the relation

$$\epsilon\tau \sim h$$

A physical discussion, similar to that carried out in **III.4** for p, q, actually leads to this result.[181] Without going into details, we can consider the case of a light quantum. Its energy uncertainty is, because of the Bohr frequency condition, h times the frequency uncertainty $\Delta\nu$: $h\Delta\nu$. But, as was discussed in Note 137, $\Delta\nu$ is at best the reciprocal $1/\tau$ of the time duration; *i.e.*, $\epsilon >\sim h/\tau$. And in order that the monochromatic nature of the light quantum be established in the time interval τ the measurement must extend over the entire duration of the interval. The case of the light quantum is characteristic, since the atomic energy levels are, as a rule, determined from the frequency of the corresponding spectral lines. Since energy behaves in such fashion, a relation between the measurement precision of other quantities $\mathcal{R}$ and the duration of the measurement might also be anticipated. But how, then, can our assumption that measurements are instantaneous be justified?

First of all, we must admit that this objection points to an essential weakness which is, in fact, the chief weakness of quantum mechanics: the theory is non-relativistic; it distinguishes time t from the three space coordinates x, y, z and presupposes an objective simultaneity concept. In fact, while all other quantities (especially those x, y, z—so closely related to t by Lorentz transformations) are represented by operators, there corresponds to time not an operator T but an ordinary number-parameter t, just as in classical mechanics. Or again: a system consisting of two particles has a wave function which depends on $2 \times 3 = 6$ space coordinates but only one time coordinate t, although from a relativistic standpoint two times would be desirable (more natural). That measurements cannot in fact be instantaneous but must be of non-vanishing finite duration has the status of natural law. That we can ignore that law may possibly have to do with the non-relativistic character of quantum mechanics. But if that provides a degree of clarification, it is not a happy one!

[180] Any textbook of classical (Hamiltonian) mechanics gives an account of this connection.

[181] The uncertainty relations for the pair time-energy have been discussed frequently. See the comprehensive treatment of Heisenberg, *Die Physikalischen Prinzipien der Quantentheorie*, II.2.d, Leipzig, 1930.

A more detailed investigation of the problem shows, however, that the situation is really not so bad as it may at first appear. For what we really need is not that the duration t of the measurement be small, but only that it have little effect in the calculation of the probabilities $(\mathsf{U}\phi_n, \phi_n)$—and therefore in the formation of

$$\mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n)\mathsf{P}_{[\phi_n]}$$

—whether we proceed from U itself or from

$$\mathsf{U}_t = e^{-\frac{i}{\hbar}t\mathsf{H}}\mathsf{U}e^{+\frac{i}{\hbar}t\mathsf{H}}$$

Because of

$$\begin{aligned}(\mathsf{U}_t\phi_n, \phi_n) &= \left(e^{-\frac{i}{\hbar}t\mathsf{H}}\mathsf{U}e^{+\frac{i}{\hbar}t\mathsf{H}}\phi_n, \phi_n\right) \\ &= \left(\mathsf{U}e^{\frac{i}{\hbar}t\mathsf{H}}\phi_n, e^{\frac{i}{\hbar}t\mathsf{H}}\phi_n\right)\end{aligned}$$

this can be accomplished by so adjusting H (by introduction of an appropriate perturbation term) that

$$e^{\frac{i}{\hbar}t\mathsf{H}}\phi_n = \phi_n \text{ to within a constant factor of absolute value 1}$$

That is, the state ϕ_n should be essentially constant with respect to **2**; *i.e.*, a stationary state. Or equivalently, $\mathsf{H}\phi_n$ must be equal to a real constant times ϕ_n; *i.e.*, ϕ_n must be an eigenfunction of H. At first glance, the possibility of such an adjustment of H—one which renders the eigenfunctions of R stationary, and therefore eigenfunctions also of H (which is to bring about the commutativity of R and H)—may seem implausible. But this is not really the case, and it will emerge that typical experimental arrangements aim to have exactly this sort of effect on H.

In point of fact, every experiment culminates in the emission of a light quantum or of a particle, with a certain energy in a certain direction. Characteristics of the emitted quantum/particle—its momentum, or the coordinates of the point where it (the "pointer") comes to rest—comprise the result of the measurement. In the case of light quanta, using the terminology of **III.6**, the desired measurement is thus equivalent to a statement as to which $m_n = 1$ (the rest being 0), *i.e.*, to an enumeration of all $m_1, m_2, \ldots$ values. For a moving (departing) mass point the corresponding statement refers to the values of the momentum components $\mathsf{P}^x, \mathsf{P}^y, \mathsf{P}^z$, while for a mass point at rest it refers its (the pointer's) cartesian coordinates x, y, z; *i.e.*, to the values of $\mathsf{Q}^x, \mathsf{Q}^y, \mathsf{Q}^z$. But the measurement is completed only if the light quantum is "borne away;" *i.e.*, when the light quantum is not in danger of absorption, or when the mass point can no longer be deflected by ambient forces, or caused to drift away from the point at which it has come to rest, in which case a large mass is necessary.[182] (This latter requirement is made necessary because of the

[182] All other details of the measuring arrangement address only the connection between the quantity of interest $\mathcal{R}$ (or of its operator R) and the m_n or the $\mathsf{P}^x, \mathsf{P}^y, \mathsf{P}^z$ (else $\mathsf{Q}^x, \mathsf{Q}^y, \mathsf{Q}^z$) mentioned above. This, of course, is the most important practical aspect of the measurement techniques.

uncertainty relations; we want the velocity and its dispersion to be small, but for the dispersion in position also to be small the dispersion in momentum—mass times velocity—must be large. Ordinarily, pointers are macroscopic objects; *i.e.*, enormous.) Now the energy operator H, so far as concerns the light quantum, is (see **III.6**, page 171)

$$\sum_{n=1}^{\infty} h\rho_n \cdot m_n + \sum_{j,n=1}^{\infty} w_{kj}^n \left\{ \sqrt{m_n + 1} \begin{pmatrix} k \to j \\ m_n \to m_n + 1 \end{pmatrix} + \sqrt{m_n} \begin{pmatrix} k \to j \\ m_n \to m_n - 1 \end{pmatrix} \right\}$$

while for both mass point models H is given by

$$\frac{(\mathsf{P}^x)^2 + (\mathsf{P}^y)^2 + (\mathsf{P}^x)^2}{2m} + V(\mathsf{Q}^x, \mathsf{Q}^y, \mathsf{Q}^z)$$

Our criteria say: the w_{kj}^n should vanish, or the potential energy V should be constant, or the mass m should be very large. But this actually produces the effect that the $\mathsf{P}^x, \mathsf{P}^y, \mathsf{P}^z$ and the $\mathsf{Q}^x, \mathsf{Q}^y, \mathsf{Q}^z$ (respectively) commute with the H given above.

In conclusion, it should be mentioned that the making stationary of the really interesting states (here the $\phi_1, \phi_2, \ldots$) plays a role elsewhere too in theoretical physics. Assumptions concerning the possibility of the interruption of chemical reactions (*i.e.*, their "poisoning"), which are often unavoidable in physical-chemical "ideal experiments," are of this nature.[183]

The two interventions **1** and **2** are fundamentally different from one another. That both are formally unique—*i.e.*, causal—is unimportant; indeed, since we are working in terms of the statistical properties of mixtures it is not surprising that each change, even if it is statistical, effects a causal change of the probabilities and expectation values. Indeed, it is for precisely this reason that one introduces statistical ensembles and probabilities! On the other hand, it is important that **2** does not increase the statistical uncertainty present in U, but that **1** does. **2** transforms states into states

$$\mathsf{P}_{[\phi]} \longrightarrow \mathsf{P}_{[\phi_t]} \quad \text{with} \quad \phi_t = e^{-\frac{i}{\hbar} t \mathsf{H}} \phi$$

while **1** can transform states into mixtures. In this sense, therefore, the development of a state according to **1** is statistical, while according to **2** it is causal.

Furthermore, for fixed H and t, **2** is simply a unitary transformation of all U: $\mathsf{U}_t = \mathsf{A}\mathsf{U}\mathsf{A}^{-1}$, $\mathsf{A} = \exp\{-\frac{i}{\hbar} t \mathsf{H}\}$ unitary. That is, $\mathsf{U}f = g$ implies $\mathsf{U}_t(\mathsf{A}f) = (\mathsf{A}g)$,

[183] See, for example, Nernst, *Theoretische Chemie*, Stuttgart (numerous editions since 1893), Book IV: Discussion of the thermodynamic proof of the "law of mass action."

so that U_t results from U by the unitary transformation A of Hilbert space; *i.e.*, by an isomorphism that leaves all of our basic geometric concepts invariant (see the principles set down in **I.4**). Therefore $\mathsf{U} \to \mathsf{U}_t$ is reversible: it suffices to replace A by A^{-1}, and this is possible since A, A^{-1} can be regarded as entirely arbitrary unitary operators—this because of the far-reaching freedom one has in the selection of H, t. Therefore **2**—like classical mechanics—fails to reproduce one of the most important and striking properties of the real world; namely, its irreversibility, the fundamental difference between "future" and "past," the directions of time.

On the other hand, **1** is of a fundamentally different character: the transition

$$\mathsf{U} \longrightarrow \mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n)\mathsf{P}_{[\phi_n]}$$

is certainly not *prima facie* reversible. We will soon see that it is in general irreversible in the sense that it is in general not possible to proceed $\mathsf{U} \longleftarrow \mathsf{U}'$ by repeated application of the processes **1**, **2**!

We have reached a point at which it becomes necessary to resort to the thermodynamic method of analysis, because it alone makes it possible for us to come to a correct understanding of the difference between **1** and **2**, a distinction into which reversibility questions obviously enter.

2. THERMODYNAMIC CONSIDERATIONS

We shall investigate the thermodynamics of quantum mechanical ensembles from two different points of view. First, let us assume the validity of both of the fundamental laws of thermodynamics, *i.e.*, the impossibility of perpetual motion of the first and second kinds (energy law and entropy law),[184] and proceed on this basis to calculation of the entropy of ensembles. In this effort the normal methods of phenomenological thermodynamics are applied, and quantum mechanics plays a role only insofar as our thermodynamic observations relate to objects whose behavior is regulated by the laws of quantum mechanics (our ensembles, as well as their statistical operators U). But the correctness of both laws will here be assumed, and not proved. Afterwards we will prove the validity of these fundamental laws in quantum mechanics. Since the energy law holds in any case, only the entropy law need be considered. Specifically, we will show that the interventions **1**, **2** never decrease the entropy, as calculated by the first method. Our decision to proceed in this order may seem somewhat

[184] The phenomenological system of thermodynamics built upon this foundation can be found in numerous texts; see, for example, Planck *Treatise on Thermodynamics* London, 1927. For the following, the statistical aspect of these laws is of chief importance. This is developed in the following treatises: Einstein, Verh. d. dtsch. physik Ges. **12**, (1914); Szilard, Z. Physik **32** (1925).

unnatural, but is based on the fact that it is from phenomenological discussion that we obtain the overall view of the problem that is required for considerations of the second kind.

We therefore begin with phenomenological considerations which will permit us to solve a well-known paradox of classical thermodynamics. First we must emphasize that the unusual character of our "ideal experiments"—*i.e.*, their practical infeasibility—does not impair their demonstrative power: in the sense of phenomenological thermodynamics, every conceivable process constitutes valid evidence, provided only that it does not conflict with the two fundamental laws of thermodynamics.

Our objective is to determine the entropy of an ensemble $[\mathsf{S}_1, \ldots, \mathsf{S}_N]$ with the statistical operator U, where U is assumed to be correctly normalized; *i.e.*, $\mathrm{Tr}\mathsf{U} = 1$. In the terminology of classical statistic mechanics we are dealing with a Gibbs ensemble: *i.e.*, the application of statistics and thermodynamics will be made not on the (interacting) components of a single, very complicated mechanical system with many (only imperfectly known) degrees of freedom,[185] but on the ensemble of very many (identical) mechanical systems, each of which may have an arbitrarily large number of degrees of freedom, and each of which is entirely separated from the others, and does not interact with any of them.[186] As a consequence of the complete separation of the systems $\mathsf{S}_1, \ldots, \mathsf{S}_N$, and of the fact that we will apply to them the ordinary enumerative methods of the calculus of probability, it is evident that the Bose-Einstein and Fermi-Dirac statistics—which differ from those, and which are applicable to certain ensembles of indistinguishable particles (namely: those comprised of light quanta or of electrons/protons: see **III.6**, particularly Note 147)—do not enter into the problem.

The method introduced by Einstein for the thermodynamic treatment of such ensembles $[\mathsf{S}_1, \ldots, \mathsf{S}_N]$ is the following:[187] Each system $\mathsf{S}_1, \ldots, \mathsf{S}_N$ is confined in a box $\mathsf{K}_1, \ldots, \mathsf{K}_N$ whose walls are impenetrable to all transmission effects, which is possible for this system because of the lack of interaction. Furthermore, each box must have a very large mass, so that the possible state (hence energy and mass) changes of the $\mathsf{S}_1, \ldots, \mathsf{S}_N$ affect their masses only slightly. Also, their velocities in the ideal experiments which are to be carried out are to be kept so small that calculations may be performed

[185] This is the Maxwell-Boltzmann method of statistical mechanics (see the review in the article by P. and T. Ehrenfest in Enzykl. d. Math. Wiss., Vol II.4.D, Leipzig, 1907). In gas theory, for example, the "very complicated system" is the gas which consists of many (interacting) molecules, and the molecules are investigated statistically.

[186] This is the Gibbs method (see the reference in Note 185). Here the individual system is the entire gas, and many replicas of the same system (*i.e.*, of the same gas) are considered simultaneously, and their properties are described statistically.

[187] See the reference in Note 184. This was further developed by L. Szilard.

non-relativistically. We imagine these boxes to be enclosed in a very large box $\overline{\mathsf{K}}$ (the volume V of $\overline{\mathsf{K}}$ is much larger than the sum of the volumes of the boxes $\mathsf{K}_1, \ldots, \mathsf{K}_N$). For simplicity, no force field will be present in $\overline{\mathsf{K}}$ (in particular, it should be free from all gravitational fields, so that the large masses of the $\mathsf{K}_1, \ldots, \mathsf{K}_N$ have no relevant effects either). We can therefore regard the $\mathsf{K}_1, \ldots, \mathsf{K}_N$ (which contain $\mathsf{S}_1, \ldots, \mathsf{S}_N$ respectively) as the molecules of a gas which is enclosed in the large container $\overline{\mathsf{K}}$. We now bring $\overline{\mathsf{K}}$ into contact with a very large heat reservoir at temperature T. The walls of $\overline{\mathsf{K}}$ then take on this temperature, and its (literal) molecules then assume the corresponding Brownian motion. Therefore they contribute momentum to the adjacent $\mathsf{K}_1, \ldots, \mathsf{K}_N$, so that these engage in motion and transfer momentum to the other $\mathsf{K}_1, \ldots, \mathsf{K}_N$. Soon all $\mathsf{K}_1, \ldots, \mathsf{K}_N$ will be in motion and will be exchanging momentum... at the wall of $\overline{\mathsf{K}}$ with the literal molecules of the wall, and with each other in the interior of $\overline{\mathsf{K}}$. The stationary state is ultimately attained in which the $\mathsf{K}_1, \ldots, \mathsf{K}_N$ have taken on the velocity distribution which is in equilibrium with the Brownian motion of the wall molecules (temperature T), that distribution being the Maxwellian velocity distribution of a gas of temperature T, the "molecules" of which are the $\mathsf{K}_1, \ldots, \mathsf{K}_N$.[188] We can now say:

The $[\mathsf{S}_1, \ldots, \mathsf{S}_N]$-gas has taken on the temperature T.

For brevity, we shall call the ensemble $[\mathsf{S}_1, \ldots, \mathsf{S}_N]$ with statistical operator U the "U-ensemble," and the $[\mathsf{S}_1, \ldots, \mathsf{S}_N]$-gas the "$\mathsf{U}$-gas."

The reason that we concern ourselves with such a gas is that we want to be in position to determine the entropy difference between a U-ensemble and a V-ensemble (here U, V are definite operators with $\mathrm{Tr}\mathsf{U} = \mathrm{Tr}\mathsf{V} = 1$ and the corresponding ensembles are denoted $[\mathsf{S}_1, \ldots, \mathsf{S}_N]$ and $[\mathsf{S}_1', \ldots, \mathsf{S}_N']$). That determination requires by definition a reversible transformation of the former ensemble into the latter,[189] and this is best accomplished with the aid of the U- and V-gases. That is, we maintain that the entropy difference between the U- and V-ensembles is exactly the same as that between the U- and V-gases if both are observed at the same temperature T but are otherwise arbitrary. If T is very near 0 then this is obviously the case with arbitrary precision because the difference between the U-gas and the V-gas vanishes as $T \to 0$ since the $\mathsf{K}_1, \ldots, \mathsf{K}_N$ of the former then have no motion of their own, and the presence of the $\mathsf{K}_1, \ldots, \mathsf{K}_N$ in $\overline{\mathsf{K}}$, when they are at rest, is thermodynamically unimportant

[188] The kinetic theory of gases, as is well known, describes in this way the process in which the walls communicate their temperature to the gas enclosed by them. See the references in Notes 184 and 185.

[189] In this transformation, if the heat quantities $Q_1, \ldots, Q_N$ are required at temperatures $T_1, \ldots, T_N$ then the entropy difference is equal to

$$\frac{Q_1}{T_1} + \frac{Q_2}{T_2} + \cdots + \frac{Q_N}{T_N}$$

See the reference in Note 184.

(likewise for V). Therefore we shall have accomplished our objective if we can show for a given change of T that the entropy of the U-gas changes just as much as the entropy of the V-gas. The entropy change of a gas which is heated from T_1 to T_2 depends only upon its caloric equation of state, or more precisely: upon its specific heat.[190] Naturally, the gas must not be assumed to be an ideal gas if—as in our case—T_1 must be chosen near 0.[191] On the other hand, it is certain that both gases (U and V) have the same equation of state and the same specific heats because, by kinetic theory, the boxes $\mathsf{K}_1, \ldots, \mathsf{K}_N$ dominate and cover completely the systems $[\mathsf{S}_1, \ldots, \mathsf{S}_N]$ and $[\mathsf{S}_1', \ldots, \mathsf{S}_N']$ which are enclosed within them. In this heating process, therefore, the difference between U and V is not noticeable, and the two entropy differences coincide, as was asserted. In the following, therefore, we shall compare only the U- and V-gases with each other, and shall take the temperature T to be so high that these can be regarded as ideal gases.[192] In this way we control its kinetic behavior completely and can apply ourselves to the real problem: to transform U-gas reversibly into V-gas. Now, in contrast to the processes contemplated so far, we shall have also to consider the $\mathsf{S}_1, \ldots, \mathsf{S}_N$ found in the interiors of the $\mathsf{K}_1, \ldots, \mathsf{K}_N$; *i.e.*, we shall have to "open" the boxes $\mathsf{K}_1, \ldots, \mathsf{K}_N$.

Next, we will show that all states $\mathsf{U} = \mathsf{P}_{[\phi]}$ have the same entropy; *i.e.*, that the reversible transformation of the $\mathsf{U} = \mathsf{P}_{[\phi]}$ ensemble into the $\mathsf{U} = \mathsf{P}_{[\psi]}$ ensemble is accomplished without the absorption or release of heat energy (mechanical energy must naturally be consumed or produced if the expectation value of the energy in $\mathsf{P}_{[\phi]}$ is different from that in $\mathsf{P}_{[\psi]}$); see Note 185. In fact, we will not even have to refer to the gases just considered. This transformation succeeds even at the zero-temperature; *i.e.*, with the ensembles themselves. It should be mentioned, furthermore, that as soon as this is proved we will be able to—and shall—so normalize the entropies of the U-ensembles that all states have entropy 0.

Moreover, the transformation $\mathsf{P}_{[\phi]} \to \mathsf{P}_{[\psi]}$ does not need to be reversible. Because if it is not so then the entropy difference must be $\geqslant$ the expression given in Note 189 (see the reference in Note 185), and therefore $\geqslant 0$. Permutation of

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[190] If $c(T)$ is the specific heat of the gas quantum under discussion, then when heated from T to $T + dT$ it takes on the quantity of heat $c(T)dT$. By Note 185, the entropy difference is then

$$\int_{T_1}^{T_2} \frac{c(T)dT}{T}$$

[191] For an ideal gas, $c(T)$ is constant, but for very small T this certainly fails. See, for example, the reference in Note 6.

[192] In addition to this, it is required that the volume V of $\overline{\mathsf{K}}$ be large in comparison with the total volume of the $\mathsf{K}_1, \ldots, \mathsf{K}_N$, and furthermore that the "energy per degree of freedom" κT (κ is Boltzmann's constant) be large in comparison with $h^2/\mu V^{\frac{2}{3}}$ (h is Planck's constant, μ is the mass of the individual molecule; this quantity has the dimensions of energy). See, for example, Fermi, Z. Physik **36** (1926).

$\mathsf{P}_{[\phi]}, \mathsf{P}_{[\psi]}$ shows that this value must also be $\leqslant 0$. Therefore the value $= 0$.

The simplest way to proceed would be to refer to the time-dependent Schrödinger equation; *i.e.*, to our process **2**, in which an energy operator H and a numerical value of t must be found such that the unitary operator $e^{-\frac{i}{\hbar}t\mathsf{H}}$ transforms ϕ into ψ. Then, in t seconds, $\mathsf{P}_{[\phi]}$ would change spontaneously into $\mathsf{P}_{[\psi]}$. That process is reversible, and entails no mention of heat (see **V.1**). We prefer, however, to avoid assumptions concerning the construction of suitable energy operators H, and instead to exploit only processes of type **1**; *i.e.*, measuring interventions. The simplest such measurement would be to measure, in the ensemble $\mathsf{P}_{[\phi]}$, a quantity $\mathcal{R}$ whose operator R has a pure discrete spectrum with simple eigenvalues $\lambda_1, \lambda_2, \ldots$ and in which ψ occurs among the eigenfunctions $\psi_1, \psi_2, \ldots$ (say $\psi_1 = \psi$). This measurement transforms ϕ into a mixture of the states $\psi_1, \psi_2, \ldots$ and therefore $\psi_1 = \psi$ will be present along with the other states ψ_n. This procedure is unsuitable, however, because $\psi_1 = \psi$ occurs only with probability $|(\phi, \psi)|^2$, while the portion $1 - |(\phi, \psi)|^2$ goes over into other states. In fact, the latter portion becomes the entire result when ϕ and ψ are orthogonal. A different experiment, however, will achieve our objective. By repetition of a great number of different measurements we will change $\mathsf{P}_{[\phi]}$ into an ensemble which differs from $\mathsf{P}_{[\psi]}$ by an arbitrarily small amount. That all these processes are (or at least can be) irreversible is unimportant, as discussed above.

We may assume ϕ and ψ to be orthogonal, since if they were not we could choose a χ ($\|\chi\| = 1$) orthogonal to both, and proceed first $\phi \to \chi$, then $\chi \to \psi$. Now assign a value to $k = 1, 2, \ldots$ and define

$$\psi^{(\nu)} = \cos \tfrac{\pi\nu}{2k} \cdot \phi + \sin \tfrac{\pi\nu}{2k} \cdot \psi \quad : \quad \nu = 0, 1, \ldots, k$$

Clearly, $\psi^{(0)} = \phi$, $\psi^{(k)} = \psi$ and $\|\psi^{(\nu)}\| = 1$. We extend each $\psi^{(\nu)}$ to a complete orthonormal set $\psi_1^{(\nu)}, \psi_2^{(\nu)}, \ldots$ with $\psi_1^{(\nu)} = \psi^{(\nu)}$. Let $\mathsf{R}^{(\nu)}$ be an operator with a pure discrete spectrum and distinct eigenvalues—say $\lambda_1^{(\nu)}, \lambda_2^{(\nu)}, \ldots$ whose eigenfunctions are the $\psi_1^{(\nu)}, \psi_2^{(\nu)}, \ldots$—and let $\mathcal{R}^{(\nu)}$ be the corresponding quantity. Observe finally that

$$\begin{aligned}\left(\psi^{(\nu-1)}, \psi^{(\nu)}\right) &= \cos \tfrac{\pi(\nu-1)}{2k} \cos \tfrac{\pi\nu}{2k} + \sin \tfrac{\pi(\nu-1)}{2k} \sin \tfrac{\pi\nu}{2k} \\ &= \cos\left(\tfrac{\pi\nu}{2k} - \tfrac{\pi(\nu-1)}{2k}\right) \\ &= \cos \tfrac{\pi}{2k}\end{aligned}$$

In the ensemble with $\mathsf{U}^{(0)} = \mathsf{P}_{\left[\psi^{(0)}\right]} = \mathsf{P}_{[\phi]} = \mathsf{U}$, we now

measure $\mathcal{R}^{(1)}$ in $\mathsf{U}^{(0)}$, producing $\mathsf{U}^{(1)}$, then
measure $\mathcal{R}^{(2)}$ in $\mathsf{U}^{(1)}$, producing $\mathsf{U}^{(2)}$, then
$\vdots$
and finally measure $\mathcal{R}^{(k)}$ in $\mathsf{U}^{(k-1)}$, producing $\mathsf{U}^{(k)}$

That $\mathsf{U}^{(k)}$, for sufficiently large k, lies arbitrarily close to $\mathsf{P}_{\left[\psi^{(k)}\right]} = \mathsf{P}_{[\psi]}$ can easily be established: If we measure $\mathcal{R}^{(\nu)}$ on $\psi^{(\nu-1)}$ then the fraction

$$|(\psi^{(\nu-1)}, \psi^{(\nu)})|^2 = (\cos \tfrac{\pi}{2k})^2$$

goes over into $\psi^{(\nu)}$, and in the successive measurements $\mathcal{R}^{(1)}, \mathcal{R}^{(2)}, \ldots, \mathcal{R}^{(k)}$ therefore at least a fraction $(\cos \frac{\pi}{2k})^{2k}$ will go from $\psi^{(0)} = \phi$ over $\psi^{(1)}, \ldots, \psi^{(k-1)}$ into $\psi^{(k)} = \psi$. And since $(\cos \frac{\pi}{2k})^{2k} \to 1$ as $k \to \infty$, the final result is as nearly ψ as one may wish, if k is sufficiently large. The exact proof runs as follows: Since the process **1** does not change the trace, and since $\mathrm{Tr}\mathsf{U}^{(0)} = \mathrm{Tr}\mathsf{P}_{[\phi]} = 1$, we have $\mathrm{Tr}\mathsf{U}^{(1)} = \mathrm{Tr}\mathsf{U}^{(2)} = \cdots = \mathrm{Tr}\mathsf{U}^{(k)} = 1$. On the other hand,

$$\begin{aligned}(\mathsf{U}^{(\nu)} f, f) &= \sum_n \left(\mathsf{U}^{(\nu-1)} \psi_n^{(\nu)}, \psi_n^{(\nu)}\right)\left(\mathsf{P}_{\left[\psi_n^{(\nu)}\right]} f, f\right) \\ &= \sum_n \left(\mathsf{U}^{(\nu-1)} \psi_n^{(\nu)}, \psi_n^{(\nu)}\right)|(\psi_n^{(\nu)}, f)|^2\end{aligned}$$

so for $\nu = 1, \ldots, k-1$ in the case $f = \psi_1^{(\nu+1)} = \psi^{(\nu+1)}$ we have

$$\begin{aligned}(\mathsf{U}^{(\nu)} \psi^{(\nu+1)}, \psi^{(\nu+1)}) &= \left(\mathsf{U}^{(\nu-1)} \psi^{(\nu)}, \psi^{(\nu)}\right)|(\psi^{(\nu)}, \psi^{(\nu+1)})|^2 \\ &\quad + \sum_{n \geqslant 2} \left(\mathsf{U}^{(\nu-1)} \psi_n^{(\nu)}, \psi_n^{(\nu)}\right)|(\psi_n^{(\nu)}, \psi^{(\nu+1)})|^2 \\ &\geqslant \left(\mathsf{U}^{(\nu-1)} \psi^{(\nu)}, \psi^{(\nu)}\right)|(\psi^{(\nu)}, \psi^{(\nu+1)})|^2 \\ &= \left(\cos \tfrac{\pi}{2k}\right)^2 \cdot \left(\mathsf{U}^{(\nu-1)} \psi^{(\nu)}, \psi^{(\nu)}\right)\end{aligned}$$

while in the case $\nu = k$ we set $f = \psi_1^{(k)} = \psi$ and obtain

$$\begin{aligned}(\mathsf{U}^{(k)} \psi^{(k)}, \psi^{(k)}) &= \sum_n \left(\mathsf{U}^{(k-1)} \psi_n^{(k)}, \psi_n^{(k)}\right)|(\psi_n^{(k)}, \psi_1^{(k)})|^2 \\ &= \left(\mathsf{U}^{(k-1)} \psi_1^{(k)}, \psi_1^{(k)}\right) \\ &= (\mathsf{U}^{(k-1)} \psi^{(k)}, \psi^{(k)})\end{aligned}$$

When taken together with

$$(\mathsf{U}^{(0)} \psi^{(1)}, \psi^{(1)}) = \left(\mathsf{P}_{\left[\psi^{(0)}\right]} \psi^{(1)}, \psi^{(1)}\right) = |(\psi^{(0)}, \psi^{(1)})| = \left(\cos \tfrac{\pi}{2k}\right)^2$$

these results give

$$(\mathsf{U}^{(k)} \psi, \psi) \geqslant \left(\cos \tfrac{\pi}{2k}\right)^{2k}$$

Since $\mathrm{Tr}\mathsf{U}^{(k)} = 1$ and $\left(\cos \frac{\pi}{2k}\right)^{2k} \to 1$ as $k \to \infty$, we can apply a result obtained in **II.11** to conclude that $\mathsf{U}^{(k)}$ converges to $\mathsf{P}_{[\psi]}$. This completes the argument and achieves our objective.

The "ideal experiments" of phenomenological thermodynamics frequently make use of structures called "semi-permeable walls" (or membranes). To what extent can one make use of those idealized elements when dealing with quantum mechanical systems?

In phenomenological thermodynamics this theorem holds: If **I** and **II** are two different states of the same system **S** then it is permissible to assume the existence of a wall which is completely permeable for **I** but not permeable for **II**:[193] this is, so to speak, the thermodynamic definition of "difference," and therefore also of "sameness" (equality) for two systems. How far is such an assumption permissible in quantum mechanics?

We first show that if $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$ is an orthonormal set then there is a semi-permeable wall which lets the system **S** in any of the states $\phi_1, \phi_2, \ldots$ pass through unhindered, and which reflects unchanged systems in any of the states $\psi_1, \psi_2, \ldots$. Systems which are on other states may, on the other hand, be changed by collision with the wall.

The system $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$ can be assumed to be complete, since otherwise it could be made so by additional $\chi_1, \chi_2, \ldots$ which one could then add to the $\phi_1, \phi_2, \ldots$. We now choose an operator R with a pure discrete spectrum and simple eigenvalues $\lambda_1, \lambda_2, \ldots, \mu_1, \mu_2, \ldots$ whose eigenfunctions are $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$ respectively. Let us suppose that in fact (for all n) $\lambda_n < 0$ and $\mu_n > 0$. Let $\mathcal{R}$ be the quantity belonging to R. We construct many "windows" in the wall, each of which is defined as follows: each "molecule" $\mathbf{K}_1, \ldots, \mathbf{K}_N$ of our gas (we are again considering U-gases at temperature $T > 0$) is detained there, opened, and the quantity $\mathcal{R}$ measured on the system $\mathbf{S}_1$ or $\mathbf{S}_2$ or ... or $\mathbf{S}_N$ contained within it. Then the box is closed again, and according to whether the measured value of $\mathcal{R}$ is > 0 or < 0, the box, together with its contents penetrates the window or is reflected, with unchanged momentum. That this contrivance achieves the desired end is clear: it remains only to discuss what changes it brings about, and how closely it is related to the so-called "Maxwell demon" of thermodynamics.[194]

In the first place, it must be said that since the measurement (under certain circumstances) changes the energy state of **S**, and perhaps the energy expectation value also, this difference in mechanical energy must be added or absorbed by the measurement device (for example, by installing a spring which can be stretched or compressed, or something similar). Since the measurement device functions quite automatically, and since only mechanical (not heat!) energies are transformed, certainly no entropy changes occur—and it is at present only this which is of interest to us. (If **S** is in one of the states $\phi_1, \phi_2, \ldots, \psi_1, \psi_2, \ldots$ then the $\mathcal{R}$-measurement does not, in general, change **S**, and no compensating changes remain in the measurement apparatus.)

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[193] See, for example, the reference in Note 184.

[194] See the reference in Note 185. The reader will find a detailed discussion of the difficulties connected with "Maxwell's demon" in L. Szilard, Z. Physik **53** (1929).

The second point is more doubtful. Our arrangement is rather similar to "Maxwell's demon"; *i.e.*, to a semi-permeable wall which transmits molecules coming from the right but reflects those coming from the left. If we use such a wall to bisect a container filled with a gas, then all the gas is soon on the left hand side of the wall; *i.e.*, the volume is halved without entropy consumption. This means an uncompensated entropy increase of the gas, and therefore, by the second law of thermodynamics, such a wall cannot exist. Our semi-permeable wall is, however, essentially different from this thermodynamically unacceptable one, because reference is made with it only to the internal properties of the "molecules" $\mathbf{K}_1, \ldots, \mathbf{K}_N$ (*i.e.*, the state of the $\mathbf{S}_1$ or $\mathbf{S}_2$ or $\ldots$ or $\mathbf{S}_N$ enclosed therein) and not to the exterior (*i.e.*, whether the molecule comes from right or left, or something similar). And this is a decisive circumstance. A thoroughgoing analysis of this question was made possible by the researches of L. Szilard, which clarified the nature of the semi-permeable wall, "Maxwell's demon," and the general role of the "intervention of an intelligent being in thermodynamical systems." We cannot go further into these things here. And need not, since the reader can find a treatment of these topics in the reference cited in Note 194.

The preceding discussion shows, in particular, that two states ϕ, ψ can certainly be separated by a semi-permeable wall if they are orthogonal. We now want to prove the converse: If ϕ, ψ are not orthogonal then the assumed existence of such a wall would contradict the second law of thermodynamics. That is, the necessary and sufficient condition for separability by semi-permeable walls is $(\phi, \psi) = 0$ and not, as in classical theory, $\phi \neq \psi$ (here we write ϕ, ψ instead of the **I**, **II** used above). This clarifies an old paradox of classical thermodynamics, which has to do with a perplexing discontinuity in the operation of semi-permeable walls: states that differ however slightly are always 100% separable, but absolutely identical states are not separable! We now have a continuous transition: It will be seen that 100% separability is possible only if $(\phi, \psi) = 0$ and that as $|(\phi, \psi)|$ increases the situation with regard to separability becomes progressively worse, until at $|(\phi, \psi)| = 1$ (here $\|\phi\| = \|\psi\| = 1$, so $|(\phi, \psi)| = 1$ entails $\phi = c\psi$ with $|c| = 1$) the states ϕ, ψ are identical and separation becomes impossible.

In order to conduct these considerations we must anticipate the final result of this section: the value of the entropy of the U-ensemble. We will, of course, not use this result in its derivation.

Let us assume there is a semi-permeable wall separating ϕ from ψ. We shall then prove $(\phi, \psi) = 0$. We consider a $\frac{1}{2}(\mathsf{P}_{[\phi]} + \mathsf{P}_{[\psi]})$-gas (*i.e.*, a gas containing $\frac{1}{2}N$ systems in state ϕ and $\frac{1}{2}N$ systems in state ψ; note that $\mathrm{Tr}\frac{1}{2}(\mathsf{P}_{[\phi]} + \mathsf{P}_{[\psi]}) = 1$) and choose V (*i.e.*, $\overline{\mathbf{K}}$) and T so that the gas is ideal. Let $\overline{\mathbf{K}}$ have the cross section 1 2 3 4 1 shown in FIGURE 3. We insert a semi-permeable wall at one end aa, and then move it halfway, up to the center bb. The temperature of the gas is kept constant by contact with a large heat reservoir $\mathbf{W}$ of temperature T at the other end 2 3. In this process, nothing happens to the ϕ-molecules, but the ψ-molecules are pushed to the right half of $\overline{\mathbf{K}}$ (between bb and 2 3). That is, the $\frac{1}{2}(\mathsf{P}_{[\phi]} + \mathsf{P}_{[\psi]})$-gas is a 1:1 mixture of $\mathsf{P}_{[\phi]}$-gas and $\mathsf{P}_{[\psi]}$-gas. Nothing

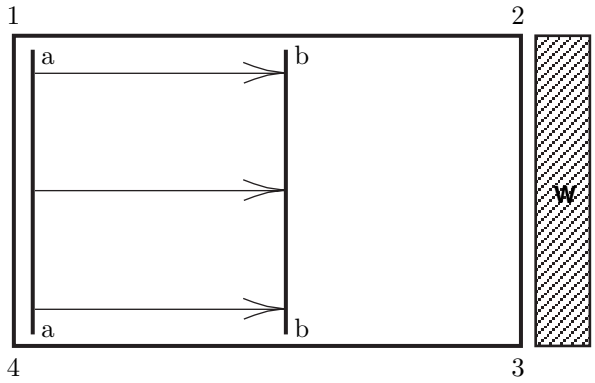

FIGURE 3: *Equal numbers of ϕ-molecules and ψ-molecules fill the cavity* $\overline{\mathsf{K}}$*, shown 1 2 3 4 in cross section. A semi-permeable wall—transparent to ϕ-molecules but opaque to ψ-molecules—is moved from position* aa *to position* bb*, with consequences developed in the text.* **W** *is a heat reservoir at temperature T. The process is isothermal.*

happens to the former, but the latter is isothermally compressed to one half of its original volume. From the equation of state of an ideal gas it follows that in this process an amount $\frac{1}{2}N\kappa T\ln 2$ of mechanical work is performed ($\frac{1}{2}N$ is the number of molecules of $\mathsf{P}_{[\psi]}$-gas, κ is Boltzmann's constant),[195] and since the energy of the gas is not changed (because the process is isothermal)[196] this energy is injected as heat into the reservoir **W**. The entropy change of the reservoir is then $Q/T = \frac{1}{2}N\kappa\ln 2$ (see Note 186).

After this process has been completed, half of the original $\mathsf{P}_{[\phi]}$-gas ($\frac{1}{4}N$ molecules) occupies the space to the left of the bb partition. The space to the right of the partition is, on the other hand, occupied by the other half of the $\mathsf{P}_{[\phi]}$-gas ($\frac{1}{4}N$ molecules) and the entire $\mathsf{P}_{[\psi]}$-gas ($\frac{1}{2}N$ molecules); *i.e.*, by $\frac{3}{4}N$ molecules of a $\frac{1}{3}\mathsf{P}_{[\phi]}+\frac{2}{3}\mathsf{P}_{[\psi]}$-gas. Now—by effectively turning off its permeability and isothermally repositioning the partition—we compress the gas on the left to volume $\frac{1}{4}V$ and expand the gas on the right to volume $\frac{3}{4}V$. The work done is

[195] If an ideal gas consists of n molecules, then its pressure is $p = n\kappa T/V$. In compression from volume V_1 to V_2 therefore mechanical work

$$\text{Work on gas} = -\int_{V_1}^{V_2} p\,dV = -n\kappa T\int_{V_1}^{V_2}\frac{dV}{V} = -n\kappa T\ln\frac{V_2}{V_1}$$

is done on the gas. In the present instance $n = \frac{1}{2}N$, $V_1 = \frac{1}{2}V$, $V_2 = V$.

[196] The energy of an ideal gas, as is well known, depends only on its temperature.

again taken from or given to the reservoir **W**: this amounts to $\frac{1}{4}N\kappa T\ln 2$ and $-\frac{3}{4}N\kappa T\ln\frac{3}{2}$, respectively (see Note 195), so the entropy increase of the reservoir is (respectively) $\frac{1}{4}N\kappa\ln 2$ and $-\frac{3}{4}N\kappa\ln\frac{3}{2}$. Altogether:

$$\tfrac{1}{2}N\kappa\ln 2+\left(\tfrac{1}{4}N\kappa\ln 2-\tfrac{3}{4}N\kappa\ln\tfrac{3}{2}\right)=N\kappa\tfrac{3}{4}\ln\tfrac{4}{3}$$

We have at this point a $\mathsf{P}_{[\phi]}$-gas and a $(\frac{1}{3}\mathsf{P}_{[\phi]}+\frac{2}{3}\mathsf{P}_{[\psi]})$-gas of $\frac{1}{4}N$ and $\frac{3}{4}N$ molecules respectively, occupying respective volumes $\frac{1}{4}V$ and $\frac{3}{4}V$. Originally we had a $(\frac{1}{2}\mathsf{P}_{[\phi]}+\frac{1}{2}\mathsf{P}_{[\psi]})$-gas of N molecules in volume V. Or, if we choose to think of it that way, two $(\frac{1}{2}\mathsf{P}_{[\phi]}+\frac{1}{2}\mathsf{P}_{[\psi]})$-gases of $\frac{1}{4}N$ and $\frac{3}{4}N$ molecules respectively, occupying respective volumes $\frac{1}{4}V$ and $\frac{3}{4}V$. The change effected by the entire process is then this: $\frac{1}{4}N$ molecules in volume $\frac{1}{4}V$ changed from a $(\frac{1}{2}\mathsf{P}_{[\phi]}+\frac{1}{2}\mathsf{P}_{[\psi]})$-gas into a $\mathsf{P}_{[\phi]}$-gas, $\frac{3}{4}N$ molecules in volume $\frac{3}{4}V$ changed from a $(\frac{1}{2}\mathsf{P}_{[\phi]}+\frac{1}{2}\mathsf{P}_{[\psi]})$-gas into a $(\frac{1}{3}\mathsf{P}_{[\phi]}+\frac{2}{3}\mathsf{P}_{[\psi]})$-gas, and the entropy of **W** increased by $N\kappa\cdot\frac{3}{4}\ln\frac{4}{3}$. Since the process was reversible, the total entropy increase must be zero; *i.e.*, the two gas-entropy changes must exactly compensate for the changed entropy of **W**. We must now find the entropy changes of the respective gases.

As we shall see, a U-gas of N molecules has entropy $-N\kappa\cdot\mathrm{Tr}(\mathsf{U}\ln\mathsf{U})$ if that of a $\mathsf{P}_{[\chi]}$-gas of equal volume and temperature is taken to be zero (see above). Therefore, if U has a pure discrete spectrum with eigenvalues $w_1, w_2, \ldots$, we have

$$\text{entropy}=-N\kappa\sum_{n=1}^{\infty}w_n\ln w_n$$

(where it is understood that $x\ln x$ is to be set equal to 0 at $x=0$). As can easily be calculated, $\mathsf{P}_{[\phi]}$, $(\frac{1}{2}\mathsf{P}_{[\phi]}+\frac{1}{2}\mathsf{P}_{[\psi]})$ and $(\frac{1}{3}\mathsf{P}_{[\phi]}+\frac{2}{3}\mathsf{P}_{[\psi]})$ have respectively the eigenvalues

$$\{1,0\}$$
$$\left\{\frac{1+\alpha}{2},\frac{1-\alpha}{2},0\right\}$$
$$\left\{\frac{3+\sqrt{1+8\alpha^2}}{6},\frac{3-\sqrt{1+8\alpha^2}}{6},0\right\}$$

where $\alpha=|(\phi,\psi)|$ (therefore $0\leqslant\alpha\leqslant 1$) and the multiplicity of 0 is always infinite but the non-zero eigenvalues are always simple.[197] Therefore the entropy

[197] We compute the eigenvalues of $a\mathsf{P}_{[\phi]}+b\mathsf{P}_{[\psi]}$. The requirement is

$$(a\mathsf{P}_{[\phi]}+b\mathsf{P}_{[\psi]})f=\lambda f$$

Since the left side is a linear combination of ϕ,ψ the right side is also, and therefore f is too if $\lambda\neq 0$. $\lambda=0$ is certainly an infinitely multiple eigenvalue, since every f orthogonal to ϕ,ψ belongs to it. It therefore suffices to assume $\lambda\neq 0$ and $f=x\phi+y\psi$ (we assume ϕ,ψ to be linearly independent; otherwise $\phi=c\psi$ with $|c|=1$ and the two states are identical). The above equation becomes

$$a(x+y(\psi,\phi))\cdot\phi+b(x(\phi,\psi)+y)\cdot\psi=\lambda x\cdot\phi+\lambda y\cdot\psi$$

of the gas has increased by

$$\begin{aligned}
&-\tfrac{1}{4}N\kappa\{1\ln 1+0\ln 0\}\\
&-\tfrac{3}{4}N\kappa\Big\{\frac{3+\sqrt{1+8\alpha^2}}{6}\ln\frac{3+\sqrt{1+8\alpha^2}}{6}+\frac{3-\sqrt{1+8\alpha^2}}{6}\ln\frac{3-\sqrt{1+8\alpha^2}}{6}\Big\}\\
&+\quad N\kappa\Big\{\frac{1+\alpha}{2}\ln\frac{1+\alpha}{2}+\frac{1-\alpha}{2}\ln\frac{1-\alpha}{2}\Big\}
\end{aligned}$$

(where the leading term vanishes). This should equal 0 when the entropy increase $N\kappa\frac{3}{4}\ln\frac{4}{3}$ of **W** is added to it. If we divide by $\frac{1}{4}N\kappa$ then we have

$$\begin{aligned}
&-\frac{3+\sqrt{1+8\alpha^2}}{2}\ln\frac{3+\sqrt{1+8\alpha^2}}{6}-\frac{3-\sqrt{1+8\alpha^2}}{2}\ln\frac{3-\sqrt{1+8\alpha^2}}{6}\\
&+2(1+\alpha)\ln\frac{1+\alpha}{2}+2(1-\alpha)\ln\frac{1-\alpha}{2}+3\ln\tfrac{4}{3}=0
\end{aligned}$$

where again: $0\leqslant\alpha\leqslant 1$.

Now it is easily seen that the expression on the left increases monotonically as α ranges from 0 to 1;[198] in fact the expression grows from 0 to $3\ln\frac{4}{3}$. We conclude that necessarily $\alpha=0$, for if it were otherwise then the process inverse

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whence

$$\begin{aligned}(a-\lambda)x+a\overline{(\phi,\psi)}y&=0\\ b(\phi,\psi)x+(b-\lambda)y&=0\end{aligned}$$

The determinant of these equations must vanish:

$$\begin{vmatrix}a-\lambda & a\overline{(\phi,\psi)}\\ b(\phi,\psi) & b-\lambda\end{vmatrix}=(a-\lambda)(b-\lambda)-ab|(\phi,\psi)|^2=0$$

i.e.,

$$\lambda^2-(a+b)\lambda+ab(1-\alpha^2)=0$$

$$\lambda=\frac{a+b\pm\sqrt{(a+b)^2-4ab(1-\alpha^2)}}{2}=\frac{a+b\pm\sqrt{(a-b)^2+4ab\alpha^2}}{2}$$

Setting $\{a,b\}=\{1,0\}$ or $\{\frac{1}{2},\frac{1}{2}\}$ or $\{\frac{1}{3},\frac{2}{3}\}$ we obtain the respective formulae given in the text.

[198] [By computer-assisted graphic display, or by the following argument:] From $(x\ln x)'=\ln x+1$ we have

$$\begin{aligned}\big(\tfrac{1+y}{2}\ln\tfrac{1+y}{2}+\tfrac{1-y}{2}\ln\tfrac{1-y}{2}\big)'&=\tfrac{1}{2}\big(\ln\tfrac{1+y}{2}+1\big)-\tfrac{1}{2}\big(\ln\tfrac{1-y}{2}+1\big)\\&=\tfrac{1}{2}\ln\tfrac{1+y}{1-y}\end{aligned}$$

so the α-derivative of our expression is

$$\begin{aligned}&-3\cdot\tfrac{1}{2}\ln\frac{3+\sqrt{1+8\alpha^2}}{3-\sqrt{1+8\alpha^2}}\cdot\tfrac{1}{3}\frac{8\alpha}{\sqrt{1+8\alpha^2}}+4\cdot\tfrac{1}{2}\ln\frac{1+\alpha}{1-\alpha}\\&=2\bigg(\ln\frac{1+\alpha}{1-\alpha}-\frac{2\alpha}{\sqrt{1+8\alpha^2}}\ln\frac{3+\sqrt{1+8\alpha^2}}{3-\sqrt{1+8\alpha^2}}\bigg)\end{aligned}$$

to that described would be entropy-decreasing, contrary to the second law. Thus have we proved that it is impossible for a semi-permeable wall to function in the manner contemplated above except in the case $(\phi, \psi) = 0$.

After these preparations we can proceed to the determination of the entropy of a U-gas of N molecules at temperature T; *i.e.*, more precisely, the entropy excess of such a gas with respect to the entropy of a $\mathsf{P}_{[\phi]}$-gas under similar conditions. By our earlier remarks, this is the entropy of a U-ensemble of N individual systems. Let $\mathrm{Tr}\mathsf{U} = 1$, as was done above.

The operator U, as we know, has a pure discrete spectrum $w_1, w_2, \ldots$ with $w_1 \geqslant 0, w_2 \geqslant 0, \ldots$ and $w_1 + w_2 + \cdots = 1$. Let the corresponding eigenfunctions be $\phi_1, \phi_2, \ldots$. Then (see **IV.3**)

$$\mathsf{U} = \sum_{n=1}^{\infty} w_n \mathsf{P}_{[\phi_n]}$$

Consequently, our gas is composed of a mixture of $\mathsf{P}_{[\phi_1]}, \mathsf{P}_{[\phi_2]}, \ldots$ gases of $w_1 N, w_2 N, \ldots$ molecules respectively, all in the volume V. Let T, V be such that all these gases are ideal, and let $\overline{\mathsf{K}}$ be of rectangular cross section. Now we will apply reversible interventions (described below: see FIGURE 4) to separate the $\phi_1, \phi_2, \ldots$ molecules from each other. We adjoin to $\overline{\mathsf{K}}$ (2 3 4 5 2) an equally large box $\overline{\mathsf{K}}'$ (1 2 5 6 1), and replace the common wall 2 5 by two contiguous walls. Let one (2 5) of those be fixed and semi-permeable—transparent for ϕ_1

That this is > 0 means that

$$\ln \frac{1+\alpha}{1-\alpha} > \frac{2\alpha}{\sqrt{1+8\alpha^2}} \ln \frac{3+\sqrt{1+8\alpha^2}}{3-\sqrt{1+8\alpha^2}}$$

i.e.,

$$\frac{1}{2\alpha} \ln \frac{1+\alpha}{1-\alpha} > \tfrac{2}{3} \cdot \frac{1}{2\beta} \ln \frac{1+\beta}{1-\beta} \qquad \text{where} \qquad \beta = \frac{\sqrt{1+8\alpha^2}}{3}$$

We shall prove the stronger inequality that results from replacing $\frac{2}{3}$ with $\frac{8}{9}$. Since $1-\beta^2 = \frac{8}{9}(1-\alpha^2)$ and $\alpha < \beta$ (which follows from the former since $\alpha < 1$) this means that

$$\frac{1-\alpha^2}{2\alpha} \ln \frac{1+\alpha}{1-\alpha} > \frac{1-\beta^2}{2\beta} \ln \frac{1+\beta}{1-\beta}$$

and this is proved if $\frac{1-x^2}{2x} \ln \frac{1+x}{1-x}$ is shown to be monotonically decreasing on the interval $0 < x < 1$. This last [graphically evident] property follows, however, from the power series expansion :

$$\begin{aligned} \tfrac{1-x^2}{2x} \ln \tfrac{1+x}{1-x} &= (1-x^2)(1 + \tfrac{1}{3}x^2 + \tfrac{1}{5}x^4 + \cdots) \\ &= 1 - (1 - \tfrac{1}{3})x^2 - (\tfrac{1}{3} - \tfrac{1}{5})x^4 - \cdots \end{aligned}$$

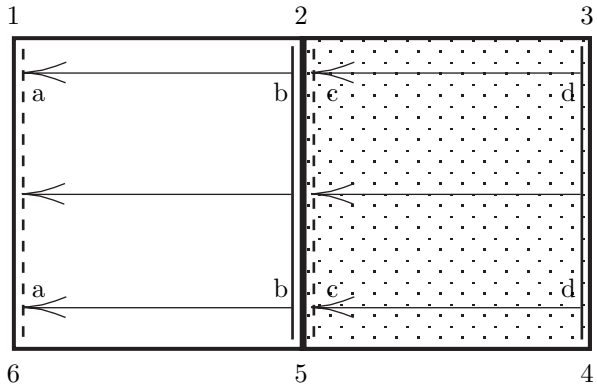

FIGURE 4: *A $(w_1, w_2, \ldots)$-weighted mixture of $(\phi_1, \phi_2, \ldots)$-gases is confined initially within box $\overline{\mathsf{K}}$ (2 3 4 5 2). Box $\overline{\mathsf{K}}'$ (1 2 5 6 1) has the same shape and volume as $\overline{\mathsf{K}}$, but is initially empty. Wall 2 5 is fixed, transparent to ϕ_1, opaque to all else. Wall bb is movable, but opaque to everything; it moves in synchrony with wall dd, which is opaque to ϕ_1, transparent to all else. Moving bb:dd to aa:cc has the effect of transporting all ϕ_1 molecules from $\overline{\mathsf{K}}$ to $\overline{\mathsf{K}}'$ without expenditure of either work or heat, while leaving the $\phi_1, \phi_2, \ldots$ molecules as undisturbed residents of $\overline{\mathsf{K}}$.*

but opaque for $\phi_2, \phi_3, \ldots$; let the other (bb) be movable, but ordinary in the sense that it is absolutely opaque to everything. In addition, we insert another semi-permeable wall dd—close to 3 4—which is transparent for $\phi_2, \phi_3, \ldots$ but opaque for ϕ_1. We now push bb and dd—keeping the distance between them constant—to aa and cc respectively (*i.e.*, close to 1 6 and 2 5 respectively). The $\phi_2, \phi_3, \ldots$ are not affected by this process, but the ϕ_1 are forced to remain between the moving walls bb and dd. Since the distance between these walls is kept constant, no work is done (against gas pressure), and no heat is developed. Finally, we replace the walls 2 5 and cc by a fixed impenetrable (*i.e.*, universally opaque) wall, and remove aa; in this way the boxes $\overline{\mathsf{K}}$, $\overline{\mathsf{K}}'$ are restored to their initial condition. There is, however, this change: all the ϕ_1 molecules reside now in $\overline{\mathsf{K}}'$. We have transferred all these from $\overline{\mathsf{K}}$ to $\overline{\mathsf{K}}'$ (a box of the same size), reversibly and without any work being done, without any evolution of heat or any temperature change.[199]

Similarly, we "tap off" the $\phi_2, \phi_3, \ldots$ molecules into boxes $\overline{\mathsf{K}}''$, $\overline{\mathsf{K}}'''$, ... (all of the same volume) and have finally $w_1 N$ molecules of $\mathsf{P}_{[\phi_1]}$-gas, $w_2 N$ molecules of $\mathsf{P}_{[\phi_2]}$-gas, ..., all at temperature T. Now we compress these isothermally to volumes $w_1 V, w_2 V, \ldots$ respectively, which requires investments of mechanical work $w_1 N\kappa T \ln w_1$, $w_2 N\kappa T \ln w_2$, ... and the transfer of those amounts of

[199] See, for example, the reference in Note 184 for an instance of this artifice, which is characteristic of the methods of phenomenological thermodynamics.

energy (as heat) to a reservoir (of temperature T, so that the process is reversible; the quantities of heat are all less than zero, since the amounts of work done in compressing the individual gases are the negatives of these values: see Note 191). The entropy increase for this process amounts to

$$\sum_{n=1}^{\infty} w_n N\kappa \ln w_n$$

Finally, we transform each of the $\mathsf{P}_{[\phi_1]}, \mathsf{P}_{[\phi_2]}, \ldots$ gases into a $\mathsf{P}_{[\phi]}$-gas (reversibly, with ϕ is some arbitrarily chosen state: see again the discussion on pages 234–5). We have then only $\mathsf{P}_{[\phi]}$-gases of $w_1 N, w_2 N, \ldots$ molecules in the respective volumes $w_1 V, w_2 V, \ldots$. Since all of these are identical, and of the same density N/V, we can mix them, and this also is reversible. We have then (since $\sum_{n=1}^{\infty} w_n = 1$) a $\mathsf{P}_{[\phi]}$-gas of N molecules in volume V.

We have at this point completed the desired reversible process. The entropy has increased by $N\kappa \sum_n w_n \ln w_n$ and since it must be zero in the final state it was

$$-N\kappa \sum_{n=1}^{\infty} w_n \ln w_n$$

in the initial state.

Since U has the eigenfunctions $\phi_1, \phi_2, \ldots$ with eigenvalues $w_1, w_2, \ldots$ the operator $\mathsf{U}\ln\mathsf{U}$ has the same eigenfunctions but eigenvalues $w_1 \ln w_1, w_2 \ln w_2, \ldots$ Consequently

$$\mathrm{Tr}(\mathsf{U}\ln\mathsf{U}) = \sum_{n=1}^{\infty} w_n \ln w_n$$

We observe that from $0 \leqslant w_n \leqslant 1$ it follows that $w_n \ln w_n \leqslant 0$, with equality only for $w_n = 0$ or 1; note also that for $w_n = 0$ we take $w_n \ln w_n$ to be zero, as follows from the fact that in the preceding discussion the vanishing w_n were not considered at all. One is led to those same conclusions by continuity considerations.

So we have determined that the entropy of a U-ensemble, consisting of N individual systems, is $-N\kappa\mathrm{Tr}(\mathsf{U}\ln\mathsf{U})$. The preceding remarks concerning $w_n \ln w_n$ establish that this is always $\geqslant 0$, and $= 0$ only if all w_n are either 0 or 1. From $\mathrm{Tr}\mathsf{U} = \sum_n w_n = 1$ it follows that in such cases only one $w_n = 1$ and all the others are 0, therefore $\mathsf{U} = \mathsf{P}_{[\phi]}$. That is, the states have entropy $= 0$, while mixtures have entropies > 0.

3. REVERSIBILITY AND EQUILIBRIUM PROBLEMS

We can now prove the irreversibility of the measurement process, as asserted in **V.1**. For example, if U is a state then $\mathsf{U} = \mathsf{P}_{[\phi]}$ and in the measurement of a quantity $\mathcal{R}$ whose operator R has the eigenfunctions $\phi_1, \phi_2, \ldots$ it goes over into the ensemble

$$\mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{P}_{[\phi]}\phi_n, \phi_n) \cdot \mathsf{P}_{[\phi_n]} = \sum_{n=1}^{\infty} |(\phi, \phi_n)|^2 \cdot \mathsf{P}_{[\phi_n]}$$

and if U' is not a state then an entropy increase has occurred (the entropy of U was 0, that of U' is > 0), so that the process is irreversible. If U' too is to be a state it must be a $\mathsf{P}_{[\phi]}$, and since the $\phi_1, \phi_2, \ldots$ are its eigenfunctions this means that all $|(\phi, \phi_n)|^2 = 0$ except one (that one being 1); *i.e.*, ϕ is orthogonal to all ϕ_n, $n \neq \bar{n}$. But then $\phi = c\phi_{\bar{n}}$ ($|c| = 1$), so $\mathsf{P}_{[\phi]} = \mathsf{P}_{[\phi_{\bar{n}}]}$, $\mathsf{U} = \mathsf{U}'$. Therefore every measurement on a state is irreversible unless the eigenvalue of the measured quantity (*i.e.*, the value of this quantity in the given state) has a sharp value, in which case the measurement does not change the state at all. As we see, the non-causal behavior here is unambiguously related to a certain concomitant thermodynamic phenomenon.

We shall now discuss in complete generality when the process **1**

$$\mathsf{U} \longrightarrow \mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n) \cdot \mathsf{P}_{[\phi_n]}$$

increases the entropy.

U has entropy $-N\kappa \mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$. If $w_1, w_2, \ldots$ are its eigenvalues and $\psi_1, \psi_2, \ldots$ its eigenfunctions then this can be written

$$-N\kappa \sum_{n=1}^{\infty} w_n \ln w_n = -N\kappa \sum_{n=1}^{\infty} (\mathsf{U}\psi_n, \psi_n) \ln (\mathsf{U}\psi_n, \psi_n)$$

U' has eigenvalues $(\mathsf{U}\phi_1, \phi_1), (\mathsf{U}\phi_2, \phi_2), \ldots$ and therefore its entropy is

$$-N\kappa \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n) \ln (\mathsf{U}\phi_n, \phi_n)$$

Consequently, the entropy of U is $\gtreqless$ that of U' according as

$$\star \qquad \sum_{n=1}^{\infty} (\mathsf{U}\psi_n, \psi_n) \ln (\mathsf{U}\psi_n, \psi_n) \gtreqless \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n) \ln (\mathsf{U}\phi_n, \phi_n)$$

We next show that in $\star$ $\geqslant$ holds in any case; *i.e.*, that the process $\mathsf{U} \to \mathsf{U}'$ is not entropy-diminishing; this is indeed clear thermodynamically, but it is important for our subsequent purposes to possess a purely mathematical proof of this fact. We proceed in such a way that U—and with it the $\psi_1, \psi_2, \ldots$—are fixed, while the $\phi_1, \phi_2, \ldots$ run through all complete orthonormal sets.

On continuity grounds we may limit ourselves to sets $\phi_1, \phi_2, \ldots$ in which only a finite number of ϕ_n are different from the corresponding ψ_n. Then, for example, $\phi_n = \psi_n$ for $n > M$. Then the $\phi_n, n \leqslant M$ are linear combinations of the $\psi_n, n \leqslant M$, and conversely:

$$\phi_m = \sum_{n=1}^{M} x_{mn}\psi_n \quad : \quad m = 1, 2, \ldots, M$$

where the M-dimensional matrix $\{x_{mn}\}$ is obviously unitary. We have

$$(\mathsf{U}\psi_m, \psi_m) = w_m$$

and, as can easily be calculated,

$$(\mathsf{U}\phi_m, \phi_m) = \sum_{n=1}^{M} w_n |x_{mn}|^2 \quad : \quad m = 1, 2, \ldots M$$

so that it is

$$\sum_{m=1}^{M} w_m \ln w_n \geqslant \sum_{m=1}^{M} \left(\sum_{n=1}^{M} w_n |x_{mn}|^2 \right) \ln \left(\sum_{n=1}^{M} w_n |x_{mn}|^2 \right)$$

that is to be proved. Since the expression on the right is a continuous function of the M^2 bounded variables x_{mn} it has a maximum, and also it actually assumes its maximum value ($\{x_{mn}\}$ is unitary!). It assumes the value of the expression on the left when

$$x_{mn} = \begin{cases} 1 & \text{for} \quad m = n \\ 0 & \text{for} \quad m \neq n \end{cases}$$

We show that matrix $\mathbb{X} = \{x_{mn}\} = \mathbb{I}$ is in fact the maximizer of the expression on the right.

To that end, let $\mathbb{X}^0 = \{x^0_{mn}\}$ where x^0_{mn} $(m, n = 1, 2, \ldots, M)$ is a set of values for which the maximum occurs. If we multiply $\mathbb{X}^0$ by the unitary matrix

$$\mathbb{A} = \begin{pmatrix} \alpha & \beta & 0 & \ldots & 0 \\ -\bar{\beta} & \bar{\alpha} & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & 1 \end{pmatrix} \quad : \quad |\alpha|^2 + |\beta|^2 = 1$$

we obtain a $\{x'_{mn}\}$ which is unitary, therefore an acceptable x_{mn}-complex. Now let $\alpha = \sqrt{1 - \epsilon^2}$, $\beta = \theta\epsilon$ (ϵ real and $|\theta| = 1$). We assume ϵ to be so small that we need only look to the $1, \epsilon, \epsilon^2$ terms and can neglect the $\epsilon^3, \epsilon^4, \ldots$ terms. Then $\alpha = 1 - \frac{1}{2}\epsilon^2$ and the elements x'_{mn} of the new matrix $\mathbb{X}' = \mathbb{A}\mathbb{X}$ become

$$\begin{aligned} x'_{1n} &\approx (1 - \tfrac{1}{2}\epsilon^2) x^0_{1n} + \theta\epsilon x^0_{2n} \\ x'_{2n} &\approx -\bar{\theta}\epsilon x^0_{1n} + (1 - \tfrac{1}{2}\epsilon^2) x^0_{2n} \\ x'_{mn} &= x^0_{mn} \quad : \quad m \geqslant 3 \end{aligned}$$

Therefore

$$\begin{aligned} \textstyle\sum_{n=1}^{M} w_n |x'_{1n}|^2 &\approx \textstyle\sum_{n=1}^{M} w_n |x^0_{1n}|^2 + \sum_{n=1}^{M} 2 w_n \Re(\bar{\theta} x^0_{1n} \bar{x}^0_{2n}) \cdot \epsilon \\ &\quad + \textstyle\sum_{n=1}^{M} w_n (-|x^0_{1n}|^2 + |x^0_{2n}|^2) \cdot \epsilon^2 \\ \textstyle\sum_{n=1}^{M} w_n |x'_{2n}|^2 &\approx \textstyle\sum_{n=1}^{M} w_n |x^0_{2n}|^2 - \sum_{n=1}^{M} 2 w_n \Re(\bar{\theta} x^0_{1n} \bar{x}^0_{2n}) \cdot \epsilon \\ &\quad - \textstyle\sum_{n=1}^{M} w_n (-|x^0_{1n}|^2 + |x^0_{2n}|^2) \cdot \epsilon^2 \\ \textstyle\sum_{n=1}^{M} w_n |x'_{mn}|^2 &= \textstyle\sum_{n=1}^{M} w_n |x^0_{mn}|^2 \quad : \quad m \geqslant 3 \end{aligned}$$

If we substitute these expressions into $f(x) = x \ln x$—which entails

$$f'(x) = \ln x + 1, \quad f''(x) = \tfrac{1}{x}$$

—and add the results together, we obtain

$$\begin{aligned}
&\sum_{m=1}^{M} \left(\sum_{n=1}^{M} w_n |x'_{mn}|^2 \right) \ln \left(\sum_{n=1}^{M} w_n |x'_{mn}|^2 \right) \\
&\approx \textstyle\sum_{n=1}^{M} \left(\sum_{n=1}^{M} w_n |x^0_{mn}|^2 \right) \ln \left(\sum_{n=1}^{M} w_n |x^0_{mn}|^2 \right) \cdot \epsilon^0 \\
&\quad + \left\{ \ln \left(\textstyle\sum_{n=1}^{M} w_n |x^0_{1n}|^2 \right) - \ln \left(\sum_{n=1}^{M} w_n |x^0_{2n}|^2 \right) \right\} \cdot \textstyle\sum_{n=1}^{M} 2 w_n \mathfrak{R}(\bar\theta x^0_{1n} \bar x^0_{2n}) \cdot \epsilon^1 \\
&\quad + \Bigg[- \left\{ \ln \left(\textstyle\sum_{n=1}^{M} w_n |x^0_{1n}|^2 \right) - \ln \left(\sum_{n=1}^{M} w_n |x^0_{2n}|^2 \right) \right\} \\
&\qquad\qquad \cdot \left\{ \left(\textstyle\sum_{n=1}^{M} w_n |x^0_{1n}|^2 \right) - \left(\sum_{n=1}^{M} w_n |x^0_{2n}|^2 \right) \right\} \\
&\qquad + \tfrac{1}{2} \left(\frac{1}{\sum_{n=1}^{M} w_n |x^0_{1n}|^2} + \frac{1}{\sum_{n=1}^{M} w_n |x^0_{2n}|^2} \right) \left(\textstyle\sum_{n=1}^{M} 2 w_n \mathfrak{R}(\bar\theta x^0_{1n} \bar x^0_{2n}) \right) \Bigg] \cdot \epsilon^2
\end{aligned}$$

For the expression on the right to be maximal the term of order ϵ^1 must vanish and the term of order ϵ^2 must be $\leqslant 0$. The first of those is the product of two factors,

$$\ln \left(\textstyle\sum_{n=1}^{M} w_n |x^0_{1n}|^2 \right) - \ln \left(\sum_{n=1}^{M} w_n |x^0_{2n}|^2 \right)$$

and

$$\textstyle\sum_{n=1}^{M} 2 w_n \mathfrak{R}(\bar\theta x^0_{1n} \bar x^0_{2n})$$

If the first of those is zero then the leading term in the ϵ^2-coefficient (which is always $\leqslant 0$) is also zero, so that the second term (which clearly is always $\geqslant 0$) must vanish in order that the entire coefficient be $\leqslant 0$. This means that

$$\textstyle\sum_{n=1}^{M} 2 w_n \mathfrak{R}(\bar\theta x^0_{1n} \bar x^0_{2n}) = 0$$

Therefore the second factor in the ϵ^1-coefficient must vanish in any event, which we may also express by writing

$$2\mathfrak{R}\left(\bar\theta \cdot \textstyle\sum_{n=1}^{M} w_n x^0_{1n} \bar x^0_{2n} \right) = 0$$

Since this goes over into absolute value of the $\sum_{n=1}^{M}$ for appropriate θ, we must have $\sum_{n=1}^{M} w_n x^0_{1n} \bar x^0_{2n} = 0$. And since we can replace the subscripts 1, 2 by any two different $k, j = 1, 2, \ldots, M$ we have

$$\sum_{n=1}^{M} w_n x^0_{kn} \bar x^0_{jn} = 0 \quad : \quad k \neq j$$

That is, the unitary coordinate transformation with the matrix $\{x^0_{mn}\}$ brings the diagonal matrix with elements $w_1, w_2, \ldots$ again into diagonal form. Since

the diagonal elements are the multipliers (or eigenvalues) of the matrix, they are not changed by the coordinate transformation, but are at most permuted. Before the transformation they were the w_m $(m = 1, \dots M)$; afterwards they are the $\sum_{n=1}^{M} w_n |x_{mn}^0|^2$ $(m = 1, \dots M)$. The sums

$$\sum_{m=1}^{M} w_m \ln w_m \quad \text{and} \quad \sum_{m=1}^{M} \left(\sum_{n=1}^{M} w_n |x_{mn}^0|^2 \right) \ln \left(\sum_{n=1}^{M} w_n |x_{mn}^0|^2 \right)$$

then have the same values. Hence there is at any rate a maximum at

$$x_{mn} = \begin{cases} 1 & \text{for} \quad m = n \\ 0 & \text{for} \quad m \neq n \end{cases}$$

as was asserted.

Let us determine when the equality holds in $\star$. If it does hold, then

$$\sum_{n=1}^{\infty} (\mathsf{U}\chi_n, \chi_n) \ln (\mathsf{U}\chi_n, \chi_n)$$

assumes its maximum value not only for $\chi_n = \psi_n$ $(n = 1, 2, \dots)$—these are the eigenfunctions of U (see above)—but also for $\chi_n = \phi_n$ $(n = 1, 2, \dots)$ with $\chi_1, \chi_2, \dots$ running through all complete orthonormal sets. This holds in particular if only the first M among the ϕ_n are transformed (*i.e.*, $\chi_n = \phi_n$ for $n > M$) and hence, of course, transformed unitarily among each other. Let $\mu_{mn} = (\mathsf{U}\phi_m, \phi_n)$ $(m, n = 1, \dots, M)$ and let $v_1, \dots, v_M$ be the eigenvalues of a finite-dimensional (Hermitian and definite) matrix $\{\mu_{mn}\}$, and let $\{\alpha_{mn}\}$ $(m, n = 1, \dots, M)$ be the matrix that transforms $\{\mu_{mn}\}$ to diagonal form. This transforms the $\phi_1, \dots, \phi_M$ into $\omega_1, \dots, \omega_M$:

$$\phi_m = \sum_{n=1}^{M} \alpha_{mn} \omega_n \quad : \quad m = 1, \dots, M$$

Then

$$\mathsf{U}\omega_n = v_n \omega_n \quad \text{and therefore} \quad (\mathsf{U}\omega_m, \omega_n) = \begin{cases} v_n & \text{for} \quad m = n \\ 0 & \text{for} \quad m \neq n \end{cases}$$

For

$$\xi_m = \sum_{n=1}^{M} x_{mn} \omega_n \quad : \quad m = 1, \dots, M \text{ and } \{x_{mn}\} \text{ unitary}$$

we have

$$(\mathsf{U}\xi_k, \xi_j) = \sum_{n=1}^{M} v_n x_{kn} \bar{x}_{jn}$$

Because of the assumption regarding the $\phi_1, \dots, \phi_M$ the expression

$$\sum_{m=1}^{M} \left(\sum_{n=1}^{M} v_n |x_{mn}|^2 \right) \ln \left(\sum_{n=1}^{M} v_n |x_{mn}|^2 \right)$$

takes on its maximum when $x_{mn} = \alpha_{mn}$. According to our previous proof, it

follows from this that

$$\sum_{n=1}^{M} v_n \alpha_{kn} \bar{\alpha}_{jn} = 0 \quad : \quad k \neq j$$

i.e., $(\mathsf{U}\phi_k, \phi_j) = 0$ for $k \neq j$ $(k, j = 1, \ldots M)$.

This must hold for all M, therefore $\mathsf{U}\phi_k$ is orthogonal to all ϕ_j, $k \neq j$, and hence it is equal to $w_k' \phi_k$ (w_k' a constant). Consequently, the $\phi_1, \phi_2, \ldots$ are eigenfunctions of U. The corresponding eigenvalues are $w_1', w_2', \ldots$ (and therefore a permutation of $w_1, w_2, \ldots$). Under these circumstances

$$\mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n) \cdot \mathsf{P}_{[\phi_n]} = \sum_{n=1}^{\infty} w_n' \cdot \mathsf{P}_{[\phi_n]} = \mathsf{U}$$

We have therefore found:

> The process **1**
>
> $$\mathsf{U} \longrightarrow \mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n) \cdot \mathsf{P}_{[\phi_n]}$$
>
> ($\phi_1, \phi_2, \ldots$ are the eigenfunctions of the operator R belonging to the measured quantity $\mathcal{R}$) never diminishes the entropy. Actually, it increases the entropy unless all $\phi_1, \phi_2, \ldots$ are eigenfunctions of U, in which case $\mathsf{U} = \mathsf{U}'$. Moreover, in the case just mentioned U commutes with R, and this is characteristic of that case (because it is equivalent to the existence of common eigenfunctions: see **II.10**). Hence the process **1** is irreversible in all cases in which it effects any change at all.

The reversibility question will now be treated for processes **1**, **2** by arguments that proceed independently of phenomenological thermodynamics, pursuant to the second point of the two-point program that was put forward at the beginning of section **V.2**. The mathematical method by which this can be accomplished we already know: if the second law of thermodynamics holds, the entropy must be equal to $-N\kappa \mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$, and this does not decrease in any process **1**, **2**. We now treat $-N\kappa \mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ merely as a calculated quantity—independently of its entropic meaning—and investigate how it responds to processes **1**, **2**.[200]

In **2** we have

$$\begin{aligned} \mathsf{U} \longrightarrow \mathsf{U}_t &= e^{-\frac{i}{\hbar} t \mathsf{H}} \mathsf{U} e^{\frac{i}{\hbar} t \mathsf{H}} \\ &= \mathsf{A}\mathsf{U}\mathsf{A}^{-1} \quad \text{with} \quad \mathsf{A} = e^{-\frac{i}{\hbar} t \mathsf{H}} \end{aligned}$$

Since $f \to \mathsf{A}f$, because of the unitary nature of A, is an isomorphic mapping of the Hilbert space on itself which transforms each operator P into $\mathsf{A}\mathsf{P}\mathsf{A}^{-1}$, it

[200] Naturally, we could neglect the factor $N\kappa$ and look only to $-\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$. Or to $-N\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ if we wish to preserve proportionality to the number N of elements.

is always the case that $F(\mathsf{APA}^{-1}) = \mathsf{A}F(\mathsf{P})\mathsf{A}^{-1}$. Consequently,

$$\mathsf{U}_t \ln \mathsf{U}_t = \mathsf{A} \cdot \mathsf{U} \ln \mathsf{U} \cdot \mathsf{A}^{-1}$$

Hence

$$\mathrm{Tr}(\mathsf{U}_t \ln \mathsf{U}_t) = \mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$$

i.e., our quantity $-N\kappa\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ is constant under **2**. We have already established what happens under **1**, and have in fact done so without reference to the second law of thermodynamics: if U changes (*i.e.*, $\mathsf{U} \neq \mathsf{U}'$) then $-N\kappa\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ increases, while for unchanged U (*i.e.*, $\mathsf{U} = \mathsf{U}'$, or $\psi_1, \psi_2, \ldots$ eigenfunctions of R, or U, R commutative) it naturally remains unchanged. In an intervention composed of several **1** and **2** (in arbitrary number and order) $-N\kappa\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ remains unchanged if each process **1** is ineffective (*i.e.*, causes no change), but in all other cases it increases.

Therefore, if only interventions **1**, **2** are taken into consideration, then each process **1** which effects any change at all is irreversible.

It is worth noting that there are other expressions—simpler than $\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$—which do not decrease under **1** and are constant under **2**. The largest eigenvalue of U provides an example. For **2** it is invariant, as are all the eigenvalues of U, while under **1** the eigenvalues $w_1, w_2, \ldots$ of U go over into the eigenvalues of U':

$$\textstyle\sum_{n=1}^{\infty} w_n |x_{1n}|^2, \quad \sum_{n=1}^{\infty} w_n |x_{2n}|^2, \quad \ldots$$

(see again the considerations earlier in this section). By the unitary nature of the matrix $\{x_{mn}\}$

$$\textstyle\sum_{n=1}^{\infty} |x_{1n}|^2 = 1, \quad \sum_{n=1}^{\infty} |x_{2n}|^2 = 1, \quad \ldots$$

so all these numbers are $\leqslant$ the largest w_n. (A maximal w_n exists since all $w_n \geqslant 0$ and $\sum_{n=1}^{M} w_n = 1$ entails $w_n \to 0$.) Now since it is possible so to change U that

$$-\mathrm{Tr}(\mathsf{U} \ln \mathsf{U}) = -\textstyle\sum_{n=1}^{\infty} w_n \ln w_n$$

remains invariant but that the largest w_m decreases, we see that these are changes which are possible according to phenomenological thermodynamics—therefore they can actually be executed by our gas processes—but which can never be brought about by successive applications of **1**, **2** alone. This proves that our introduction of gas processes was indeed necessary.

Instead of $-\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ we could also consider $\mathrm{Tr}(F(\mathsf{U}))$ for appropriate functions $F(x)$. That this increases under **1** when $\mathsf{U} \neq \mathsf{U}'$ (for $\mathsf{U} = \mathsf{U}'$, as well as under **2**, it is of course invariant) can be proved, as was done for $F(x) = -x \ln x$, if the special properties of this function of which we made use also pertain to $F(x)$. These are: $F''(x) < 0$ and the monotonic decrease of $F'(x)$, but the latter follows from the former. Therefore, for our non-thermodynamic irreversibility considerations we could use any $\mathrm{Tr}(F(\mathsf{U}))$ in

which $F(x)$ is convex from above (meaning $F''(x) < 0$) on the interval $0 \leqslant x \leqslant 1$ which contains all the eigenvalues of U.

Finally, it should be shown that the mixing of two ensembles U, V (say in the ratio $\alpha : \beta$, $\alpha > 0$, $\beta > 0$, $\alpha + \beta = 1$) is also not entropy-diminishing

$$-\mathrm{Tr}\big((\alpha\mathsf{U} + \beta\mathsf{V}) \ln(\alpha\mathsf{U} + \beta\mathsf{V})\big) \geqslant -\alpha\mathrm{Tr}(\mathsf{U} \ln \mathsf{U}) - \beta\,\mathrm{Tr}(\mathsf{V} \ln \mathsf{V})$$

and that this also holds when $-x \ln x$ is replaced by any convex $F(x)$. The proof is left to the reader.

We turn now to an investigation of the stationary equilibrium distribution; *i.e.*, the mixture of maximum entropy, when the energy is given. The latter is, of course, to be understood to mean that the expectation value of the energy is prescribed: only this interpretation is admissible in view of the method indicated in Note 184 for the thermodynamical investigation of statistical ensembles. Consequently, only such mixtures will be allowed for the U of which $\mathrm{Tr}\mathsf{U} = 1$ and $\mathrm{Tr}\mathsf{U}\mathsf{H} = E$, where H is the energy operator and E is the prescribed energy expectation value. Under these auxiliary conditions, $-N\kappa\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ is to be made a maximum. We also make the simplifying assumption that H has a pure discrete spectrum, with eigenvalues $W_1, W_2, \ldots$ (some of which may be multiple) and eigenfunctions $\phi_1, \phi_2, \ldots$.

Let $\mathcal{R}$ be a quantity whose operator R has the same eigenfunctions $\phi_1, \phi_2, \ldots$ as H but only distinct (or simple) eigenvalues. Measurement of $\mathcal{R}$ transforms U (by **2**) into

$$\mathsf{U}' = \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n)\mathsf{P}_{[\phi_n]}$$

and therefore $-N\kappa\mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$ increases unless $\mathsf{U} = \mathsf{U}'$. Also, $\mathrm{Tr}\mathsf{U}$ and $\mathrm{Tr}\mathsf{U}\mathsf{H}$ do not change—the latter because the ϕ_n are eigenfunctions of H, and therefore $(\mathsf{H}\phi_m, \phi_n)$ vanishes for $m \neq n$:

$$\begin{aligned}
\mathrm{Tr}(\mathsf{U}'\mathsf{H}) &= \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n)\mathrm{Tr}(\mathsf{P}_{[\phi_n]}\mathsf{H}) \\
&= \sum_{n=1}^{\infty} (\mathsf{U}\phi_n, \phi_n)(\mathsf{H}\phi_n, \phi_n) \\
&= \sum_{m,n=1}^{\infty} (\mathsf{U}\phi_m, \phi_n)(\mathsf{H}\phi_n, \phi_m) = \mathrm{Tr}(\mathsf{U}\mathsf{H})
\end{aligned}$$

as follows also from the commutativity of R and H (*i.e.*, from the simultaneous measurability of $\mathcal{R}$ and energy). Consequently, the desired maximum is the same if we limit ourselves to such U'; *i.e.*, to statistical operators with eigenfunctions $\phi_1, \phi_2, \ldots$. And furthermore, it is assumed only among these.

Therefore

$$\mathsf{U} = \sum_{n=1}^{\infty} w_n \mathsf{P}_{[\phi_n]}$$

and—since U, UH and $\mathsf{U}\ln\mathsf{U}$ all have the same eigenfunctions ϕ_n but the respective eigenvalues w_n, $w_n W_n$ and $w_n \ln w_n$—it suffices to make

$$-N\kappa \sum_{n=1}^{\infty} w_n \ln w_n$$

a maximum, subject to the auxiliary conditions

$$\sum_{n=1}^{\infty} w_n = 1 \qquad \text{and} \qquad \sum_{n=1}^{\infty} w_n W_n = E$$

This is exactly the same problem as that which is encountered in connection with the corresponding equilibrium problem in ordinary gas theory,[201] and is solved in the same way. According to the well-known procedure for extremum calculations, we must solve

$$\frac{\partial}{\partial w_n}\Big(\sum_{m=1}^{\infty} w_m \ln w_m\Big) + \alpha \frac{\partial}{\partial w_n}\Big(\sum_{m=1}^{\infty} w_m\Big) + \beta \frac{\partial}{\partial w_n}\Big(\sum_{m=1}^{\infty} w_m W_m\Big) = 0$$

in which α, β are suitable constants (Lagrange multipliers) and $n = 1, 2, \ldots$. That is,

$$(\ln w_n + 1) + \alpha + \beta W_n = 0$$

whence

$$w_n = e^{-1-\alpha-\beta W_n} = a e^{-\beta W_n} \quad \text{where} \quad a = e^{-1-\alpha}$$

From $\sum_{n=1}^{\infty} w_n = 1$ it follows that

$$a = \frac{1}{\sum_{n=1}^{\infty} e^{-\beta W_n}}$$

and therefore

$$w_n = \frac{e^{-\beta W_n}}{\sum_{m=1}^{\infty} e^{-\beta W_m}}$$

And because of $\sum_{n=1}^{\infty} w_n W_n = E$ we have

$$\frac{\sum_{n=1}^{\infty} W_n e^{-\beta W_n}}{\sum_{m=1}^{\infty} e^{-\beta W_m}} = E$$

which determines β. If, as is customary, we introduce the "partition function"

$$Z(\beta) = \sum_{n=1}^{\infty} e^{-\beta W_n} = \mathrm{Tr}(e^{-\beta \mathsf{H}})$$

[201] See, for example, Planck, *Theorie der Wärmstrahlung*, Leipzig, 1913.

(see Notes 183, 184 for this and the following) then

$$Z'(\beta) = -\sum_{n=1}^{\infty} W_n e^{-\beta W_n} = -\mathrm{Tr}(\mathsf{H}e^{-\beta \mathsf{H}})$$

and the condition that determines β becomes

$$-\frac{Z'(\beta)}{Z(\beta)} = E$$

(We are making the assumption here that $\sum_{n=1}^{\infty} e^{-\beta W_n}$ and $\sum_{n=1}^{\infty} W_m e^{-\beta W_n}$ converge for all $\beta > 0$; *i.e.*, that $W_n \to \infty$ for $n \to \infty$, and that in fact they do so with sufficient rapidity: for example, $W_n / \ln n \to \infty$ suffices.) We then obtain the following expressions for U itself:

$$\mathsf{U} = \sum_{n=1}^{\infty} a e^{-\beta W_n} \mathsf{P}_{[\phi_n]} = a e^{-\beta \mathsf{H}} = \frac{e^{-\beta \mathsf{H}}}{\mathrm{Tr}(e^{-\beta \mathsf{H}})} = \frac{e^{-\beta \mathsf{H}}}{Z(\beta)}$$

The properties of the equilibrium ensemble U (which is determined by the values of E or of β, and which therefore depends on a parameter, as it must) can now be determined by methods customary in gas theory.

The entropy of our equilibrium ensemble is

$$\begin{aligned} S = -N\kappa \mathrm{Tr}(\mathsf{U} \ln \mathsf{U}) &= -N\kappa \mathrm{Tr}\Big(\frac{e^{-\beta \mathsf{H}}}{Z(\beta)} \ln \frac{e^{-\beta \mathsf{H}}}{Z(\beta)}\Big) \\ &= -\frac{N\kappa}{Z(\beta)} \mathrm{Tr}\big[e^{-\beta \mathsf{H}}\big(-\beta \mathsf{H} - \ln Z(\beta)\big)\big] \\ &= \frac{\beta N \kappa}{Z(\beta)} \mathrm{Tr}(\mathsf{H}e^{-\beta \mathsf{H}}) + \frac{N\kappa \ln Z(\beta)}{Z(\beta)} \mathrm{Tr}(e^{-\beta \mathsf{H}}) \\ &= N\kappa \Big[-\beta \frac{Z'(\beta)}{Z(\beta)} + \ln Z(\beta)\Big] \end{aligned}$$

and the total energy is

$$NE = -N \frac{Z'(\beta)}{Z(\beta)}$$

(This—not E itself—is to be considered in conjunction with S.) Thus U, S and NE are expressed as functions of β. Instead of inverting the last equation (*i.e.*, expressing β as a function of E) it is more practical to determine the temperature T of the equilibrium mixture, and to reduce everything to this. This is done as follows:

Our equilibrium mixture is brought into contact with a heat reservoir of temperature T' and energy $N dE$ is transferred to it from that reservoir. The two laws of thermodynamics require, then, that the total energy must remain unchanged, and that the entropy must not decrease. Consequently, the heat

reservoir loses the energy NdE and therefore its entropy increase is $-NdE/T'$, and we must now have

$$dS - \frac{NdE}{T'} = \Big(\frac{1}{N}\frac{dS}{dE} - \frac{1}{T'}\Big)NdE \geqslant 0$$

On the other hand, $NdE \gtrless 0$ must hold according to whether $T' \gtrless T$ because the colder body absorbs energy from the warmer. Consequently $T' \gtrless T$ implies

$$\frac{1}{N}\frac{dS}{dE} - \frac{1}{T'} \gtrless 0$$

i.e.,

$$T' \gtrless N\frac{dE}{dS} = \frac{N\frac{dE}{d\beta}}{\frac{dS}{d\beta}}$$

Hence

$$T = \frac{N\frac{dE}{d\beta}}{\frac{dS}{d\beta}} = -\frac{1}{\kappa}\frac{\big(\frac{Z'(\beta)}{Z(\beta)}\big)'}{\big(\ln Z(\beta) - \beta\frac{Z'(\beta)}{Z(\beta)}\big)'}$$
$$= -\frac{1}{\kappa}\frac{\big(\frac{Z'(\beta)}{Z(\beta)}\big)'}{-\beta\big(\frac{Z'(\beta)}{Z(\beta)}\big)'} = \frac{1}{\kappa\beta}$$

i.e.,

$$\beta = \frac{1}{\kappa T}$$

which we can use to express U, S and NE as functions of temperature.

The similarity of the expressions obtained above for the entropy, equilibrium ensemble, etc. to the corresponding results of classical thermodynamical theory is striking. Look first to the entropy $-N\kappa\mathrm{Tr}(\mathsf{U}\ln\mathsf{U})$:

$$\mathsf{U} = \sum_{n=1}^{\infty} w_n \mathsf{P}_{[\phi_n]}$$

refers to a mixture of ensembles $\mathsf{P}_{[\phi_1]}, \mathsf{P}_{[\phi_2]}, \ldots$ with relative weights $w_1, w_2, \ldots$; *i.e.*, Nw_1 ϕ_1-systems, Nw_2 ϕ_2-systems, ... The Boltzmann entropy of this ensemble is obtained with the aid of the "thermodynamic probability"

$$\frac{N!}{(Nw_1)!(Nw_2)!\cdots}$$

It is the "κ-fold logarithm."[201] Since N is large, we may approximate the factorials by the Stirling formula $x! \approx \sqrt{2\pi x}\,e^{-x}x^x$ and then $\frac{N!}{(Nw_1)!(Nw_2)!\cdots}$ becomes essentially

$$-N\kappa\sum_{n=1}^{\infty} w_n \ln w_n$$

—and this is exactly $-N\kappa\mathrm{Tr}(\mathsf{U}\ln\mathsf{U})$.

Consider now the equilibrium ensemble

$$\mathsf{U} = e^{-\mathsf{H}/\kappa T}$$

(we neglect the normalization factor $1/Z(\beta)$), which can be written

$$\sum_{n=1}^{\infty} e^{-W_n/\kappa T}\mathsf{P}_{[\phi_n]}$$

and refers therefore to a mixture of states $\mathsf{P}_{[\phi_1]}, \mathsf{P}_{[\phi_2]}, \ldots$; *i.e.*, of stationary states with energies $W_1, W_2, \ldots$ with the respective (relative) weights

$$e^{-W_1/\kappa T}, \quad e^{-W_2/\kappa T}, \quad \ldots$$

If an energy value is multiple, say $W_{n_1} = W_{n_2} = \cdots = W_{n_\nu} = W$, then

$$\mathsf{P}_{[\phi_{n_1}]} + \mathsf{P}_{[\phi_{n_2}]} + \cdots + q\mathsf{P}_{[\phi_{n_\nu}]}$$

appears in the equilibrium ensemble with weight $e^{-W/\kappa T}$, which is to say: in the correctly normalized mixture

$$\tfrac{1}{\nu}\left(\mathsf{P}_{[\phi_{n_1}]} + \mathsf{P}_{[\phi_{n_2}]} + \cdots + q\mathsf{P}_{[\phi_{n_\nu}]}\right)$$

appears (see the beginning of **IV.3**) with weight $\nu e^{-W/\kappa T}$. But the classical "canonical ensemble" is—apart from the appearance of the specifically quantum mechanical construct $\frac{1}{\nu}\left(\mathsf{P}_{[\phi_{n_1}]} + \mathsf{P}_{[\phi_{n_2}]} + \cdots + q\mathsf{P}_{[\phi_{n_\nu}]}\right)$—defined in exactly the same way: this is known as Boltzmann's Theorem.[201]

For $T \to 0$ the weights $e^{-W_n/\kappa T}$ approach 1, and therefore our U tends to

$$\sum_{n=1}^{\infty} \mathsf{P}_{[\phi_n]} = \mathsf{I}$$

Consequently, $\mathsf{U} \approx \mathsf{I}$ is the absolute equilibrium state if no energy restrictions apply—a result we had obtained already in **IV.3**. We see that the "*a priori* equal probability of the quantum orbits" (*i.e.*, of the simple non-degenerate ones—in general the multiplicity of the eigenvalues is the *a priori* weight: see discussion above) follows automatically from this theory.

It remains to ascertain how much can be said non-thermodynamically about the equilibrium ensemble U of a given energy; *i.e.*, what can be deduced only from the fact that U is stationary (does not change in the course of time, under process **2**), and that it remains unchanged in all measurements which do not affect the energy (*i.e.*, measurements of quantities $\mathcal{R}$ that are, under process **1**, measurable simultaneously with energy, and that correspond therefore to operators R that commute with H and have the same eigenfunctions $\phi_1, \phi_2, \ldots$ as H).

Because of the differential equation $\frac{\partial}{\partial t}\mathsf{U} = \frac{i}{\hbar}(\mathsf{UH}-\mathsf{HU})$ the former condition requires only that H, U commute. The latter condition means that if $\phi_1, \phi_2, \ldots$ comprise a complete eigenfunction set of H then $\mathsf{U} = \mathsf{U}'$. Let the corresponding eigenvalues of H be $W_1, W_2, \ldots$ and those of U be $w_1, w_2, \ldots$. If $W_j = W_k$ we can replace ϕ_j, ϕ_k by

$$\frac{\phi_j + \phi_k}{\sqrt{2}}, \quad \frac{\phi_j - \phi_k}{\sqrt{2}}$$

for H. These, therefore, are also eigenfunctions of U, from which it follows that $w_j = w_k$. Therefore, a function $F(x)$ with $F(W_n) = w_n$ $(n = 1, 2, \ldots)$ can be constructed, and $F(\mathsf{H}) = \mathsf{U}$. It is clear that this is sufficient, and that it implies the commutativity of H and U.

So we have $\mathsf{U} = F(\mathsf{H})$, but no specific form is assigned to $F(x)$. In particular, the result

$$F(x) = \frac{1}{Z(\beta)} e^{-\beta x} \quad : \quad \beta = \frac{1}{\kappa T}$$

we achieved by other means is not enforced. From $\mathrm{Tr}\mathsf{U} = 1$ and $\mathrm{Tr}(\mathsf{UH}) = 1$ it follows that

$$\sum_{n=1}^{\infty} F(W_n) = 1 \quad \text{and} \quad \sum_{n=1}^{\infty} W_n F(W_n) = E$$

but with this, all that this method can supply is exhausted.

4. THE MACROSCOPIC MEASUREMENT

Although our entropy expression is, as we saw, completely analogous to classical entropy, it is still surprising that it is invariant under normal temporal evolution of the system (process **2**), and increases only in consequence of measurements (process **1**). In classical theory—where measurements in general played no role—its increase, as a rule, resulted from the ordinary mechanical evolution of the system. It is incumbent upon us to clear up this apparently paradoxical situation.

A familiar classical thermodynamic argument runs as follows: Imagine a container of volume V which is bisected by a partition. On one side of the partition are M molecules of gas (assumed, for simplicity, to be an ideal gas) at temperature T. We allow the gas to expand isothermally and reversibly $\frac{1}{2}V \to V$ by pushing against the partition, doing work which we utilize, and remaining isothermal by drawing heat from a large heat reservoir at temperature T. The entropy of the reservoir decreases by $M\kappa \ln 2$ (see Note 195), and therefore the entropy of the gas increases by that same amount. If, on the other hand, we had simply removed (or punctured) the partition the gas would have diffused into the (previously empty) other half of the enclosure; the gas entropy would again have increased by $M\kappa \ln 2$, but now without any corresponding entropy compensation taking place. The process is consequently irreversible, for the

entropy has increased in the course of the simple temporal evolution of the system (diffusion). Why does our theory give nothing similar?

The situation is best clarified if we set $M = 1$. Thermodynamics is still valid for such a one-molecule gas, and it is true that its entropy increases by $\kappa \ln 2$ if its volume is doubled. Nevertheless, this difference is actually $\kappa \ln 2$ only if one knows no more about the molecule than that it was found initially in volume $\frac{1}{2}V$ and later in volume V. For example, if the molecule is in the volume V but it is known whether it is on the right or left side of the middle of the enclosure, then we could insert a partition in the middle and allow this to be pushed by the molecule (isothermally and reversibly) to (respectively) the left or right end of the cylindrical enclosure. During this process, mechanical work $\kappa T \ln 2$ is performed; *i.e.*, this amount of energy is drawn from the reservoir. Consequently, at the end of the process the molecule is again in volume V, but we no longer know whether it is left or right of the middle and there has been a compensating entropy decrease of $\kappa \ln 2$ (in the reservoir). That is, we have exchanged our knowledge for the entropy decrease $\kappa \ln 2$.[202] Or: the entropy is the same in volume V as in volume $\frac{1}{2}V$, provided we know, in the first-mentioned case, in which half of the enclosure the molecule is to be found. Therefore, if we knew all the properties (position and momentum) of the molecule before the diffusion process was initiated we could calculate at each subsequent moment whether it is on left or right, and entropy would not have changed. If, however, the only information at our disposal were the macroscopic information that the molecule was initially in the right (or left) half of the enclosure, then entropy would increase upon diffusion.

For a classical observer, who knows all coordinates and momenta, the entropy is therefore constant, and is in fact 0, since the Boltzmann "thermodynamic probability" is 1 (see the reference in Note 201)—just as in our theory for states $\mathsf{U} = \mathsf{P}_{[\phi]}$, since these again correspond to the highest possible state of knowledge of the observer, relative to the system.

The time-variations of entropy are based then on the fact that the observer does not know everything—that he cannot find out (measure) everything that is measurable in principle. His senses allow him to perceive only the so-called macroscopic quantities. But this clarification of the apparent contradiction mentioned at the outset imposes upon us an obligation to investigate the precise analog of classical macroscopic entropy for quantum mechanical ensembles; *i.e.*, the entropy as seen by an observer who cannot measure all quantities, but only a few special quantities, namely, the macroscopic ones. And even

[202] L. Szilard (see the reference in Note 194) has shown that one cannot get this "knowledge" without a compensating entropy increase $\kappa \ln 2$. In general, $\kappa \ln 2$ is the "thermodynamic value" of knowledge which takes the form of distinguishing between two alternative cases. All attempts to carry out the process described above without knowledge of in which half of the enclosure the molecule is initially located can be shown to be invalid, though they may occasionally lead to very complicated automatic mechanisms.

these, under certain circumstances, with only limited accuracy.

In **III.3** we learned that all measurements of limited accuracy can be replaced by absolutely accurate measurement of other quantities which are functions of them, and which have discrete spectra. Now if $\mathcal{R}$ is such a quantity, and R its operator, and if $\lambda^{(1)}, \lambda^{(2)}, \ldots$ are the distinct eigenvalues, then the measurement of $\mathcal{R}$ is equivalent to answering the following questions:

$$\text{“Is } \mathcal{R} = \lambda^{(1)}\text{?”}, \quad \text{“Is } \mathcal{R} = \lambda^{(2)}\text{?”}, \quad \ldots$$

In fact, we can also say directly: Assume that $\mathcal{S}$, with operator S, is to be measured with limited accuracy—say that one wishes to determine within which of the intervals $c_{n-1} < \lambda \leqslant c_n$ $(\cdots c_{-2} < c_{-1} < c_0 < c_1 < c_2 < \cdots)$ it lies. This becomes a case of answering these questions:

$$\text{“Does } \mathcal{S} \text{ lie in } c_{n-1} < \lambda \leqslant c_n\text{?”} \quad : \quad n = 0, \pm 1, \pm 2, \ldots$$

Now, such questions correspond, by **III.5**, to projections E whose quantities $\mathfrak{E}$ (which have only two values: 0 or 1) are actually to be measured. In our examples, the $\mathfrak{E}$ are the functions $F_n(\mathcal{R})$, $n = 1, 2, \ldots$ in which

$$F_n(\lambda) = \begin{cases} 1 & \text{for} \quad \lambda = \lambda^{(n)} \\ 0 & \text{otherwise} \end{cases}$$

or the functions $G_n(\mathcal{S})$, $n = 0, \pm 1, \pm 2, \ldots$ in which

$$G_n(\lambda) = \begin{cases} 1 & \text{for} \quad c_{n-1} < \lambda \leqslant c_n \\ 0 & \text{otherwise} \end{cases}$$

and the corresponding E are $F_n(\mathsf{R})$ or $G(\mathsf{S})$, respectively. Therefore, instead of giving the macroscopically measurable quantities $\mathcal{S}$ (together with statements of the macroscopically attainable measurement precision), we may equivalently give the questions $\mathfrak{E}$ that are answered by the macroscopic measurements, or their projections E (see **III.5**). Characterization of the macroscopic observer comes therefore to this: specification of his E. (Thus, classically, one might characterize him by stating that he can measure temperature and pressure in each cm^3 of the gas volume—perhaps with certain precision limitations—but nothing else.[203])

Let us consider the method by which two non-simultaneously measurable quantities (for example: the coordinate q and the momentum p; see **III.4**) can be measured simultaneously with limited precision. Let the mean errors be ϵ, η respectively (according to the uncertainty principle $\epsilon\eta \sim h$). The discussion in **III.4** showed that with such limited precision requirements such measurements are indeed possible: the q (position) measurement is performed with light wave lengths that are not too short, and the p (momentum) measurement is performed with light wave trains that are not too long. If everything is

[203] This characterization of the macroscopic observer is due to E. Wigner.

properly arranged, then the actual measurements consist in detecting two light quanta in some way (perhaps by means of photographic plates): one (in the q measurement) is the light quantum scattered by the Compton effect; the other (in the p measurement) is reflected, changed in frequency (by the Doppler effect) and then (to measure that changed frequency) deflected by an optical device (prism, diffraction grating). By the end of the experiment, two light quanta have produced two black spots on two photographic plates, and from the locations of the spots (directions of the light quanta) we can calculate q and p. We must emphasize here that nothing prevents us from determining (with arbitrary precision) the locations of the spots (directions of the light quanta), because these are obviously simultaneously measurable (they are coordinates of two different objects). However, excessive precision at this point is not of much help for the measurement of q and p. As was shown in **III.4**, the relation of the spot-coordinates to q and p is such that the uncertainties ϵ, η persist, even if the spot-coordinates are measured with arbitrarily great precision, and the apparatus cannot be arranged so that $\epsilon\eta \ll h$.

Therefore, if we introduce the spot-coordinates themselves (or directions of the light quanta) as physical quantities (with operators Q', P') then we see that Q', P' are commutative, but the operators Q, P belonging to q, p can be described in terms of them with no higher precision than ϵ, η respectively. Let the quantities belonging to Q', P' be q', p'. The interpretation that the actual macroscopically measurable quantities are not the q, p themselves but are in fact q', p' is a very plausible one (it is, indeed, the q', p' that are in fact measured), and it is in accord with our postulated simultaneous measurability of all macroscopic quantities.

It is reasonable to attribute to this result a general significance, and to view it as disclosing a characteristic of the macroscopic method of observation. According to this, the macroscopic procedure consists of replacing all possible operators $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$, which as a rule do not commute with each other, by other operators $\mathsf{A}', \mathsf{B}', \mathsf{C}', \ldots$ (of which these are functions to within a certain approximation) which do commute with each other. Since we can just as well denote these functions of $\mathsf{A}', \mathsf{B}', \mathsf{C}', \ldots$ themselves by $\mathsf{A}', \mathsf{B}', \mathsf{C}', \ldots$, we may say this: the $\mathsf{A}', \mathsf{B}', \mathsf{C}', \ldots$ are approximations to the $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$, but commute exactly with each other. If the respective numbers $\epsilon_{\mathsf{A}}, \epsilon_{\mathsf{B}}, \epsilon_{\mathsf{C}}, \ldots$ give measure to the magnitudes of $\mathsf{A}' - \mathsf{A}, \mathsf{B}' - \mathsf{B}, \mathsf{C}' - \mathsf{C}, \ldots$ then we see that $\epsilon_{\mathsf{A}}\epsilon_{\mathsf{B}}$ will give order of magnitude measure to $\mathsf{AB} - \mathsf{BA}$ (generally $\neq 0$), etc. This sets the limit on the approximations that can be achieved. It is, of course, advisable when enumerating the $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ to restrict oneself to those operators whose physical quantities are accessible to macroscopic observation, at least to within a reasonable approximation.

These wholly qualitative observations remain an empty program so long as we cannot show that they require only things that are mathematically practicable. Therefore, for the characteristic case Q, P, we shall discuss further the question of the existence of the above Q', P' on a mathematical basis. For this purpose, let ϵ, η be two positive numbers with $\epsilon\eta = \frac{1}{2}\hbar$. We seek two

commuting Q', P' such that $\mathsf{Q}' - \mathsf{Q}, \mathsf{P}' - \mathsf{P}$ have (in a sense still to be defined more precisely) the respective orders of magnitude ϵ, η.

We do this with quantities q', p' which are measurable with perfect precision; *i.e.*, Q', P' have pure discrete spectra. Since they commute there is a complete orthonormal set $\phi_1, \phi_2, \ldots$ of eigenfunctions common to both (see **II.10**). Let the corresponding eigenvalues of Q', P' be $a_1, a_2, \ldots$ and $b_1, b_2, \ldots$, respectively. Then

$$\mathsf{Q}' = \sum_{n=1}^{\infty} a_n \mathsf{P}_{[\phi_n]} \qquad \mathsf{P}' = \sum_{n=1}^{\infty} b_n \mathsf{P}_{[\phi_n]}$$

Arrange their measurement in such a manner that it creates one of the states $\phi_1, \phi_2, \ldots$. To that end: measure a quantity $\mathcal{R}$ whose operator R has eigenfunctions $\phi_1, \phi_2, \ldots$ and distinct eigenvalues $c_1, c_2, \ldots$. Then Q', P' are functions of R. That this measurement implies measurement of Q and P in approximate fashion is clearly implied by this: In the state ϕ_n the values of Q, P are expressed approximately by the values of Q', P'; *i.e.*, by a_n, b_n. That is, their dispersions about these values are small. These dispersions are the expectation values of the quantities $(q - a_n)^2$, $(p - b_n)^2$; *i.e.*,

$$\big((\mathsf{Q} - a_n \mathsf{I})^2 \phi_n, \phi_n\big) = \|(\mathsf{Q} - a_n \mathsf{I})\phi_n\|^2 = \|\mathsf{Q}\phi_n - a_n \phi_n\|^2$$
$$\big((\mathsf{P} - b_n \mathsf{I})^2 \phi_n, \phi_n\big) = \|(\mathsf{P} - b_n \mathsf{I})\phi_n\|^2 = \|\mathsf{P}\phi_n - b_n \phi_n\|^2$$

They are measures of the squares of the differences of (respectively) Q' and Q, P' and P, so must be approximately ϵ^2 and η^2, respectively. We therefore require

$$\|\mathsf{Q}\phi_n - a_n \phi_n\| \lesssim \epsilon \qquad \|\mathsf{P}\phi_n - b_n \phi_n\| \lesssim \eta$$

Instead of speaking of Q', P' it becomes then more appropriate only to seek a complete orthonormal set $\phi_1, \phi_2, \ldots$ for which, for a suitable choice of $a_1, a_2, \ldots$ and $b_1, b_2, \ldots$, the above estimates hold.

Individual ϕ (with $\|\phi\| = 1$) for which (for suitable a, b)

$$\|\mathsf{Q}\phi - a\phi\| = \epsilon \qquad \|\mathsf{P}\phi - b\phi\| = \eta$$

are known from **III.4**:

$$\phi_{\sigma,\rho,\gamma} = \phi_{\sigma,\rho,\gamma}(q) = \left(\tfrac{2\gamma}{h}\right)^{\frac{1}{4}} \exp\left\{-\tfrac{\pi\gamma}{h}(q-\sigma)^2 + i\tfrac{2\pi\rho}{h}q\right\}$$

Because of $\epsilon\eta = \frac{1}{2}\hbar = \frac{h}{4\pi}$ we have again

$$\epsilon = \sqrt{\tfrac{h\gamma}{4\pi}} \qquad \eta = \sqrt{\tfrac{h}{4\pi\gamma}}$$

(*i.e.*, $\gamma = \epsilon/\eta$) and we now choose $a = \sigma, b = \rho$.

We now must construct a complete orthonormal set with the help of these $\phi_{\rho,\sigma,\gamma}$. Since σ is the Q expectation value, and ρ is the P expectation value, it is plausible that σ, ρ should each run through a set of numbers independently of each other. And, in fact, that they should do so in such a way that the σ-set has approximately the density ϵ and the ρ-set approximately the density η. It proves practical in view of $2\sqrt{\pi} \cdot \epsilon = \sqrt{h\gamma}$ and $2\sqrt{\pi} \cdot \eta = \sqrt{h/\gamma}$ to choose units so that

$$\sigma = \sqrt{h\gamma} \cdot \mu \quad \text{and} \quad \rho = \sqrt{h/\gamma} \cdot \nu \quad : \quad \mu, \nu = 0, \pm 1, \pm 2, \ldots$$

The functions

$$\psi_{\mu,\nu}(q) = \phi_{\mu\sqrt{h\gamma},\nu\sqrt{h/\gamma},\gamma}(q)$$

ought then to correspond to the ϕ_n $(n = 1, 2, \ldots)$. It is obviously irrelevant that we have two indices μ, ν in place of the one n.

These functions are normalized, and satisfy

$$\|\mathsf{Q}\psi_{\mu,\nu} - \mu\sqrt{h\gamma}\cdot\psi_{\mu,\nu}\| = \epsilon \qquad \|\mathsf{P}\psi_{\mu,\nu} - \nu\sqrt{h/\gamma}\cdot\psi_{\mu,\nu}\| = \eta$$

but are not orthogonal. If we now orthogonalize them (in sequence) by the Schmidt process (see **II.2**, proof of THEOREM 8) then we can prove completeness of the resulting orthonormal set $\psi'_{\mu,\nu}$ without any particular difficulties, and can also establish the estimates

$$\|\mathsf{Q}\psi'_{\mu,\nu} - \mu\sqrt{h\gamma}\cdot\psi'_{\mu,\nu}\| = C\epsilon \qquad \|\mathsf{P}\psi'_{\mu,\nu} - \nu\sqrt{h/\gamma}\cdot\psi'_{\mu,\nu}\| = C\eta$$

The value $C \approx 60$ has been obtained in this way, and could probably be reduced. The proof of this fact leads to rather tedious calculations which, however, require no new concepts, so we will omit them. The factors $C \approx 60$ are not important since $\epsilon\eta = \frac{1}{2}\hbar$, measured in macroscopic (CGS) units, is exceedingly small (of the order 10^{-28}).

Summing up, we can say that it is justified to assume the commutativity of all macroscopic operators, and in particular of the macroscopic projections E introduced above.

The E correspond to all macroscopically answerable questions $\mathfrak{E}$; *i.e.*, to all discriminations between alternatives in the system under investigation that can be carried out macroscopically. They are all commutative. We can conclude from **II.5** that $\mathsf{I} - \mathsf{E}$ belongs along with E to the set of all projectors associated with macroscopically answerable questions (propositions), and that EF, $\mathsf{E} + \mathsf{F} - \mathsf{EF}$, $\mathsf{E} - \mathsf{EF}$ belong along with E, F. It is reasonable to assume that every system **S** admits of only a finite number of such questions; *i.e.*, only a finite number of such operators: $\mathsf{E}_1, \mathsf{E}_2, \ldots, \mathsf{E}_n$. We introduce the notation

$$\mathsf{E}^{(+)} = \mathsf{E}, \qquad \mathsf{E}^{(-)} = \mathsf{I} - \mathsf{E}$$

and consider all 2^n products

$$\mathsf{E}_1^{(s_1)}\mathsf{E}_2^{(s_2)}\cdots\mathsf{E}_n^{(s_n)} \quad : \quad (s_1, s_2, \ldots, s_n = \pm)$$

Any two different ones among these have the product O, for if $\mathsf{E}_1^{(s_1)}\cdots\mathsf{E}_n^{(s_n)}$ and $\mathsf{E}_1^{(t_1)}\cdots\mathsf{E}_n^{(t_n)}$ are two such which differ in (say) the ν^{th} place, then their product presents the factor $\mathsf{E}_\nu^{(+)}\mathsf{E}_\nu^{(-)}$, which is O. Each E_ν is the sum of several such products: indeed

$$\mathsf{E}_\nu = \sum_{s_1\ldots\not{s}_\nu\ldots s_n = \pm} \mathsf{E}_1^{(s_1)}\cdots\mathsf{E}_{\nu-1}^{(s_{\nu-1})}\mathsf{E}_\nu^{(+)}\mathsf{E}_{\nu+1}^{(s_{\nu+1})}\cdots\mathsf{E}_n^{(s_n)}$$

Among these products, consider the ones which are different from O. Call them $\mathsf{E}'_1, \mathsf{E}'_2, \ldots, \mathsf{E}'_m$. (Evidently $m \leqslant 2^n$, but actually $m \leqslant n-1$ since these must occur among the $\mathsf{E}_1, \mathsf{E}_2, \ldots, \mathsf{E}_n$ and be $\neq \mathsf{O}$.) Now clearly: $\mathsf{E}'_\mu \neq \mathsf{O}$; $\mathsf{E}'_\mu \mathsf{E}'_\nu = \mathsf{O}$ for $\mu \neq \nu$; each E_μ is the sum of several E'_μ. (From the latter it follows that $n = 2^m$.) It should be noted that $\mathsf{E}_\mu + \mathsf{E}_\nu = \mathsf{E}'_\rho$ can never occur unless $\mathsf{E}_\mu = \mathsf{O}$ and $\mathsf{E}_\nu = \mathsf{E}'_\rho$ or $\mathsf{E}_\mu = \mathsf{E}'_\rho$ and $\mathsf{E}_\nu = \mathsf{O}$; otherwise $\mathsf{E}_\mu, \mathsf{E}_\nu$ would be sums of several $\mathsf{E}'_\pi = \mathsf{O}$ and therefore E'_ρ the sum of $\geqslant 2$ terms E'_π (possibly with repetitions). By **II.4**, THEOREMS 15,16 these would all differ from one another; since their number is $\geqslant 2$ and all are $\neq \mathsf{O}$ they also differ from E'_ρ. Therefore their product with E'_ρ would be O. Hence the product of their sum with E'_ρ would also be O, but this contradicts the assertion that their sum is equal to E'_ρ.

The properties $\mathfrak{E}'_1, \mathfrak{E}'_2, \ldots, \mathfrak{E}'_m$ corresponding to the $\mathsf{E}'_1, \mathsf{E}'_2, \ldots, \mathsf{E}'_m$ are then macroscopic properties of the following type: None is absurd. Every two are mutually exclusive. Each macroscopic property obtains by disjunction of several of them. None can be resolved by disjunction into two sharper macroscopic properties. $\mathfrak{E}'_1, \mathfrak{E}'_2, \ldots, \mathfrak{E}'_m$ therefore represent the farthest that one can go in macroscopic discrimination, for they are macroscopically indecomposable.

In the following we shall not require that their number be finite, but only that there exist macroscopically indecomposable properties $\mathfrak{E}'_1, \mathfrak{E}'_2, \ldots$. Let their projections be $\mathsf{E}'_1, \mathsf{E}'_2, \ldots$, all again different from O, mutually orthogonal, and each macroscopic E the sum of several of them.

Therefore I is also a sum of several of them. If E'_ν did not occur in this sum it would be orthogonal to each term and hence to the sum—that is, to I: $\mathsf{E}'_\nu = \mathsf{E}'_\nu \cdot \mathsf{I} = \mathsf{O}$, which is impossible. Therefore $\mathsf{E}'_1 + \mathsf{E}'_2 + \cdots = \mathsf{I}$. We now drop the prime notation, writing simply $\mathfrak{E}_1, \mathfrak{E}_2, \ldots$ and $\mathsf{E}_1, \mathsf{E}_2 \ldots$. The closed linear manifolds belonging to these will be called $\mathfrak{M}_1, \mathfrak{M}_2, \ldots$ and their dimension numbers $s_1, s_2, \ldots$

If all the $s_n = 1$ (*i.e.*, all the $\mathfrak{M}_n$ are one-dimensional) then $\mathfrak{M}_n = [\phi_n]$ and $\mathsf{E}_n = \mathsf{P}_{[\phi_n]}$, and because $\mathsf{E}_1 + \mathsf{E}_2 + \cdots = \mathsf{I}$ the $\phi_1, \phi_2, \ldots$ would form a complete orthonormal set. This would mean that macroscopic measurements would themselves make possible a complete determination of the state of the observed system. Since this is ordinarily not the case, we have in general $s_n > 1$, and in fact $s_n \gg 1$.

It should be observed, additionally, that the E_n—which are the elementary building blocks of the macroscopic description of the world—correspond in a certain sense to the cell division of phase space in classical theory. We have already seen that they can reproduce the behavior of non-commutative operators in an approximate fashion—in particular, that of Q and P, which are so important for phase space.

Now... what entropy does the mixture U have for an observer whose indecomposable projections are $\mathsf{E}_1, \mathsf{E}_2 \ldots$? Or, more precisely: How much entropy can such an observer maximally obtain by transforming U into V —*i.e.*, what entropy increase (or decrease) can he (under suitable conditions

and the most favorable circumstances) produce in external objects as compensation for the transition $\mathsf{U} \to \mathsf{V}$?

First, it must be emphasized that he cannot distinguish between two ensembles U, U' if both give the same expectation value to E_n for each n; *i.e.*, if $\mathrm{Tr}(\mathsf{U}\mathsf{E}_n) = \mathrm{Tr}(\mathsf{U}'\mathsf{E}_n) : n = 1, 2, \ldots$. After some time, of course, such discrimination may become possible, since U, U' change according to **2**, and

$$\mathrm{Tr}(\mathsf{A}\mathsf{U}\mathsf{A}^{-1}\mathsf{E}_n) = \mathrm{Tr}(\mathsf{A}\mathsf{U}'\mathsf{A}^{-1}\mathsf{E}_n) \quad : \quad \mathsf{A} = e^{-\frac{i}{\hbar}t\mathsf{H}}$$

must no longer hold.[204] But we consider only measurements which are carried out immediately. Under the above conditions we may therefore regard U, U' as indistinguishable. The observer—making use only of such semi-permeable walls as transmit the ϕ of some E_n and reflect the remainder unchanged—can use the method of **V.2** to transform a $\mathsf{U}' = \sum_{n=1}^{\infty} x_n \mathsf{E}_n$ into a $\mathsf{V}' = \sum_{n=1}^{\infty} y_n \mathsf{E}_n$ reversibly, and the entropy difference, since the entropy of U' is $-\kappa \mathrm{Tr}(\mathsf{U}' \ln \mathsf{U}')$, will be given by

$$-\kappa \mathrm{Tr}(\mathsf{V}' \ln \mathsf{V}') + \kappa \mathrm{Tr}(\mathsf{U}' \ln \mathsf{U}')$$

To be sure, in order that such U' with $\mathrm{Tr}(\mathsf{U}') = 1$ exist in general, the $\mathrm{Tr}\mathsf{E}_n$ —*i.e.*, the numbers s_n—must be finite: we therefore assume that to be the case. U' has the s_1-fold eigenvalue x_1, the s_2-fold eigenvalue x_2 ... . Therefore $-\mathsf{U}' \ln \mathsf{U}'$ has the s_1-fold eigenvalue $-x_1 \ln x_1$, the s_2-fold eigenvalue $-x_2 \ln x_2$, etc. Consequently $\mathrm{Tr}(\mathsf{U}') = 1$ implies

$$\sum_{n=1}^{\infty} s_n x_n = 1$$

and the entropy of U' is given by

$$-\kappa \sum_{n=1}^{\infty} s_n x_n \ln x_n$$

Because of $\mathsf{U}'\mathsf{E}_m = \sum_n x_n \mathsf{E}_n \mathsf{E}_m = x_m \mathsf{E}_m$ we have $\mathrm{Tr}(\mathsf{U}'\mathsf{E}_m) = x_m \mathrm{Tr}\mathsf{E}_m = s_m x_m$ whence

$$x_m = \frac{\mathrm{Tr}(\mathsf{U}'\mathsf{E}_m)}{s_m}$$

and the entropy of U' becomes

$$-\kappa \sum_{n=1}^{\infty} \mathrm{Tr}(\mathsf{U}'\mathsf{E}_n) \ln \frac{\mathrm{Tr}(\mathsf{U}'\mathsf{E}_n)}{s_n}$$

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[204] If E_n commutes with H, and therefore with A, the equality still holds, because

$$\mathrm{Tr}(\mathsf{A}\cdot\mathsf{U}\mathsf{A}^{-1}\mathsf{E}_n) = \mathrm{Tr}(\mathsf{U}\mathsf{A}^{-1}\mathsf{E}_n\cdot\mathsf{A}) = \mathrm{Tr}(\mathsf{U}\mathsf{A}^{-1}\mathsf{A}\mathsf{E}_n) = \mathrm{Tr}(\mathsf{U}\mathsf{E}_n)$$

But all E_n—*i.e.*, all macroscopically observable quantities—are in no way all commutative with H. Indeed, many such quantities—for example, the center of gravity of a gas in diffusion—change appreciably with t; *i.e.*, $\mathrm{Tr}(\mathsf{U}\mathsf{E}_n)$ is not constant. Since all macroscopic quantities do commute, H is never a macroscopic quantity; *i.e.*, the energy cannot be measured macroscopically with complete precision. This is plausible without additional comment.

For arbitrary U ($\mathrm{Tr}\mathsf{U} = 1$) the entropy must given similarly by

$$-\kappa \sum_{n=1}^{\infty} \mathrm{Tr}(\mathsf{U}\mathsf{E}_n) \ln \frac{\mathrm{Tr}(\mathsf{U}\mathsf{E}_n)}{s_n}$$

because if we set

$$x_n = \frac{\mathrm{Tr}(\mathsf{U}\mathsf{E}_n)}{s_n}, \quad \mathsf{U}' = \sum_{n=1}^{\infty} x_n \mathsf{E}_n$$

then $\mathrm{Tr}(\mathsf{U}\mathsf{E}_n) = \mathrm{Tr}(\mathsf{U}'\mathsf{E}_n)$, and since U, U' are indistinguishable they must have the same entropy.

We must also mention the fact that this entropy is never less than the customary entropy:

$$-\kappa \sum_{n=1}^{\infty} \mathrm{Tr}(\mathsf{U}\mathsf{E}_n) \ln \frac{\mathrm{Tr}(\mathsf{U}\mathsf{E}_n)}{s_n} \geqslant -\kappa \mathrm{Tr}(\mathsf{U} \ln \mathsf{U})$$

with equality only in the case $\mathsf{U} = \sum_{n=1}^{\infty} x_n \mathsf{E}_n$. By the results of **V.3** this is certainly the case if

$$\mathsf{U}' = \sum_{n=1}^{\infty} \frac{\mathrm{Tr}(\mathsf{U}\mathsf{E}_n)}{s_n} \mathsf{E}_n$$

can be obtained from U by several (not necessarily macroscopic) applications of process **1** because on the left we then have $-\kappa \mathrm{Tr}(\mathsf{U}' \ln \mathsf{U}')$, and $\mathsf{U} = \sum_{n=1}^{\infty} x_n \mathsf{E}_n$ means $\mathsf{U} = \mathsf{U}'$. Now consider an orthonormal set $\phi_1^{(n)}, \ldots, \phi_{s_n}^{(n)}$ which spans the closed linear manifold $\mathfrak{M}_n$ belonging to E_n. Because of

$$\sum_{n=1}^{\infty} \mathsf{E}_n = \mathsf{I}$$

all $\phi_\nu^{(n)}$ ($n = 1, 2, \ldots$; $\nu = 1, 2, \ldots, s_n$) form a complete orthonormal set. Let R be an operator with these eigenfunctions (and only distinct eigenvalues), and $\mathcal{R}$ the physical quantity to which R corresponds. In the measurement of $\mathcal{R}$ we get from U (by **1**)

$$\mathsf{U}'' = \sum_{n=1}^{\infty} \sum_{\nu=1}^{s_n} (\mathsf{U}\phi_\nu^{(n)}, \phi_\nu^{(n)}) \cdot \mathsf{P}_{[\phi_\nu^{(n)}]}$$

Then, if we set

$$\psi_\mu^{(n)} = \frac{1}{\sqrt{s_n}} \sum_{\nu=1}^{s_n} e^{i2\pi \frac{\mu\nu}{s_n}} \phi_\nu^{(n)} \quad : \quad \mu = 1, \ldots, s_n$$

the $\psi_1^{(n)}, \ldots, \psi_{s_n}^{(n)}$ form an orthogonal set which spans the same closed linear manifold $\mathfrak{M}_n$ as the $\phi_1^{(n)}, \ldots, \phi_{s_n}^{(n)}$. Therefore the

$$\psi_\nu^{(n)} \quad : \quad n = 1, 2, \ldots; \ \nu = 1, 2, \ldots, s_n$$

also form a complete orthonormal set, and we form an operator S with these eigenfunctions, distinct eigenvalues and corresponding physical quantity $\mathcal{S}$. We

note the validity of the following formulas:

$$\left(\mathsf{P}_{[\phi_\nu^{(n)}]}\psi_\mu^{(m)}, \psi_\mu^{(m)}\right) = \begin{cases} 0 & \text{for} \quad m \neq n \\ \frac{1}{s_n} & \text{for} \quad m = n \end{cases}$$

$$\sum_{\nu=1}^{s_n} \mathsf{P}_{[\phi_\nu^{(n)}]} = \sum_{\nu=1}^{s_n} \mathsf{P}_{[\psi_\nu^{(n)}]} = \mathsf{E}_n$$

In the measurement of $\mathcal{S}$, therefore, U'' becomes (by **1**)

$$\begin{aligned}
&\sum_{m=1}^{\infty}\sum_{\mu=1}^{s_m}(\mathsf{U}''\psi_\mu^{(m)}, \psi_\mu^{(m)})\mathsf{P}_{[\psi_\mu^{(m)}]} \\
&= \sum_{m=1}^{\infty}\sum_{\mu=1}^{s_m}\left[\sum_{n=1}^{\infty}\sum_{\nu=1}^{s_n}(\mathsf{U}\phi_\nu^{(n)}, \phi_\nu^{(n)})\left(\mathsf{P}_{[\phi_\nu^{(n)}]}\psi_\mu^{(m)}, \psi_\mu^{(m)}\right)\right]\mathsf{P}_{[\psi_\mu^{(m)}]} \\
&= \sum_{m=1}^{\infty}\sum_{\mu=1}^{s_m}\left[\sum_{\nu=1}^{s_m}\frac{(\mathsf{U}\phi_\nu^{(m)}, \phi_\nu^{(m)})}{s_m}\right]\mathsf{P}_{[\psi_\mu^{(m)}]} \\
&= \sum_{m=1}^{\infty}\sum_{\mu=1}^{s_m}\frac{\mathrm{Tr}(\mathsf{U}\mathsf{E}_m)}{s_m}\cdot\mathsf{P}_{[\psi_\mu^{(m)}]} \\
&= \sum_{m=1}^{\infty}\frac{\mathrm{Tr}(\mathsf{U}\mathsf{E}_m)}{s_m}\mathsf{E}_m = \mathsf{U}'
\end{aligned}$$

Consequently, two processes **1** suffice to transform U into U', and this is all we need for the proof.

For states ($\mathsf{U} = \mathsf{P}_{[\phi]}$, $\mathrm{Tr}(\mathsf{U}\mathsf{E}_n) = (\mathsf{E}_n\phi, \phi) = \|\mathsf{E}_n\phi\|^2$) this entropy

$$-\kappa\sum_{n=1}^{\infty}\|\mathsf{E}_n\phi\|^2 \ln\frac{\|\mathsf{E}_n\phi\|^2}{s_n}$$

is no longer subject to the inconveniences of the "macroscopic" entropy. In general, it is not constant in time (*i.e.*, under process **2**), and does not vanish for all states $\mathsf{U} = \mathsf{P}_{[\phi]}$. That the $\mathrm{Tr}(\mathsf{U}\mathsf{E}_n)$, from which our entropy was formed, are not generally constant in time was discussed already in Note 204. It is easy to determine when the state $\mathsf{U} = \mathsf{P}_{[\phi]}$ has entropy 0: since

$$0 \leqslant \frac{\|\mathsf{E}_n\phi\|^2}{s_n} \leqslant 1$$

all summands

$$\|\mathsf{E}_n\phi\|^2 \ln\frac{\|\mathsf{E}_n\phi\|^2}{s_n}$$

in the entropy expression are $\leqslant 0$. All these must therefore vanish, which requires

$$\frac{\|\mathsf{E}_n\phi\|^2}{s_n} = 0 \text{ else } 1$$

The former means $\mathsf{E}_n\phi = 0$, and the latter that $\|\mathsf{E}_n\phi\| = \sqrt{s_n}$, but since

$$\|\mathsf{E}_n\phi\| \leqslant 1 \quad \text{and} \quad s_n \geqslant 1$$

this implies $s_n = 1$ and $\|\mathsf{E}_n\phi\| = \|\phi\|$; *i.e.*, $\mathsf{E}_n\phi = \phi_n$. That is: $s_n = 1$, ϕ in $\mathfrak{M}_n$. The latter certainly cannot hold for two different n, but also it cannot hold at all because then $\mathsf{E}_n\phi = 0$ would always be true, and therefore $\phi = 0$ since $\sum_{n=1}^{\infty} \mathsf{E}_n = \mathsf{I}$. Hence for exactly one n is it the case that ϕ is in $\mathfrak{M}_n$, and then s_n=1. But, since we determined that in general all $s_n \gg 1$, this is impossible. So our entropy is always > 0.

Since the macroscopic entropy is always time variable, the next question to be answered is this: Does it behave like the phenomenological thermodynamics of the real world; *i.e.*, does it predominantly increase? This question is answered affirmatively in classical mechanical theory by the so-called Boltzmann H-theorem. In that, however, certain statistical assumptions—namely, the so-called "disorder assumptions"—must be made.[205] In quantum mechanics it was possible for the author to prove the corresponding theorem without such assumptions.[206] Since the detailed discussion of this subject, as well of the ergodic theorem closely connected with it (see the reference cited in Note 206, where this theorem is also proved) would go beyond the scope of this volume, we cannot report on these investigations. The reader who is interested in this problem can refer to the treatments in the references.

[205] For the classical H-theorem, see Boltzmann, *Vorlesungen über Gastheorie*, Leipzig, 1896, as well as the extremely instructive discussion by P. and T. Ehrenfest in the article cited in Note 185. The "disorder assumptions" which can take the place (in quantum mechanics) of those of Boltzmann have been formulated by W. Pauli (*Sommerfeld-Festschrift*, 1928), and the H-theorem is proved there with their help. More recently, the author has also succeeded in proving the classical-mechanical ergodic theorem, see PNAS, January & March, 1932 as well as the improved treatment of G. D. Birkhoff, PNAS December, 1931 & March, 1932.

[206] Z. Physik **57** (1929).

CHAPTER VI

THE MEASURING PROCESS

1. FORMULATION OF THE PROBLEM

In the discussion so far we have treated the relation of quantum mechanics to the various causal and statistical methods of describing nature. In the course of this we have found a peculiar dual nature of the quantum mechanical procedure which could not be satisfactorily explained. Namely, we found that on the one hand a state ϕ is transformed into the state ϕ' under the action of an energy operator H in the time interval $0 \leqslant \tau \leqslant t$:

$$\frac{\partial}{\partial t}\phi_\tau = -\frac{i}{\hbar}\mathsf{H}\phi_\tau \quad : \quad 0 \leqslant \tau \leqslant t$$

so if we write $\phi_0 = \phi,\ \phi_t = \phi'$ then

$$\phi' = e^{-\frac{i}{\hbar}t\mathsf{H}}\phi$$

which is purely causal. A mixture U is correspondingly transformed into

$$\mathsf{U}' = e^{-\frac{i}{\hbar}t\mathsf{H}}\mathsf{U}e^{+\frac{i}{\hbar}t\mathsf{H}}$$

Therefore, as a consequence of the causal change of ϕ into ϕ' the states $\mathsf{U} = \mathsf{P}_{[\phi]}$ go over into the states $\mathsf{U}' = \mathsf{P}_{[\phi']}$ (process **2** in **V.1**). On the other hand, the state ϕ—which may refer to a quantity with a pure discrete spectrum, distinct eigenvalues and eigenfunctions $\phi_1, \phi_2, \ldots$—undergoes in a measurement a change in which any of the states $\phi_1, \phi_2, \ldots$ may result, and in fact do result with the respective probabilities $|(\phi, \phi_1)|^2, |(\phi, \phi_2)|^2, \ldots$. That is, the mixture

$$\mathsf{U}' = \sum_{n=1}^{\infty} |(\phi, \phi_n)|^2 \mathsf{P}_{[\phi_n]}$$

obtains. More generally, the mixture U goes over into

$$\mathsf{U}' = \sum_{n=1}^{\infty} |(\mathsf{U}\phi_n, \phi_n)|^2 \mathsf{P}_{[\phi_n]}$$

(process **1** in **V.1**). Since the states go over into mixtures, the process is not causal.

The difference between these two processes $U \to U'$ is a very fundamental one: aside from their different statuses with regard to the principle of causality, they also differ in that the former is (thermodynamically) reversible, while the latter is not (see **V.3**).

Let us now compare these circumstances with those which actually exist in nature, or in its observation. First, it is inherently correct that measurement or the related process of subjective perception is a new entity relative to the physical environment, and is not reducible to the latter. Indeed, subjective perception leads us into the intellectual inner life of the individual, which is extra-observational by its very nature, since it must be taken for granted by any conceivable observation or experiment. (See the discussion above.) Nevertheless, it is a fundamental requirement of the scientific viewpoint—the so-called *principle of psycho-physical parallelism*—that it must be possible so to describe the extra-physical process of subjective perception as if it were in the reality of the physical world; *i.e.*, to assign to its parts equivalent physical processes in the objective environment, in ordinary space. (Of course, in this correlating procedure there arises the frequent necessity of localizing some of these processes at points which lie within the portion of space occupied by our own bodies. But this does not alter the fact of their belonging to "the world about us," the objective environment referred to above.) In a simple example, these concepts might be applied as follows: We wish to measure the temperature. If we want, we can proceed numerically by looking to the mercury column in a thermometer, and then say: "This is the temperature as measured by the thermometer." But we can carry the process further, and from the properties of mercury (which can be explained in kinetic and molecular terms) we can calculate its heating, expansion, and the resultant length of the mercury column, and then say: "This length is seen by the observer." Going still further, and taking the light source into consideration, we could find out the reflection of the light quanta on the opaque mercury column, and the path taken by the reflected light quanta into the eye of the observer, their refraction in the eye lens, and the formation of an image on the retina, and then we would say: "This image is registered by the retina of the observer." And were our physiological knowledge greater than it is today, we could go still further, tracing the chemical reactions which produce the impression of this image on the retina, and in the optic nerve and in the brain, and then in the end say: "These chemical changes of his brain cells are perceived by the observer." But in any case, no matter how far we proceed—from the thermometer scale, to the mercury, to the retina, or into the brain—at some point we must say: "And this is perceived by the observer." That is, we are obliged always to divide the world into two parts, the one being the observed system, the other the observer. In the former we can follow all physical processes (in principle at least) arbitrarily precisely. In the latter, this is meaningless. The boundary between the two is arbitrary to a very large extent. In particular, we saw in the four different possibilities considered in the preceding example that the "observer"—in this sense—need not be identified with the body of the actual observer: in one instance we included even the thermometer in it, while in another instance even the eyes and optic nerve

were not included. That this boundary can be pushed arbitrarily far into the interior of the body of the actual observer is the content of the principle of psycho-physical parallelism. But this does not change the fact that in every account the boundary must be put somewhere if the principle is not to be rendered vacuous; *i.e.*, if a comparison with experience is to be possible. Indeed, experience only makes statements of this type: "An observer has made a certain (subjective) observation," and never any like this: "A physical quantity has a certain value."

Now quantum mechanics describes events which occur in observed portions of the world, so long as they do not interact with the observing portion, and does so by means of process **2** (**V.1**). But as soon such an interaction does occur—*i.e.*, a measurement is made—the theory requires application of process **1**. This duality is therefore fundamental to the theory.[207] Danger, however, lies in the fact that the principle of psycho-physical parallelism is violated so long as it is not shown that the boundary between the observed system and the observer can be displaced arbitrarily, in the sense given above.

In order to discuss this, let us divide the world into three parts: I, II, III. Let I be the system actually observed, II the measuring instrument, and III the actual observer.[208] It is to be shown that the boundary can just as well be drawn between I and II+III as between I+II and III. In comparison of the first and second cases of our introductory example, viewed in this light: I was the system to be observed, II the thermometer, and III the light plus the observer. In comparison of the second and third cases, I was the system to be observed plus the thermometer, II was the light plus the eye of the observer, III was the observer, from the retina on. In comparison of the third and fourth cases, I was everything up to the retina of the observer, II was his retina, optic nerve and brain, III was his abstract "ego." That is, in one case **2** is to be applied to I and **1** to the interaction between I and II+III; in the other case **2** is to be applied to I+II and **1** to the interaction between I+II and III. In both cases, III itself remains outside of the calculation. Proof of the following assertion—that both procedures give the same results regarding I (in both cases, this and only this belongs to the observed part of the world)—is then our problem.

But in order to be able to accomplish this we must first investigate more closely the process of forming the union of two physical systems (such as leads from I and II to I+II).

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[207] N. Bohr, Naturwiss. **17** (1929) was the first to point out that the duality which is necessitated by quantum formalism, by the quantum mechanical description of nature, is fully justified by the physical nature of things, and that it may be connected with the principle of psycho-physical parallelism.

[208] The discussion which is carried out below, as well as in **VI.3**, contains essential elements which the author owes to conversations with L. Szilard. See also the similar considerations of Heisenberg in the reference cited in Note 181.

2. COMPOSITE SYSTEMS

As was stated at the end of the preceding section, we consider two physical systems I, II (which do not necessarily have the meaning of I, II above) and their combination I+II. In classical mechanics, I would have k degrees of freedom, and therefore coordinates $q_1, \ldots, q_k$, which we will abbreviate with the single symbol q. Correspondingly, let II have ℓ degrees of freedom, and coordinates $r_1, \ldots, r_\ell$ which will be denoted r. Therefore, I+II has $k+\ell$ degrees of freedom and coordinates $q_1, \ldots, q_k, r_1, \ldots, r_\ell$ or, more briefly, q, r. In quantum mechanics then the wave functions of I have the form $\phi(q)$, those of II the form $\xi(r)$ and those of I+II the form $\Phi(q, r)$. In the corresponding Hilbert spaces $\mathfrak{R}^{\mathrm{I}}$, $\mathfrak{R}^{\mathrm{II}}$ and $\mathfrak{R}^{\mathrm{I+II}}$ the inner product is defined

$$\int \phi(q)\overline{\psi(q)}dq, \quad \int \xi(r)\overline{\eta(r)}dr \quad \text{and} \quad \iint \Phi(q,r)\overline{\Psi(q,r)}dqdr$$

respectively. Corresponding to physical quantities in I, II and I+II are the (hypermaximal) Hermitian operators $\dot{\mathsf{A}}$, $\ddot{\mathsf{A}}$, A in $\mathfrak{R}^{\mathrm{I}}$, $\mathfrak{R}^{\mathrm{II}}$, $\mathfrak{R}^{\mathrm{I+II}}$ respectively.

Each physical quantity in I is naturally also one in I+II, and its A is to be obtained from its $\dot{\mathsf{A}}$ in this way: to obtain $\mathsf{A}\Phi(q, r)$ consider r as a constant and apply $\dot{\mathsf{A}}$ to the q-function $\Phi(q, r)$.[209] This transformation rule is correct in any case for the coordinate and momentum operators $\mathsf{Q}_1, \ldots, \mathsf{Q}_k$ and $\mathsf{P}_1, \ldots, \mathsf{P}_k$; *i.e.*,

$$q_1, \ldots, q_k, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_1}, \ldots, \tfrac{\hbar}{i}\tfrac{\partial}{\partial q_k}$$

(see **I.2**), and it conforms with the principles **I**, **II** in **IV.2**.[210] We therefore adopt the rule as a general postulate. (This is the customary procedure in quantum mechanics.)

In the same way, each physical quantity in II is one also in I+II, and its $\ddot{\mathsf{A}}$ gives its A by the same rule: $\mathsf{A}\Phi(q, r)$ equals $\ddot{\mathsf{A}}\Phi(q, r)$ if in the latter expression q is taken as a constant, and $\Phi(q, r)$ is considered to be a function of r.

If $\phi_m(q)$ $(m = 1, 2, \ldots)$ is a complete orthonormal set in $\mathfrak{R}^{\mathrm{I}}$, and $\xi_n(r)$ $(n = 1, 2, \ldots)$ one in $\mathfrak{R}^{\mathrm{II}}$, then $\Phi_{m|n}(q, r) = \phi_m(q)\xi_n(r)$ $(m, n = 1, 2, \ldots)$ is clearly one in $\mathfrak{R}^{\mathrm{I+II}}$. The operators $\dot{\mathsf{A}}$, $\ddot{\mathsf{A}}$ and A can therefore be represented by matrices $\{\dot{a}_{m|m'}\}$, $\{\ddot{a}_{n|n'}\}$ and $\{a_{mn|m'n'}\}$ respectively $(m, m', n, n' = 1, 2, \ldots)$.[211]

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[209] It can easily be shown that if $\dot{\mathsf{A}}$ is Hermitian or hypermaximal, then so is A.

[210] For **I** this is clear, and for **II** also so long as only polynomials are concerned. For general functions it can be inferred from the fact that the correspondence between a resolution of the identity and a Hermitian operator is not disturbed in our transition $\dot{\mathsf{A}} \to \mathsf{A}$.

[211] Because of the large number and variety of indices, we here denote matrices in a way which differs from the notation used thus far.

We shall make frequent use of this. The matrix representation means that

$$\dot{\mathsf{A}}\phi_m(q) = \sum_{m'=1}^{\infty} \dot{a}_{m|m'}\phi_{m'}(q), \qquad \ddot{\mathsf{A}}\xi_n(r) = \sum_{n'=1}^{\infty} \ddot{a}_{n|n'}\xi_{n'}(r)$$

and

$$\mathsf{A}\Phi_{mn}(q,r) = \sum_{m',n'=1}^{\infty} a_{mn|m'n'}\Phi_{m'n'}(q,r)$$

i.e.,

$$\mathsf{A}\phi_m(q)\xi_n(r) = \sum_{m',n'=1}^{\infty} a_{mn|m'n'}\phi_{m'}(q)\xi_{n'}(r)$$

In particular, the correspondence $\dot{\mathsf{A}} \to \mathsf{A}$ means that

$$\mathsf{A}\phi_m(q)\xi_n(r) = [\dot{\mathsf{A}}\phi_m(q)]\xi_n(r) = \sum_{m'=1}^{\infty} \dot{a}_{m|m'}\phi_{m'}(q)\xi_n(r)$$

i.e.,

$$a_{mn|m'n'} = \dot{a}_{m|m'} \cdot \delta_{n|n'} \quad \text{where} \quad \delta_{n|n'} = \begin{cases} 1 & \text{for} \quad n = n' \\ 0 & \text{for} \quad n \neq n' \end{cases}$$

Similarly, the correspondence $\ddot{\mathsf{A}} \to \mathsf{A}$ implies $a_{mn|m'n'} = \delta_{m|m'} \cdot \ddot{a}_{n|n'}$.

A statistical ensemble in I+II is characterized by its statistical operator U or (equivalently) by its matrix $\{u_{mn|m'n'}\}$. This determines the statistical properties of all quantities in I+II, and therefore also in I (and II). Consequently there corresponds to it a statistical ensemble in I (or II) alone. In fact, an observer who could perceive only I, and not II, would view the ensemble of systems I+II as an instance of a system I. What, now, is the operator $\dot{\mathsf{U}}$ or matrix $\{\dot{u}_{m|m'}\}$ that belongs to this I ensemble? We determine it as follows: The I quantity with matrix $\{\dot{a}_{m|m'}\}$ has the matrix $\{\dot{a}_{m|m'}\delta_{n|n'}\}$ as an I+II quantity, and therefore, by reason of a calculation in I, has the expectation value

$$\sum_{m,m'=1}^{\infty} \dot{u}_{m|m'}\dot{a}_{m'|m}$$

while calculation in I+II gives

$$\begin{aligned} \sum_{m,n,m',n'=1}^{\infty} u_{mn|m'n'}\dot{a}_{m'|m}\delta_{n'|n} &= \sum_{m,m',n=1}^{\infty} u_{mn|m'n}\dot{a}_{m'|m} \\ &= \sum_{m,m'=1}^{\infty} \left(\sum_{n=1}^{\infty} u_{mn|m'n} \right) \dot{a}_{m'|m} \end{aligned}$$

For those expressions to be equal, we must have

$$\dot{u}_{m|m'} = \sum_{n=1}^{\infty} u_{mn|m'n}$$

In the same way, our I+II ensemble, if only II is considered and I is ignored, determines a statistical operator $\ddot{\mathsf{U}}$ and matrix $\{\ddot{u}_{n|n'}\}$. By analogy, we obtain

$$\ddot{u}_{n|n'} = \sum_{m=1}^{\infty} u_{mn|mn'}$$

We have thus established the rules of correspondence for the statistical operators of I, II and I+II, *i.e.*, for $\dot{\mathsf{U}}$, $\ddot{\mathsf{U}}$ and U. They proved to be essentially different from the rules or correspondence among the operators $\dot{\mathsf{A}}$, $\ddot{\mathsf{A}}$ and A of physical quantities.

It should be mentioned that our $\dot{\mathsf{U}}$, $\ddot{\mathsf{U}}$, U correspondence depends only apparently on the choice of the $\phi_m(q)$ and $\xi_n(r)$. Indeed, it was derived from an invariant condition (the implications of which are unique): namely, that expectation values in I—whether obtained from $\dot{\mathsf{U}}$ or from U—are identical (and similarly, for expectation values in II, whether obtained from $\ddot{\mathsf{U}}$ or U).

U expresses the statistics in I+II, $\dot{\mathsf{U}}$ and $\ddot{\mathsf{U}}$ those statistics restricted to I and II. The question now arises: Do $\dot{\mathsf{U}}$, $\ddot{\mathsf{U}}$ determine U uniquely or not? In general, one expects a negative answer because all "probability dependencies" which may exist between between the two systems disappear as information is reduced to that conveyed solely by $\dot{\mathsf{U}}$ and $\ddot{\mathsf{U}}$; *i.e.*, to that concerning the separated systems I and II. But if one knows the state of I precisely, and also that of II, then "probability questions" do not arise: the state of I+II too is then precisely known. An exact mathematical discussion is, however, preferable to these qualitative considerations, and that we proceed now to provide.

The problem is, then: For two definite matrices $\{\dot{u}_{m|m'}\}$ and $\{\ddot{u}_{n|n'}\}$, find a third definite matrix $\{u_{mn|m'n'}\}$ such that

$$\sum_{n=1}^{\infty} u_{mn|m'n} = \dot{u}_{m|m'} \quad \text{and} \quad \sum_{m=1}^{\infty} u_{mn|mn'} = \ddot{u}_{n|n'}$$

(We note in passing that from

$$\sum_{m=1}^{\infty} \dot{u}_{m|m} = 1 \quad \text{and} \quad \sum_{n=1}^{\infty} \ddot{u}_{n|n} = 1$$

it follows directly that

$$\sum_{m,n=1}^{\infty} u_{mn|mn} = 1$$

i.e., that correct normalization is preserved.) This problem is always solvable: for example, $u_{mn|m'n'} = \dot{u}_{m|m'} \cdot \ddot{u}_{n|n'}$ is always a solution (it is easily seen that this matrix is definite). But the question arises as to whether this is the only solution.

We will show that this is the case if and only if at least one of the two matrices $\{\dot{u}_{m|m'}\}$ and $\{\ddot{u}_{n|n'}\}$ refers to a pure state. First we prove the necessity of this condition; *i.e.*, the existence of multiple solutions if both matrices correspond to mixtures. In such a case (see **IV.2**)

$$\begin{aligned}\dot{u}_{m|m'} &= \alpha\,\dot{v}_{m|m'} + \beta\,\dot{w}_{m|m'}\\ \ddot{u}_{n|n'} &= \gamma\,\ddot{v}_{n|n'} + \delta\,\ddot{w}_{n|n'}\end{aligned}$$

where $\dot{v}_{m|m'}$, $\dot{w}_{m|m'}$,$\ddot{v}_{n|n'}$, $\ddot{w}_{n|n'}$ (all definite) differ by more than a constant factor, and where also

$$\sum_{m=1}^{\infty}\dot{v}_{m|m} = \sum_{m=1}^{\infty}\dot{w}_{m|m} = \sum_{n=1}^{\infty}\ddot{v}_{n|n} = \sum_{n=1}^{\infty}\ddot{w}_{n|n} = 1$$

$\alpha,\beta,\gamma,\delta > 0$, $\alpha+\beta=1$ and $\gamma+\delta=1$. We easily verify that every matrix of the form

$$u_{mn|m'n'} = \pi\,\dot{v}_{m|m'}\ddot{v}_{n|n'} + \rho\,\dot{w}_{m|m'}\ddot{v}_{n|n'} + \sigma\,\dot{v}_{m|m'}\ddot{w}_{n|n'} + \tau\,\dot{w}_{m|m'}\ddot{w}_{n|n'}$$

with

$$\begin{aligned}\pi+\sigma&=\alpha\\ \rho+\tau&=\beta\\ \pi+\rho&=\gamma\\ \sigma+\tau&=\delta\end{aligned}\quad\text{and}\quad \pi,\rho,\sigma,\tau>0$$

is a solution. Then π,ρ,σ,τ can be chosen in an infinite number of ways. Because of $\alpha+\beta=\gamma+\delta$ $(=\pi+\rho+\sigma+\tau)$ only three of the four equations are independent. We can therefore write

$$\begin{aligned}\sigma &= \alpha-\pi\\ \rho &= \gamma-\pi\\ \tau &= (\delta-\alpha)+\pi\end{aligned}$$

and in order that all be >0 we must require $\alpha-\delta=\gamma-\beta<\pi<\alpha,\gamma$, which is the case for infinitely many π. Now different π,ρ,σ,τ lead to different $u_{mn|m'n'}$ because the $\dot{v}_{m|m'}\ddot{v}_{n|n'}$, $\dot{w}_{m|m'}\ddot{v}_{n|n'}$, $\dot{v}_{m|m'}\ddot{w}_{n|n'}$, $\dot{w}_{m|m'}\ddot{w}_{n|n'}$ are linearly independent, since the $\dot{v}_{m|m'}$, $\dot{w}_{m|m'}$ are, and so are the $\ddot{v}_{n|n'}$, $\ddot{w}_{n|n'}$.

Next we prove sufficiency, and here we may assume that $\dot{u}_{m|m'}$ corresponds to a state (the other case is dealt with in the same way). Then $\dot{\mathsf{U}} = \mathsf{P}_{[\phi]}$ and since the complete orthonormal set $\phi_1,\phi_2,\ldots$ was arbitrary, we can assume $\phi=\phi_1$. $\dot{\mathsf{U}} = \mathsf{P}_{[\phi_1]}$ has the matrix

$$\dot{u}_{m|m'} = \begin{cases}1 & \text{for}\quad m=m'=1\\ 0 & \text{otherwise}\end{cases}$$

Therefore

$$\sum_{n=1}^{\infty}u_{mn|m'n} = \begin{cases}1 & \text{for}\quad m=m'=1\\ 0 & \text{otherwise}\end{cases}$$

In particular,

$$\sum_{n=1}^{\infty} u_{mn|mn} = 0 \quad \text{for} \quad m \neq 1$$

But because of the definiteness of $u_{mn|m'n'}$ all $u_{mn|mn} = (\mathsf{U}\Phi_{mn}, \Phi_{mn}) \geqslant 0$, therefore in this case $u_{mn|mn} = 0$. That is, $(\mathsf{U}\Phi_{mn}, \Phi_{mn}) = 0$ and hence, because of the definiteness of U, also $(\mathsf{U}\Phi_{mn}, \Phi_{m'n'}) = 0$ (see **II.5**, THEOREM 19) where m', n' are arbitrary. That is, it follows from $m \neq 1$ that $u_{mn|m'n'} = 0$, and by Hermiticity this follows also from $m' \neq 1$. For $m = m' = 1$, however, we have

$$u_{1n|1n'} = \sum_{m=1}^{\infty} u_{mn|mn'} = \ddot{u}_{n|n'}$$

Consequently, as was asserted, the solution $u_{mn|m'n}$ is determined uniquely.

We can thus summarize our result as follows: A statistical ensemble in I+II with operator $\mathsf{U} = \{u_{mn|m'n'}\}$ is determined uniquely by the statistical ensembles in I and II individually, with respective operators $\dot{\mathsf{U}} = \{\dot{u}_{m|m'}\}$ and $\ddot{\mathsf{U}} = \{\ddot{u}_{n|n'}\}$, if and only if the following two conditions are satisfied:

1.

$$u_{mn|m'n'} = \dot{v}_{m|m'} \cdot \ddot{v}_{n|n'}$$

From $\mathrm{Tr}\mathsf{U} = \sum_{m,n} u_{mn|mn} = \sum_m \dot{v}_{m|m} \cdot \sum_n \ddot{v}_{n|n} = 1$ it follows that if we multiply $\dot{v}_{m|m}$ and $\ddot{v}_{n|n}$ by appropriate reciprocal factors we can obtain

$$\sum_{m=1}^{\infty} \dot{v}_{m|m} = 1, \qquad \sum_{n=1}^{\infty} \ddot{v}_{n|n} = 1$$

But then we see that $\dot{u}_{m|m'} = \dot{v}_{m|m'}$, $\ddot{u}_{n|n'} = \ddot{v}_{n|n'}$.

2. Either

$$\dot{v}_{m|m'} = \overline{x}_m x_{m'} \quad \text{or} \quad \ddot{v}_{n|n'} = \overline{x}_n x_{n'}$$

Indeed, $\dot{\mathsf{U}} = \mathsf{P}_{[\phi]}$ means that $\phi = \sum_m y_m \phi_m$ and therefore

$$\dot{u}_{m|m'} = \overline{y}_m y_{m'}$$

Correspondingly for $\dot{v}_{m|m'}$. By analogy, the same is true with $\ddot{\mathsf{U}} = \mathsf{P}_{[\xi]}$.

We shall call $\dot{\mathsf{U}}$ and $\ddot{\mathsf{U}}$ the projections of U in I and II respectively.[212]

We now apply ourselves to the states of I+II: $\mathsf{U} = \mathsf{P}_{[\Phi]}$. The corresponding wave functions $\Phi(q, r)$ can be expanded in the complete orthonormal set $\Phi_{mn}(q, r) = \phi_m(q)\xi_n(r)$:

$$\Phi(q, r) = \sum_{m,n=1}^{\infty} f_{mn}\phi_m(q)\xi_n(r)$$

[212] As will emerge, the projections of a state in I+II are in general mixtures in I or II. This circumstance was discovered by Landau, Z. Physik **45** (1927).

We can therefore replace them by the coefficients f_{mn} $(m, n = 1, 2, \ldots)$ which are subject only to the condition that $\sum_{m,n} |f_{mn}|^2 = \|\Phi\|^2$ be finite.

We now define two operators F, F^* by

$$\mathsf{F}\ \phi(q) = \int \overline{\Phi(q,r)}\ \phi(q)dq$$
$$\mathsf{F}^*\xi(r) = \int \Phi(q,r)\ \xi(r)\,dr$$

F

These are linear, but have the peculiarity of being defined in $\mathfrak{R}^{\mathrm{I}}$ and $\mathfrak{R}^{\mathrm{II}}$ respectively while taking on values from $\mathfrak{R}^{\mathrm{II}}$ and $\mathfrak{R}^{\mathrm{I}}$ respectively. Their relation is that of adjoints, since obviously $(\mathsf{F}\phi, \xi) = (\phi, \mathsf{F}^*\xi)$ (the inner product on the left is to be formed in $\mathfrak{R}^{\mathrm{II}}$, while that on the right is to be formed in $\mathfrak{R}^{\mathrm{I}}$). Since the difference between $\mathfrak{R}^{\mathrm{I}}$ and $\mathfrak{R}^{\mathrm{II}}$ is mathematically unimportant, we can apply the results of **II.11**: then, since we are dealing with integral operators, $\Sigma(\mathsf{F})$ and $\Sigma(\mathsf{F}^*)$ are both equal to

$$\iint |\Phi(q,r)|^2 dqdr = \|\Phi\|^2 = 1$$

($\|\Phi\|$ in $\mathfrak{R}^{\mathrm{I+II}}$!), and are therefore finite. Consequently F, F^* are continuous—in fact, are completely continuous—operators, and $\mathsf{F}^*\mathsf{F}$ as well as $\mathsf{F}\mathsf{F}^*$ are definite operators: $\mathrm{Tr}(\mathsf{F}^*\mathsf{F}) = \Sigma(\mathsf{F}) = 1$, $\mathrm{Tr}(\mathsf{F}\mathsf{F}^*) = \Sigma(\mathsf{F}^*) = 1$.

If we again consider the difference between $\mathfrak{R}^{\mathrm{I}}$ and $\mathfrak{R}^{\mathrm{II}}$ we see that $\mathsf{F}^*\mathsf{F}$ is defined and assumes values in $\mathfrak{R}^{\mathrm{I}}$, $\mathsf{F}\mathsf{F}^*$ is defined and assumes values in $\mathfrak{R}^{\mathrm{II}}$.

Since

$$\mathsf{F}\phi_m(q) = \sum_{n=1}^{\infty} \overline{f}_{mn}\xi_n(r)$$

F has the matrix $\{\overline{f}_{mn}\}$, as is discovered by use of the complete orthonormal sets $\phi_m(q)$ and $\overline{\xi}_n(r)$ (note that the latter is a complete orthonormal set along with $\xi_n(r)$). Likewise, F^* has the matrix $\{f_{mn}\}$ (obtained with the aid of the same complete orthonormal systems). Therefore (using the complete orthonormal set $\phi_m(q)$ in $\mathfrak{R}^{\mathrm{I}}$)

$$\mathsf{F}^*\mathsf{F} \quad \text{has the matrix} \quad \Big\{ \sum_{n=1}^{\infty} \overline{f}_{mn} f_{m'n} \Big\}$$

and (using the complete orthonormal set $\overline{\xi}_n(r)$ in $\mathfrak{R}^{\mathrm{II}}$)

$$\mathsf{F}\mathsf{F}^* \quad \text{has the matrix} \quad \Big\{ \sum_{m=1}^{\infty} \overline{f}_{mn} f_{mn'} \Big\}$$

On the other hand (using the complete orthonormal set $\Phi_{mn}(q,r) = \phi_m(q)\xi_n(r)$ in $\mathfrak{R}^{\mathrm{I+II}}$), $\mathsf{U} = \mathsf{P}_{[\Phi]}$ has the matrix $\{\overline{f}_{mn} f_{m'n'}\}$, so that $\dot{\mathsf{U}}$ and $\ddot{\mathsf{U}}$—its projections in $\mathfrak{R}^{\mathrm{I}}$ and $\mathfrak{R}^{\mathrm{II}}$—have the matrices

$$\Big\{ \sum_{n=1}^{\infty} \overline{f}_{mn} f_{m'n} \Big\} \quad \text{and} \quad \Big\{ \sum_{m=1}^{\infty} \overline{f}_{mn} f_{mn'} \Big\}$$

respectively (with the complete orthonormal sets given above).[213] Consequently

U $$\dot{\mathsf{U}} = \mathsf{F}^*\mathsf{F}, \qquad \ddot{\mathsf{U}} = \mathsf{F}\mathsf{F}^*$$

Note that the definitions **F** and the equations **U** make no use of ϕ_m, ξ_n, so hold independently of any particular basis selections.

The operators $\dot{\mathsf{U}}$ and $\ddot{\mathsf{U}}$ are completely continuous, and by **II.11** and **IV.3** they can be written in the form

$$\dot{\mathsf{U}} = \sum_{k=1}^{\infty} w_k' \mathsf{P}_{[\psi_k]}, \qquad \ddot{\mathsf{U}} = \sum_{k=1}^{\infty} w_k'' \mathsf{P}_{[\eta_k]}$$

in which the ψ_k comprise a complete orthonormal set in $\mathfrak{R}^{\mathrm{I}}$, the η_k one in $\mathfrak{R}^{\mathrm{II}}$, and all $w_k', w_k'' \geqslant 0$. We now neglect the terms in the preceding formulas with $w_k' = 0$ or $w_k'' = 0$ respectively, and re-number the remaining terms with $k = 1, 2, \ldots$. Then the ψ_k and η_k again form orthonormal—but now not necessarily complete—sets; the sums

$$\sum_{k=1}^{M'} \quad \text{and} \quad \sum_{k=1}^{M''} \quad \text{appear now in place of} \quad \sum_{k=1}^{\infty}$$

where M', M'' can be either ∞ of finite. Also, all w_k', w_k'' are now > 0.

Let us now consider a ψ_k. $\dot{\mathsf{U}}\psi_k = w_k'\psi_k$ and therefore $\mathsf{F}^*\mathsf{F}\psi_k = w_k'\psi_k$ which gives $\mathsf{F}\mathsf{F}^*\mathsf{F}\psi_k = w_k'\mathsf{F}\psi_k$ whence $\ddot{\mathsf{U}}\mathsf{F}\psi_k = w_k'\mathsf{F}\psi_k$, Furthermore

$$\begin{aligned}(\mathsf{F}\psi_k, \mathsf{F}\psi_\ell) = (\mathsf{F}^*\mathsf{F}\psi_k, \psi_\ell) &= (\dot{\mathsf{U}}\psi_k, \psi_\ell) \\ &= w_k'(\psi_k, \psi_\ell) \\ &= \begin{cases} w_k' & \text{for} \quad k = \ell \\ 0 & \text{for} \quad k \neq \ell \end{cases}\end{aligned}$$

Therefore, in particular, $\|\mathsf{F}\psi_k\| = w_k'$. The $\frac{1}{\sqrt{w_k'}}\mathsf{F}\psi_k$ then form an orthonormal set in $\mathfrak{R}^{\mathrm{II}}$ and they are eigenfunctions of $\ddot{\mathsf{U}}$, with the same eigenvalues as the ψ_k have for $\dot{\mathsf{U}}$ (*i.e.*, w_k'). That is, each eigenvalue of $\dot{\mathsf{U}}$ is an eigenvalue also of $\ddot{\mathsf{U}}$, with at least the same multiplicity. Interchanging $\dot{\mathsf{U}}$ and $\ddot{\mathsf{U}}$ shows that same eigenvalues have in fact the same multiplicities. The w_k' and w_k'' therefore coincide except for their order. Hence $M' = M'' = M$, and by re-enumeration of the w_k'' we obtain $w_k' = w_k'' = w_k$. This done, we can then clearly choose

$$\eta_k = \frac{1}{\sqrt{w_k}}\mathsf{F}\psi_k$$

in general. Then

$$\frac{1}{\sqrt{w_k}}\mathsf{F}^*\eta_k = \frac{1}{w_k}\mathsf{F}^*\mathsf{F}\psi_k = \frac{1}{w_k}\dot{\mathsf{U}}\psi_k = \psi_k$$

[213] The preceding mathematical discussion is based on a paper by E. Schmidt, Math. Ann. **83** (1907).

Therefore[212]

V $$\eta_k = \frac{1}{\sqrt{w_k}}\mathsf{F}\psi_k \qquad \psi_k = \frac{1}{\sqrt{w_k}}\mathsf{F}^*\eta_k$$

Let us now extend the orthonormal set $\psi_1, \psi_2, \ldots$ to a complete orthonormal set $\psi_1, \psi_2, \ldots, \psi_1', \psi_2', \ldots$ and likewise the $\eta_1, \eta_2, \ldots$ to a complete orthonormal set $\eta_1, \eta_2, \ldots, \eta_1', \eta_2', \ldots$ where each of the two sets $\psi_1', \psi_2', \ldots$ and $\eta_1', \eta_2', \ldots$ can be empty, finite or infinite, and each can be selected independently of the other. As previously remarked, **F** and **U** make no reference to any specific orthonormal bases. We are free therefore to use **V**, as well as the above constructions, to determine the selection of the complete orthonormal sets $\phi_1, \phi_2, \ldots$ and $\xi_1, \xi_2, \ldots$. Specifically, we let these coincide with the

$$\psi_1, \psi_2, \ldots, \psi_1', \psi_2', \ldots \quad \text{and} \quad \eta_1, \eta_2, \ldots \eta_1', \eta_2', \ldots$$

respectively: let ψ_k correspond to ϕ_{μ_k} and η_k to ξ_{ν_k} ($k = 1, 2, \ldots$: $\mu_1, \mu_2, \ldots$ different from one another, and $\nu_1, \nu_2, \ldots$ likewise). Then

$$\begin{aligned} \mathsf{F}\phi_{\mu_k} &= \sqrt{w_k}\,\xi_{\nu_k} \\ \mathsf{F}\phi_m &= 0 \quad \text{for} \quad m \neq \mu_1, \mu_2, \ldots \end{aligned}$$

Therefore

$$f_{mn} = \begin{cases} \sqrt{w_k} & \text{for} \quad m = \mu_k,\ n = \nu_k,\ k = 1, 2, \ldots \\ 0 & \text{otherwise} \end{cases}$$

or equivalently

$$\Phi(q, r) = \sum_{k=1}^{M} \sqrt{w_k}\,\phi_{\mu_k}(q)\,\xi_{\nu_k}(r)$$

By suitable choice of the complete orthonormal sets $\phi_m(q)$ and $\xi_n(r)$ we have thus established that each column of the matrix $\{f_{mn}\}$ contains at most one non-zero element (that this is real and > 0, namely $\sqrt{w_k}$, is unimportant for what follows). What is the physical meaning of this mathematical statement?

Let A be an operator with eigenfunctions $\phi_1, \phi_2, \ldots$ and with only distinct eigenvalues (say $a_1, a_2, \ldots$), and likewise, let B have eigenfunctions $\xi_1, \xi_2, \ldots$ and distinct eigenvalues $b_1, b_2, \ldots$. A corresponds to a physical quantity in I, B to one in II. They are therefore simultaneously measurable. It is easily seen that the statement "$\mathcal{A}$ has the value a_m and $\mathcal{B}$ has the value b_n" determines the state $\Phi_{mn}(q, r) = \phi_m(q)\,\xi_n(r)$, and that if the composite system I+II is in state Φ this occurs with probability $(\mathsf{P}_{[\Phi_{mn}]}\Phi, \Phi) = |(\Phi, \Phi_{mn})|^2 = |f_{mn}|^2$. Consequently, our statement means that $\mathcal{A}$, $\mathcal{B}$ are simultaneously measurable, and that if one of them is measured in Φ then the other is uniquely determined by it. (An a_m with all $f_{mn} = 0$ cannot result, because its total probability $\sum_{n=1}^{\infty} |f_{mn}|^2$ cannot be 0; if a_m is ever observed then for exactly one n is

$f_{mn} \neq 0$; likewise for b_n.) There may be several possible $\mathcal{A}$-values in the state Φ (namely, those a_m for which

$$\sum_{n-1}^{\infty} |f_{mn}|^2 > 0$$

i.e., for which there exists an n with $f_{mn} \neq 0$—usually all a_m are such), and an equal number of possible $\mathcal{B}$-values (those b_n for which there exists an m with $f_{mn} \neq 0$), but Φ establishes a one-to-one correspondence between the possible $\mathcal{A}$-values and the possible $\mathcal{B}$-values.

If we call the possible m values $\mu_1, \mu_2, \ldots$ and the corresponding possible n values $\nu_1, \nu_2, \ldots$ then

$$f_{mn} = \begin{cases} c_k \neq 0 & \text{for} \quad m = \mu_k, \ n = \nu_k, \ k = 1, 2, \ldots \\ 0 & \text{otherwise} \end{cases}$$

and therefore (whether M be finite or ∞)

$$\Phi(q, r) = \sum_{k=1}^{M} c_k \phi_{\mu_k}(q)\, \xi_{\nu_k}(r)$$

hence

$$\dot{u}_{mm'} = \sum_{n=1}^{\infty} \overline{f}_{mn} f_{m'n} = \begin{cases} |c_k|^2 & \text{for} \quad m = m' = \mu_k, \ k = 1, 2, \ldots \\ 0 & \text{otherwise} \end{cases}$$

$$\ddot{u}_{nn'} = \sum_{m=1}^{\infty} \overline{f}_{mn} f_{mn'} = \begin{cases} |c_k|^2 & \text{for} \quad n = n' = \nu_k, \ k = 1, 2, \ldots \\ 0 & \text{otherwise} \end{cases}$$

from which we obtain finally

$$\dot{\mathsf{U}} = \sum_{k=1}^{M} |c_k|^2 \mathsf{P}_{[\phi_{\mu_k}]}$$

$$\ddot{\mathsf{U}} = \sum_{k=1}^{M} |c_k|^2 \mathsf{P}_{[\xi_{\nu_k}]}$$

Hence, when Φ is projected in I or II it in general becomes a mixture, though it is a pure state in I+II. Indeed, it provides certain information regarding I+II which cannot be made use of in I alone or in II alone; namely, the one-to-one correspondence between $\mathcal{A}$-values and $\mathcal{B}$-values.

For each Φ we can therefore choose A, B—*i.e.*, the ϕ_m and the ξ_n—such that our condition is satisfied; for arbitrary A, B it may, of course, be violated. Each state Φ then establishes a particular relation between I and II, while the related quantities $\mathcal{A}$, $\mathcal{B}$ depend upon Φ. How far Φ determines them—*i.e.*, the ϕ_m and the ξ_n—is not difficult to answer. If all $|c_k|$ are different and non-zero,

then $\dot{\mathsf{U}}, \ddot{\mathsf{U}}$ (which are determined by Φ) determine the respective ϕ_m, ξ_n uniquely (see **IV.3**). The general discussion is left to the reader.

Finally, let us mention the fact that for $M \neq 1$ neither $\dot{\mathsf{U}}$ nor $\ddot{\mathsf{U}}$ is a state (because several $|c_k|^2 > 0$), while for $M = 1$ both are: $\dot{\mathsf{U}} = \mathsf{P}_{[\phi_{\mu_1}]}$, $\ddot{\mathsf{U}} = \mathsf{P}_{[\xi_{\nu_1}]}$. Then $\Phi(q,r) = c_1 \phi_{\mu_1}(q)\, \xi_{\nu_1}(r)$. We can absorb the c_1 into ϕ_{μ_k}. In short: $\dot{\mathsf{U}}, \ddot{\mathsf{U}}$ are states if and only if $\Phi(q,r)$ has the form $\phi(q)\xi(r)$, in which case $\dot{\mathsf{U}} = \mathsf{P}_{[\phi]}$ and $\ddot{\mathsf{U}} = \mathsf{P}_{[\xi]}$ respectively.

On the basis of the above results, we in summary note: If I is in the state $\phi(q)$ and II in the state $\xi(r)$, then I+II is in the state $\Phi(q,r) = \phi(q) \cdot \xi(r)$. If, on the other hand, I+II is in a state $\Phi(q,r)$ which is not a product $\phi(q) \cdot \xi(r)$ then I and II are mixtures and not states, but Φ establishes a one-to-one correspondence between the possible values of certain quantities in I and II.

3. DISCUSSION OF THE MEASURING PROCESS

Before we complete the discussion of the measuring process in the sense of the ideas developed in **VI.1** (with the aid of the formal tools developed in **VI.2**) we shall make use of the results of **VI.2** to exclude an explanation often proposed to account for the statistical character of the process **1** (see again **V.1**). This rests on the following idea: Let I be the observed system, and II the observer. If I is in the state $\dot{\mathsf{U}} = \mathsf{P}_{[\phi]}$ before the measurement, while II on the other hand is in a mixture

$$\ddot{\mathsf{U}} = \sum_{n-1}^{\infty} w_n \mathsf{P}_{[\xi_n]}$$

then I+II is a uniquely determined mixture U which we can easily calculate from **VI.2**:

$$\mathsf{U} = \sum_{n-1}^{\infty} w_n \mathsf{P}_{[\Phi_n]} \quad \text{where} \quad \Phi_n(q,r) = \phi(q)\xi_n(r)$$

If now a measurement takes place in I, then this is to be regarded as a dynamical interaction of I and II; *i.e.*, as a process **2** (see **V.1**) with an energy operator H. If the process has a time duration t then

$$\mathsf{U} \to \mathsf{U}' = e^{-\frac{i}{\hbar}t\mathsf{H}}\, \mathsf{U}\, e^{\frac{i}{\hbar}t\mathsf{H}}$$

where in fact

$$= \sum_{n=1}^{\infty} w_k \mathsf{P}_{[\Phi_n^{(t)}]} \quad \text{where} \quad \Phi_n^{(t)} = e^{-\frac{i}{\hbar}t\mathsf{H}} \Phi_n$$

Now if each $\Phi_n^{(t)}(q,r)$ were of the form $\psi_n(q)\eta_n(r)$, where the ψ_n are the eigenfunctions of A and the η_n any complete orthonormal set, then this intervention would have the character of a measurement. For it transforms each state ϕ of I into a mixture of the eigenfunctions of A. The statistical character of the result would then arise in this way: Before the measurement,

I was in a (unique) state, but II was a mixture, and that mixture has, in the course of the interaction, associated itself with I+II. And, in particular, it has made a mixture of their projection in I. But the result of such a measurement is indeterminate because the initial state of the observer (before the measurement) is not known exactly. It is conceivable that such a mechanism might function, because the information available to the observer regarding his own state could have absolute limitations, by the laws of nature. These limitations would be expressed in the values of the w_n, which are characteristic of the observer alone (and therefore independent of ϕ).

It is at this point that the attempted explanation breaks down. For quantum mechanics requires that $w_n = (\mathsf{P}_{[\psi_n]}\phi, \phi) = |(\phi, \psi_n)|^2$; *i.e.*, w_n is dependent on ϕ! There might exist another decomposition

$$\mathsf{U}' = \sum_{n=1}^{\infty} w_n' \mathsf{P}_{[\Phi_n']}$$

(the $\Phi_n' = \psi_n(q)\eta_n(r)$ are orthonormal) but this is of no use either, because the w_n' are (except for order), determined uniquely by U' (**IV.3**), and are therefore equal to the w_n.[214]

Therefore, the non-causal nature of the process **1** cannot be attributed to incomplete knowledge of the state of the observer, and we will therefore assume in all that follows that the state of the observer is completely known.

Let us now apply ourselves again to the problem formulated at the end of **VI.1**. I, II and III shall have the meanings given there, and for the quantum mechanical investigation of I, II we shall use the notation of **VI.2**, while III remains outside of the calculations (see the discussion of this in **VI.1**). Let $\mathcal{A}$ be the quantity (in I) actually to be measured, represented by the operator A with eigenfunctions $\phi_1(q), \phi_2(q), \ldots$. Let I be in the state $\phi(q)$.

If I is the observed system, and II+III the observer, then we must apply process **I** and expect to find that the measurement transforms I from the state ϕ to one of the states ϕ_n $(n = 1, 2, \ldots)$. Now, what mode of description must we adopt if I+II is taken to be the observed system, and only III the observer?

In this case we must say that II is a measuring instrument which shows on a scale the value of $\mathcal{A}$ (in I): the position of the pointer on this scale is a physical quantity $\mathcal{B}$ (in II), which is actually observed by III. (If II is already within the body of the observer we have the corresponding physiological concepts in place of the scale and pointer; e.g., retina and image on the retina, etc.) Let $\mathcal{A}$ have the values $a_1, a_2, \ldots$, $\mathcal{B}$ have the values $b_1, b_2, \ldots$, and let the numbering be such that a_n is associated with b_n.

[214] This approach admits of still more variants, all of which must be rejected for similar reasons.

Initially, I is in the (unknown) state $\phi(q)$ and II in the (known) state $\xi(r)$, so I+II is in the state $\Phi(q,r) = \phi(q) \cdot \xi(r)$. The measurement (so far as it is performed by II on I) is, as in the earlier example, carried out by an energy operator H (in I+II) in time t: this is the process **2** which transforms

$$\Phi \longrightarrow \Phi' = e^{-\frac{i}{\hbar} t \mathsf{H}} \Phi$$

Viewed by the observer III, one has a measurement only if the following is the case: If III were to measure (by process **1**) the simultaneously measurable quantities $\mathcal{A}$, $\mathcal{B}$ (in I or II respectively, or both in I+II) then the pair of values a_m, b_n would have probability 0 for $m \neq n$ and probability w_n for $m = n$. That is, it suffices "to look at" II, whereupon $\mathcal{A}$ will have been measured in I. Quantum mechanics imposes the requirement that $w_n = |(\phi, \phi_n)|^2$.

If this is established then the measuring process, so far as it occurs in II, is "explained" theoretically; *i.e.*, the division I | II+III discussed in **VI.1** has been shifted to I+II | III.

The mathematical problem is then the following: A complete orthonormal set $\phi_1, \phi_2, \ldots$ is given in I. We seek such a set $\xi_1, \xi_2, \ldots$ in $\mathfrak{R}^{\mathrm{II}}$, and a state ξ in $\mathfrak{R}^{\mathrm{II}}$, and an energy operator H in $\mathfrak{R}^{\mathrm{I+II}}$, and a time t such that the following holds: If ϕ is an arbitrary state in $\mathfrak{R}^{\mathrm{I}}$ and

$$\Phi'(q,r) = e^{-\frac{i}{\hbar} t \mathsf{H}} \Phi(q,r) \qquad \text{with} \qquad \Phi(q,r) = \phi(q)\xi(r)$$

then Φ' has necessarily the form

$$\Phi'(q,r) = \sum_{n=1}^{\infty} c_n \phi_n(q) \xi_n(r)$$

(where the c_k are naturally dependent upon ϕ). Therefore $|c_m|^2 = |(\phi, \phi_m)|^2$. That the latter is equivalent to the physical requirement formulated above was discussed in **VI.2**.

In the following we shall use a fixed set $\xi_1, \xi_2, \ldots$ and a fixed ξ along with the fixed $\phi_1, \phi_2, \ldots$ and shall investigate the unitary operator

$$\Delta = e^{-\frac{i}{\hbar} t \mathsf{H}}$$

instead of H.

This mathematical problem leads us back to a problem solved in **VI.2**. There a quantity corresponding to our present Φ' was given, and we established the existence of c_n, ϕ_n, ξ_n. Now ϕ_n, ξ_n are fixed, Φ and c_n dependent upon ϕ are given, and we seek to establish the existence of a Δ such that $\Phi' = \Delta\Phi$ gives back these c_n, ϕ_n, ξ_n.

We shall show that such a determination of Δ is indeed possible. In this case, only the principle is of importance to us; *i.e.*, the existence of such a

Δ. The further question—whether the unitary operators Δ corresponding to simple and plausible measuring arrangements also have this property—will not concern us. We have, as it happens, already seen that our requirements coincide with those enlisted in a plausible iterative approach to the measurement process. The arrangements in question are to possess the characteristics of measurement; quantum mechanics would be in blatant contradiction with experience if these Δ did not satisfy our requirements (at least approximately).[215] In the following we will be content to exhibit an abstract Δ—one which in fact satisfies our requirements exactly.

Let the ϕ_m $(m = 0, \pm1, \pm2, \ldots)$ and the ξ_n $(n = 0, \pm1, \pm2, \ldots)$ be two given complete orthonormal sets in $\mathfrak{R}^{\mathrm{I}}$ and $\mathfrak{R}^{\mathrm{II}}$ respectively. (It is simply as a fundamentally irrelevant technical convenience that our indices run now on $0, \pm1, \pm2, \ldots$, rather than on $1, 2, \ldots$.) Let the state ξ be, for simplicity, ξ_0. We define the operator Δ by its action:

$$\Delta \cdot \sum_{m,n=-\infty}^{\infty} x_{mn}\phi_m(q)\xi_n(r) = \sum_{m,n=-\infty}^{\infty} x_{mn}\phi_m(q)\xi_{m+n}(r)$$

Since the $\phi_m(q)\xi_n(r)$ and the $\phi_m(q)\xi_{m+n}(r)$ are both complete orthonormal sets in $\mathfrak{R}^{\mathrm{I+II}}$, this Δ is unitary. Now

$$\phi(q) = \sum_{m=-\infty}^{\infty} (\phi, \phi_m) \cdot \phi_m(q), \qquad \xi(r) = \xi_0(r)$$

so

$$\Phi(q, r) = \phi(q)\xi(r) = \sum_{m=-\infty}^{\infty} (\phi, \phi_m) \cdot \phi_m(q)\xi_0(r)$$

and therefore

$$\Phi'(q, r) = \Delta\Phi(q, r) = \sum_{m=-\infty}^{\infty} (\phi, \phi_m) \cdot \phi_m(q)\xi_m(r)$$

Our purpose is thus accomplished [though in this abstract discussion the structure of $t\mathsf{H} = i\hbar \ln \Delta$ remains unaddressed]. We have in addition $c_m = (\phi, \phi_m)$.

A better overall view of the mechanism of this process can be obtained if we exemplify it by concrete Schrödinger wave functions, and give H in place of Δ.

The observed object, as well as the observer (*i.e.*, I and II respectively) will be characterized by single variables q and r respectively, both running continuously from $-\infty$ to $+\infty$. That is, let both be thought of as points that can move along the line. Their wave functions have then the form $\psi(q)$ and $\eta(r)$ respectively. We will assume that their masses m_1 and m_2 are so large

[215] The corresponding calculation for the case of the position measurement discussed in **III.4** is contained in a paper by Weizsäcker, Z. Physik **70** (1931).

that the kinetic term

$$\mathsf{T} = \tfrac{1}{m_1}\dot{\mathsf{P}}^2 + \tfrac{1}{m_2}\ddot{\mathsf{P}}^2 = \tfrac{1}{m_1}(\tfrac{\hbar}{i}\tfrac{\partial}{\partial q})^2 + \tfrac{1}{m_2}(\tfrac{\hbar}{i}\tfrac{\partial}{\partial r})^2$$

in the composite energy operator $\mathsf{H} = \mathsf{T} + \mathsf{V}_{\text{interaction}}$ can be neglected, and to the interaction term—which is decisive for the measurement—assign the particular form

$$\mathsf{V}_{\text{interaction}} = \tfrac{1}{\tau}\dot{\mathsf{Q}}\ddot{\mathsf{P}} = \tfrac{1}{\tau}q(\tfrac{\hbar}{i}\tfrac{\partial}{\partial r})$$

where τ is a constant with the dimensions of time. Schrödinger's time-dependent differential equation (for the I+II wave functions $\psi_t = \psi_t(q,r)$) then reads

$$\tfrac{1}{\tau}q(\tfrac{\hbar}{i}\tfrac{\partial}{\partial r})\psi_t(q,r) = i\hbar\tfrac{\partial}{\partial t}\psi_t(q,r)$$

or

$$\big(\tau\tfrac{\partial}{\partial t} + q\tfrac{\partial}{\partial r}\big)\psi_t(q,r) = 0$$

of which the general [unnormalized] solution has the form

$$\psi_t(q,r) = f(q, r - \tfrac{1}{\tau}qt)$$

If, at $t = 0$, we have $\psi_0(q,r) = \Phi(q,r)$ then we have $f(q,r) = \Phi(q,r)$ and therefore

$$\psi_t(q,r) = \Phi(q, r - \tfrac{1}{\tau}qt)$$

In particular, if the initial states of I and II are represented by $\phi(q)$ and $\xi(r)$ respectively, then in the sense of our calculational scheme (if the time t appearing therein is chosen to be τ)

$$\Phi(q,r) = \phi(q)\xi(r)$$
$$\Phi'(q,r) = \psi_\tau(q,r) = \phi(q)\xi(r-q)$$

We wish now to show that this can be used by II for a position measurement of I; *i.e.*, that the coordinates are tied to each other. (Since q, r have continuous spectra they are measurable with only arbitrary precision, so this can be accomplished only approximately.)

For this purpose we will assume that $\xi(r)$ differs from 0 only in a very small interval $-\epsilon < r < +\epsilon$ (*i.e.*, that the coordinate of the observer before the measurement is very accurately known); additionally, $\xi(r)$ should, of course, be normalized:

$$\|\xi\| = 1; \quad i.e., \quad \int |\xi(r)|^2 dr = 1$$

The probability that [at time τ] q lies in the interval $[q_0 \pm \delta\,]$ and r in the interval $[r_0 \pm \delta'\,]$ is

$$\int_{q_0-\delta}^{q_0+\delta}\int_{r_0-\delta'}^{r_0+\delta'} |\Phi'(q,r)|^2 dq dr = \int_{q_0-\delta}^{q_0+\delta}\int_{r_0-\delta'}^{r_0+\delta'} |\phi(q)|^2|\xi(r-q)|^2 dq dr$$

Because of the assumption imposed upon $\xi(r)$, this vanishes if q_0 and r_0 differ by more than $\delta + \delta' + \epsilon$, which is to say: q, r are so closely tied to each other that their difference can never be greater than $\delta + \delta' + \epsilon$. And for $r_0 = q_0$ this becomes

$$\int_{q_0-\delta}^{q_0+\delta} |\phi(q)|^2 dq$$

if we choose $\delta' \geqslant \delta + \epsilon$. Since we can choose $\delta, \delta', \epsilon$ to be arbitrarily small (they must, however, be greater than zero) this means that q, r are tied together with arbitrary closeness, and the probability density has the value stipulated by quantum mechanics: $|\phi(q)|^2$.

That is, the properties of measurements, as we have discussed them in **VI.1** and in this section, are realized.

The discussion of more complicated examples—of (say) an analog of the four-term example discussed in **VI.1**, or of the control that a second observer III might effect upon the measurement of I by II—can also be carried out in this fashion. But that will be left to the reader.

NAME INDEX

SUBJECT INDEX

LOCATIONS OF FLAGGED PROPOSITIONS

Although von Neumann did not number his equations, he did attach identifying flags—sometimes arbitrarily, sometimes with mnemonic intent—to principles, defining properties, conditions, rules and equations of special significance. Flags which pertained only to immediate arguments were sometimes used again to identify different propositions in subsequent portions of the text. Those with mnemonic intent were adjusted by Beyer to onform to the translated mnemonic. Here follows a sequential list of the pages on which those flags appear:

ARTICLES CITED

To cite sources in the periodical literature, von Neumann employed a convention rendered so terse by the systematic omission of page numbers and article titles as to become ambiguous when several articles by the same author appear in the same volume. Those citations are spelled out here in searchable detail. Article titles (when not originally in English) are presented here in English translation. The following abbreviations (which occasionally depart from those adopted in the text) are employed in the following list:

Ann. Phys.	=	Annalen der Physik
Ann. Math.	=	Annals of Mathematics
Circ. Math. di Pal.	=	Rendiconti del Circolo di Mathematico di Palermo
Gött. Nachr.	=	Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen
J. für Reine Math.	=	Journal für reine und angewandte Mathematik
Lond. Math. Soc. Proc.	=	Proceedings of the London Mathematical Society
Math. Ann.	=	Mathematische Annalen
Math. Z.	=	Mathematische Zeitschrift
Naturwiss.	=	Naturwissenschaften
Proc. Roy. Soc. London	=	Proceedings of the Royal Society of London
Phil. Mag.	=	Philosophical Magazine
PNAS	=	Proceedings of the National Academy of Sciences
Phys. Rev.	=	Physical Review
Phys. Z.	=	Physikalische Zeitschrift
Verh. d. Physik. Ges.	=	Verhandlungen der Deutschen Physikalische Gesellschaft
Z. Phys.	=	Zeitschrift für Physik

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At several points, von Neumann cites specific passages in Courant & Hilbert's *Methoden der Mathematischen Physik* (1931). Readers will be familiar with the substantially revised English translation of that classic work, which was published as *Methods of Mathematical Physics* (MMP) in 1953. Here follows indication of where (if at all) the passages cited by von Neumann are to be found in MMP:

Note 30, page 17
Note 71, page 69
Note 89, page 88 } : MMP Chapter II, "Linear Integral Equations"

Note 140, page 167 : { MMP ChapterVI, "Application of the Calculus of Variations to Eigenvalue Problems," especially §4. "The maximum-minimum property of eigenvalues"

Page 172 : { MMP page 328, equations (48) & (49) / MMP page 92, equations (31) & (32) } Hermite polynomials

Note 152, page 189 : Omitted in MMP from discussion of Fourier series

LOCATIONS OF THE FOOTNOTES

Von Neumann's notes (displayed originally as endnotes, but here as footnotes) refer fairly frequently to previous notes, which themselves refer occasionally to still earlier notes. It is to reduce the tedium of tracing such references to their root that the following index has been constructed.