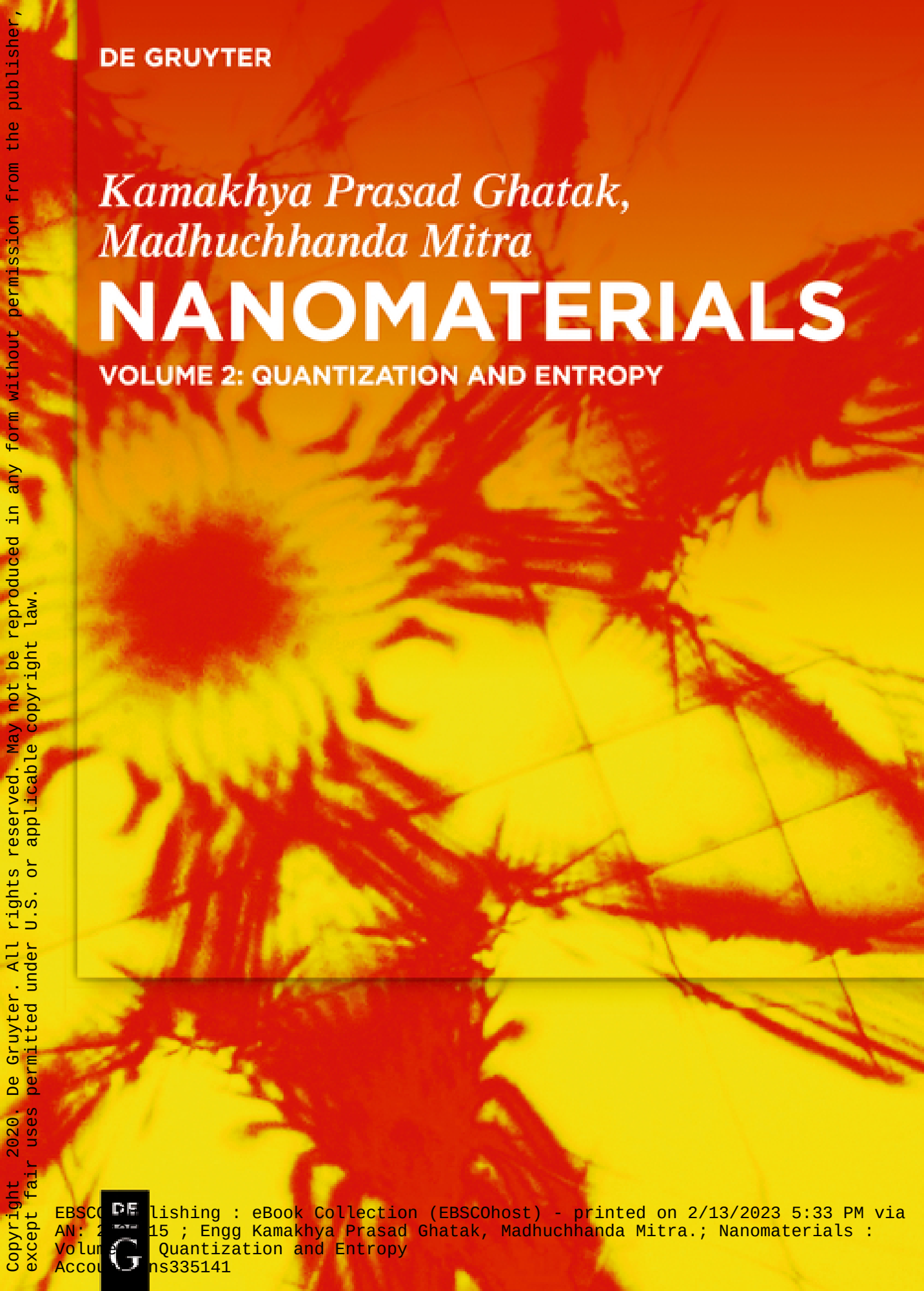

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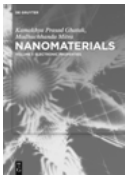

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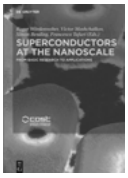

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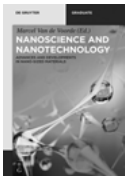

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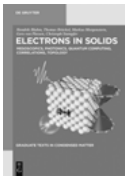

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Nanomaterials

Volume 2: Quantization and Entropy

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After spending forty years in Nanomaterials, I have finally realized that my education is nothing but heducation and my real I, is not at all equal to the sum of the body I wear and the mind which drives the body.

From the desk of the first author:
The author dedicates this book to the following beautiful trio whose combined effort is just like a Decadron to him to revive the last phase of his academic life.

1. Professor Dr. S. Chakrabarti, the Hon'ble Director of the Institute of Engineering and Management, his present mentor for kindly picking him from National Institute of Technology at Agartala at rather academic turbulent moments and transforming myself as a member of IEM and UEM family.
2. Professor Dr. B. Chatterjee, the Hon'ble Vice-Chancellor of the University of Engineering and Management, Jaipur for his warm personality which generates in the mind the confidence that "*Yes, I can*".
3. Professor R. Paul Dean Research (Associate) of the University of Engineering and Management, Kolkata for behaving like the academic daughter of the author to feel that at least in odd times she will be besides him.

From the desk of the Second author:
The second author dedicates this book to Mr. B. Nag, her colleague and lifelong time tested friend for making her life always pleasant in the Department of Applied Physics of the University of Calcutta.

Preface

Calmness and tolerance act like air conditioning in a hot room and increase everyone's efficiency.

The applications and the importance of nanomaterials in many dimensions are already well known since its creation in the domain of low dimensional science and technology. An enormous range of powerful applications of such low dimensional structures in the quantum regime together with a rapid increase in computing power, have generated considerable interest in the study of the quantum effect devices based on various new materials of reduced dimensionality. Examples of such new applications include quantum registers, quantum switches, quantum sensors, quantum logic gates, quantum well (QWs), nanowires (NWs), quantum box (QBs), quantum wire transistors, quantum cascade lasers, high-speed digital networks, high-resolution terahertz spectroscopy, advanced integrated circuits, superlattice photo-oscillator, superlattice photo-cathodes, resonant tunneling diodes and transistors, superlattice coolers, thermoelectric devices, thin film transistors, micro-optical systems, high performance infrared imaging systems, single electron/molecule electronics, nano-tube based diodes, and other nano-electronic devices [1–14].

In volume 1 of the series on nanomaterials, we have investigated ***few Electronic Properties of Opto electronic nanomaterials having various band structures under different physical conditions in the presence of intense photon field with the use of the Heisenberg's Uncertainty Principle (HUP)***. In this context, it may be written that the available reports on the said areas cannot afford to cover even an entire chapter regarding the ***ENTROPY*** in heavily doped (HD) nanomaterials and after thirty years of continuous effort, we see that the complete investigations of the entropy comprising of the whole set of materials and allied sciences is really a sea and is a permanent member of the domain of impossibility theorems.

It may be noted that the entropy is a significant concept and a physical phenomenon which occupies a singular position in the whole arena of science and technology in general and whose importance has already been established since the inception of second law of thermodynamics which in recent years finds extensive applications in modern thermodynamics of nanomaterials, characterization and investigation of condensed matter systems, thermal properties of thermal semiconducting devices and related aspects in connection with the investigations of the thermal properties of nanomaterials [15–19].

It is well known that the entropy is the measure of disorder or uncertainty about a system [15–19]. The equilibrium state of a system maximizes the entropy as all the information about the initial conditions except that the conserved variables are lost. According to the second law of thermodynamics the total entropy of any system will not decrease other than by increasing the entropy of some other system. A reduction in the increase of entropy in a specified process, such as a chemical

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reaction, means that it is energetically more efficient. In accordance to the second law of thermodynamics the entropy of a system that is not isolated may decrease. In mechanics, the second law in conjunction with the fundamental thermodynamic relation places limits on a system's ability to do useful work. The entropy change of a system at temperature T absorbing an infinitesimal amount of heat δq in a reversible way is given by $\delta q/T$. Statistical mechanics demonstrates that entropy is governed by probability, thus allowing for a decrease in disorder even in an isolated system. According to Boltzmann's the entropy is a measure of the number of possible microscopic states (or microstates) of a system in thermodynamic equilibrium. Entropy is the only quantity in the physical sciences that seems to imply a particular direction of progress, sometimes called an arrow of time.

The significant work of Zawadzki [20] reflects the fact that the entropy for materials having degenerate electron concentration is independent of scattering mechanisms and is exclusively determined by the dispersion laws of the respective carriers. It will, therefore, assume different values for different systems and varies with the doping, the magnitude of the reciprocal quantizing magnetic field under magnetic quantization, the nanothickness in ultrathin films, quantum wires and dots, the quantizing electric field as in inversion layers, the carrier statistics in various types of quantum confined superlattices having different carrier energy spectra and other types of low-dimensional field assisted systems.

It is well known that heavy doping and carrier degeneracy are the keys to unlock the important properties of Materials and they are especially instrumental in dictating the characteristics of Ohomic contacts and Schottky contacts, respectively [21–31]. It is an amazing fact that although the heavily doped materials (HDS) have been investigated in the literature but the study of the corresponding entropies of HDS ***is still one of the open research problems***. **This first monograph solely investigates the entropy** *in HD non-linear optical, III-V, II-VI, Gallium Phosphide, Germanium, Platinum Antimonide, stressed, IV-VI, Lead Germanium Telluride, Tellurium, II-V, Zinc and Cadmium di-phosphides, Bismuth Telluride, III-V, II-VI, IV-VI and HgTe/CdTequantum well HD superlattices with graded interfaces under magnetic quantization, III-V, II-VI, IV-VI and HgTe/CdTe HD effective mass superlattices under magnetic quantization, quantum confined effective mass superlattices and superlattices of HD optoelectronic materials with graded interfaces respectively*. Our method is not at all related with the Density-of-States (DOS) technique as used in the literature. From the electron energy spectrum, one can obtain the DOS but the DOS technique, as used in the literature cannot provide the *E-k* dispersion relation. *Therefore, our study is more fundamental than those in the existing literature, because the Boltzmann transport equation, which controls the study of the charge transport properties of the semiconductor devices, can be solved if and only if the E-k* dispersion relation *is known.*

This book is divided into two parts each containing 5 and 4 chapters and 5 appendices is partially based on our on-going researches on the entropy in HDS and

an attempt has been made to present a cross section of the entropy for wide range of HDS and their quantized-structures with varying carrier energy spectra under various physical conditions.

It is well known that the band tails are being formed in the forbidden zone of the HDS and can be explained by the overlapping of the impurity band with the conduction and valence bands [32]. Kane [33] and Bonch Bruevich [34] have independently derived the theory of band tailing for materials having unperturbed parabolic energy bands. Kane's model [33] was used to explain the experimental results on tunneling [35] and the optical absorption edges [36, 37] in this context. Halperin and Lax [38] developed a model for band tailing applicable only to the deep tailing states. Although Kane's concept is often used in the literature for the investigation of band tailing [39, 40], it may be noted that this model [33, 41] suffers from serious assumptions in the sense that the local impurity potential is assumed to be small and slowly varying in space coordinates [40]. In this respect, the local impurity potential may be assumed to be a constant. In order to avoid these approximations, we have developed in this book, the electron energy spectra for HDS for studying the entropy based on the concept of the variation of the kinetic energy [32, 40] of the electron with the local point in space coordinates. This kinetic energy is then averaged over the entire region of variation using a Gaussian type potential energy. On the basis of the E–k dispersion relation, we have obtained the electron statistics for different HDS for the purpose of numerical computation of the respective entropy. It may be noted that, a more general treatment of many-body theory for the DOS of HDS merges with one-electron theory under macroscopic conditions [32]. Also, the experimental results for the Fermi energy and others are the average effect of this macroscopic case. So, the present treatment of the one-electron system is more applicable to the experimental point of view and it is also easy to understand the overall effect in such a case [31]. In a HDS, each impurity atom is surrounded by the electrons, assuming a regular distribution of atoms, and it is screened independently [39, 42, 43]. The interaction energy between electrons and impurities is known as the impurity screening potential. This energy is determined by the inter-impurity distance and the screening radius (popularly known as the Debye screening length). The screening length changes with the band structure. Furthermore, these entities are important for HDS in characterizing the semiconductor properties [44–47] and the modern electronic devices [39, 46]. The works on Fermi energy and the screening length in an n-type GaAs have already been initiated in the literature [47], based on Kane's model. Incidentally, the limitations of Kane's model [33, 40], as mentioned above, are also present in their studies.

The part one deals with the influence of quantum confinement on the entropy of non-parabolic HDS and in chapter one we study the entropy in QWs of HD nonlinear optical materials on the basis of a generalized electron dispersion law introducing the anisotropies of the effective masses and the spin orbit splitting constants respectively together with the inclusion of the crystal field splitting within the framework of

the $\vec{k}.\vec{p}$ formalism. ***We will observe that the complex electron dispersion law in HDS instead of real one occurs from the existence of the essential poles in the corresponding electron energy spectrum in the absence of band tails***. The physical picture behind the existence of the complex energy spectrum in HD non-linear optical Materials is the interaction of the impurity atoms in the tails with the splitting constants of the valance bands. The more is the interaction, the more the prominence of the complex part than the other case. In the absence of band tails, there is no interaction of the impurity atoms in the tails with the spin orbit constants and consequently, the complex part vanishes. One important consequence of the HDS forming band tails is that ***the effective electron mass (EEM) exists in the forbidden zone, which is impossible without the effect of band tailing. In the absence of band tails, the effective mass in the band gap of Materials is infinity. Besides, depending on the type of the unperturbed carrier energy spectrum, the new forbidden zone will appear within the normal energy band gap for HDS.***

The results of HD III-V (e.g. *InAs*, *InSb*, *GaAs* etc.), ternary (e.g. $Hg_{1-x}Cd_xTe$), quaternary (e.g. $In_{1-x}Ga_xAs_{1-y}P_y$ *lattice matched to InP*) compounds form a special case of our generalized analysis under certain limiting conditions. The entropy in HD QWs of II-VI, IV-VI, stressed Kane type materials, *Te*, *GaP*, $PtSb_2, Bi_2Te_3$, *Ge*, *GaSb*, II-V, Lead Germanium Telluride, Zinc and Cadmium Diphosphides has also been investigated in the appropriate sections. The importance of the aforementioned materials has also been described in the same chapter. In the absence of band tails and under the condition of extreme carrier degeneracy together with certain limiting conditions, all the results for all the entropies for all the HD QWs of chapter one get simplified into the form of isotropic parabolic energy bands exhibiting the necessary mathematical compatibility test. In the second and third chapters, the entropy for HD nanowires (NWs) and quantum boxes (QBs) of all the materials of chapter 1 have respectively been investigated. As a collateral study we shall observe that the EEM in such QWs and NWs becomes a function of size quantum number, the Fermi energy, the scattering potential and other constants of the system which is the intrinsic property of such 2D and 1D electronic materials.

In this context, it may be noted that the effects of quantizing magnetic field (B) on the band structures of compound materials are most striking than that of the parabolic one and are easily observed in experiments. A number of interesting physical features originate from the significant changes in the basic energy wave vector relation of the carriers caused by the magnetic field. The valuable information could also be obtained from experiments under magnetic quantization regarding the important physical properties such as Fermi energy and effective masses of the carriers, which affect almost all the transport properties of the electron devices [48] of various materials having different carrier dispersion relations [49].

Specifically in chapter four we study the entropy in HD non-linear optical materials in the presence of strong magnetic field leading to the magnetic quantization of the energy band states of the corresponding bulk HD materials. The results

of HD III-V (e.g. *InAs*, *InSb*, *GaAs* etc.), ternary (e.g. $Hg_{1-x}Cd_xTe$), quaternary (e.g. $In_{1-x}Ga_xAs_{1-y}P_y$ *lattice matched to InP*) compounds form a special case of our generalized analysis under certain limiting conditions. The entropy for HD II-VI, IV-VI, stressed Kane type materials, *Te*, *GaP*, $PtSb_2, Bi_2Te_3$, *Ge*, *and GaSb* has also been investigated by formulating the respective appropriate HD energy band structure. In the absence of band tails and under the condition of extreme carrier degeneracy together with certain limiting conditions, all the results for all the entropies for all the HD materials of this chapter one get simplified into the well-known parabolic energy bands under strong magnetic quantization exhibiting the necessary mathematical compatibility test. In chapter five we have studied the entropy for all the HD materials of chapter four in the presence of magneto size quantization.

In part two we have studied the entropies in HD quantum confined superlattices (SLs). It is well known that Keldysh [50] first suggested the fundamental concept of a SL, although it was successfully experimental realized by Esaki and Tsu [51]. The importance of SLs in the field of nano-electronics has already been described in [52–53]. The most extensively studied III-V SL is the one consisting of alternate layers of *GaAs* and $Ga_{1-x}Al_xAs$ owing to the relative ease of fabrication. The *GaAs*layer forms quantum wells and $Ga_{1-x}Al_xAs$ form potential barriers. The III-V SL's are attractive for the realization of high speed electronic and optoelectronic devices [54]. In addition to SLs with usual structure, SLs with more complex structures such as II-VI [55], IV-VI [56] and *HgTe*/*CdTe* [57] SL's have also been proposed. The IV-VI SLs exhibit quite different properties as compared to the III-V SL due to the peculiar band structure of the constituent materials [58]. The epitaxial growth of II-VI SL is a relatively recent development and the primary motivation for studying the mentioned SLs made of materials with the large band gap is in their potential for optoelectronic operation in the blue [59]. *HgTe*/*CdTe*SL's have raised a great deal of attention since 1979, when as a promising new materials for long wavelength infrared detectors and other electro-optical applications [60]. Interest in Hg-based SL's has been further increased as new properties with potential device applications were revealed [61]. These features arise from the unique zero band gap material *HgTe* [62] and the direct band gap materials *CdTe* which can be described by the three band mode of Kane [63]. The combination of the aforementioned materials with specified dispersion relation makes *HgTe*/*CdTe* SL very attractive, especially because of the possibility to tailor the material properties for various applications by varying the energy band constants of the SLs. In addition to it, for effective mass SLs, the electronic sub-bands appear continually in real space [64, 65, 66].

We note that all the aforementioned SLs have been proposed with the assumption that the interfaces between the layers are sharply defined, of zero thickness, i.e., devoid of any interface effects. The SL potential distribution may be then considered as a one dimensional array of rectangular potential wells. The aforementioned advanced experimental techniques may produce SLs with physical interfaces between

the two materials crystallographically abrupt; adjoining their interface will change at least on an atomic scale. As the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the electrons. The influence of finite thickness of the interfaces on the electron dispersion law is very important, since the electron energy spectrum governs the electron transport in SLs.

The chapter six explores the entropy in III-V, II-VI, IV-VI, *HgTe*/*CdTe* and strained layer heavily doped Quantum wire superlattices (QWHDSLs) with graded interfaces and heavily doped quantum wire effective mass super lattices respectively. The chapter seven investigates the entropy in quantum dot HDSLs for all cases of chapter six. The chapter eight of part two of this book contains the study of the entropy in HD SLs under magnetic quantization for all the cases of chapter six. The chapter nine contains the conclusions and future research in this context.

With the advent of nano-devices, the built-in electric field becomes so large that the electron energy spectrum changes fundamentally instead of being invariant and the chapter 10 (**Appendix A**) of this book investigates the entropy under intense electric field in bulk specimens of HD III-V, ternary and quaternary materials. The same chapter explores the influence of electric field on the entropy in the presence of magnetic quantization, cross-fields configuration, QWs, NWs, QBs, magneto size quantum effect, inversion and accumulation layers, magneto inversion and magneto accumulation layers, doping superlattices, magneto doping superlattices, QWHD, NWHD and QBHD effective mass superlattices, magneto QWHD effective mass superlattices, magneto HD effective mass superlattices, QWHD, NWHD and QBHD superlattices with graded interfaces, magneto QWHD superlattices with graded interfaces and magneto HD superlattices with graded interfaces and respectively magnetic quantization, size quantization, accumulation layers, HD doping superlattices and effective mass HD superlattices under magnetic quantization respectively. **It is interesting to note that the EEM depends on the strong electric field** (which is not observed elsewhere) together with the fact that the EEM in the said systems depends on the respective quantum numbers in addition to the Fermi energy, the scattering potential and others system constants which are the characteristics features of such hetero-structures.

The Chapter 10 (**Appendix A**) investigates the entropy in bulk specimens HD Kane type materials under intense electric field in the presence of strong magnetic quantization after formulating the electron dispersion law in the present case. The same appendix studies the entropy under cross-fields configuration, QWs, NWs, QBs, magneto size quantum effect, inversion and accumulation layers, magneto inversion and magneto accumulation layers, doping superlattices, magneto doping superlattices, QWHD, NWHD and QBHD effective mass superlattices, magneto QWHD effective mass superlattices, magneto HD effective mass superlattices, QWHD, NWHD and QBHD superlattices with graded interfaces, magneto QWHD superlattices with graded interfaces and magneto HD superlattices with graded interfaces and respectively.

In this context we have already noted that the semiconductor superlattices (SLs) composed of alternative layers of two different degenerate layers with controlled thickness [67] have found wide applications in many new devices such as photodiodes, photo-resistors [67, 68], transistors [69], light emitters [70], tunneling devices [71], etc. [72–84]. The investigations of the physical properties of narrow gap SLs have increased extensively; since they are important for optoelectronic devices and because of the quality of hereto-structures, involving narrow gap materials have been improved. It may be noted in this context that the doping superlattices, are crystals with a periodic sequence of ultrathin film layers [85, 86] of the same semiconductor with the intrinsic layer in between together with the opposite sign of doping. All the donors will be positively charged and all the acceptors negatively. This periodic space charge causes a periodic space charge potential which quantizes the motions of the carriers in the z-direction together with the formation of the sub-band energies. *In Chapter 11(**Appendix B**), the* entropy *in doping superlattices of HD nonlinear optical, III-V, II-VI, IV-VI, and stressed Kane type Materials has been investigated. In this case we will note that the EEM in such doping supper lattices becomes a function of nipi sub-band index, surface electron concentration, Fermi energy, the scattering potential and other constants of the system which is the intrinsic property of such 2D quantized systems. In Chapter 12 (**Appendix C**) the entropy in QWHDSLs under magnetic quantization have been studied.*

It is well known that the electrons in bulk materials in general, have three dimensional freedom of motion. When, these electrons are confined in a one dimensional potential well whose width is of the order of the carrier wavelength, the motion in that particular direction gets quantized while that along the other two directions remains as free. Thus, the energy spectrum appears in the shape of discrete levels for the one dimensional quantization, each of which has a continuum for the two dimensional free motion. The transport phenomena of such one dimensional confined carriers have recently studied [87] with great interest. For the metal-oxide-semiconductor (MOS) structures, the work functions of the metal and the semiconductor substrate are different and the application of an external voltage at the metal-gate causes the change in the charge density at the oxide semiconductor interface leading to a bending of the energy bands of the semiconductor near the surface. As a result, a one dimensional potential well is formed at the semiconductor interface. The spatial variation of the potential profile is so sharp that for considerable large values of the electric field, the width of the potential well becomes of the order of the de Broglie wavelength of the carriers. The Fermi energy, which is near the edge of the conduction band in the bulk, becomes nearer to the edge of the valance band at the surface creating inversion layers. The energy levels of the carriers bound within the potential well get quantized and form electric sub bands. Each of the sub-band corresponds to a quantized level in a plane perpendicular to the surface leading to a quasi two dimensional electron gas. Thus, the extreme band bending at low temperature allows us to observe the quantum effects at

the surface. Although, considerable work has already been done regarding the various physical properties of different types of inversion layers having various band structures, nevertheless it appears from the literature that there lies scopes in the investigations made while the interest for studying different other features of accumulation layers is becoming increasingly important. In *chapter 13* (**Appendix D**), the Entropy in accumulation layers of HD nonlinear optical, III-V, II-VI, IV-VI, stressed Kane type Materials and *Ge* have been investigated. For the purpose of relative comparisons, we have also studied the entropy in inversion layers of the afore-mentioned materials. *It is interesting to note that the EEM in such layers is a function of electric sub-band index, surface electric field, Fermi energy, the scattering potential and other constants of the system which is the intrinsic property of such 2D electrons*.

It is worth remarking that the influence of crossed electric and quantizing magnetic fields on the transport properties of materials having various band structures has relatively less investigated as compared with the corresponding magnetic quantization, although, the cross-fields are fundamental with respect to the addition of new physics and the related experimental findings in modern quantum effect devices. It is well known that in the presence of electric field (E_0) along x-axis and the quantizing magnetic field (B) along z-axis, the mass of the carriers in materials become modified and for which the carrier moves in both the z and y directions. The motion along y-direction is purely due to the presence of E_O along x-axis and in the absence of electric field, the effective electron mass along y-axis tends to infinity which indicates the fact that the electron motion along y-axis is forbidden. The effective electron mass of the isotropic, bulk materials having parabolic energy bands exhibits mass anisotropy in the presence of cross fields and this anisotropy depends on the electron energy, the magnetic quantum number, the electric and the magnetic fields respectively, although, the effective electron mass along z- axis is a constant quantity. In 1966, Zawadzki and Lax [88] formulated the entropy for III-V materials in accordance with the two band model of Kane under cross fields configuration which generates the interest to study this particular topic of solid state science in general [89].

The chapter 14 (**Appendix E**) investigates the entropy under cross-field configuration in HD nonlinear optical, III-V, II-VI, IV-VI and stressed Kane type materials respectively. This chapter also tells us that the EEM in all the cases is a function of the finite scattering potential, the magnetic quantum number and the Fermi energy even for HD materials whose bulk electrons in the absence of band tails are defined by the parabolic energy bands. The last chapter 15 (Appendix F) contains the numerical values of the energy band constants of few materials.

It is needless to say that this monograph is based on the ***'iceberg principle'*** [90] and the rest of which will be explored by the researchers of different appropriate fields. Since, there is no existing report devoted solely to the study of entropy for HD quantized structures to the best of our knowledge, we hope that the present book will a useful reference source for the present and the next generation of the

readers and the researchers of nano-materials and allied sciences in general. We have discussed enough regarding the Entropies in different quantized HD materials although lots of new computer oriented numerical analysis are being left for the purpose of being computed by the readers, to generate the new graphs and the inferences from them which all together is a sea in itself. The production of error free first edition of any book from every point of view is a permanent member in the domain of impossibility theorems, the same stands very true for this monograph also. Various expressions and a few chapters of this book have been appearing for the first time in printed form. The suggestions from the readers for the development of the book will be highly appreciated for the purpose of inclusion in the future edition, if any. In this book, from chapter one to till chapter fourteen, we have presented circa ***200 open research problems*** for the graduate students, PhD aspirants, researchers, engineers in this pinpointed research topic. We strongly hope that alert readers of this monograph will not only solve the said problems by removing all the mathematical approximations and establishing the appropriate uniqueness conditions, but also will generate new research problems both theoretical and experimental and, thereby, transforming this monograph into a solid book. Incidentally, our readers after reading this book will easily understand that how little is presented and how much more is yet to be investigated in this exciting topic which is the signature of coexistence of new physics, advanced mathematics combined with the inner fire for performing creative researches in this context from the young scientists since like Kikoin [91] we feel that ***"A young scientist is no good if his teacher learns nothing from him and gives his teacher nothing to be proud of"***. We emphatically write that the problems presented here form the integral part of this book and will be useful for the readers to initiate their own contributions on the entropy for HDS and their quantized counter parts since like Sakurai [92] we firmly believe *"The reader who has read the book but cannot do the exercise has learned nothing"*.

In this monograph, we have formulated ***the expressions of effective electron mass and the sub-band energy throughout this monograph as a collateral study, for the purpose of in-depth investigations of the said important pinpointed research topics***. Thus, in this book, the readers will get much information regarding the influence of quantization in HD low dimensional materials having different band structures. Although the name of the book is extremely specific, from the content, one can easily infer that it should be useful in graduate courses on materials science, condensed matter physics, solid states electronics, nano-science and technology and solid-state sciences and devices in many Universities and the Institutions in addition to both Ph.D. students and researchers in the aforementioned fields. *Last but not the least, we do hope that our humble effort will kindle the desire to delve deeper into this fascinating and deep topic by any one engaged in materials research and device development either in academics or in industries.*

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Real gentleness in a person is the power that sees, understands, yet never interferes.

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I am grateful to all my friends and colleagues for the last 40 years from my school days till date for forming my inner fire to solve independently the problems from five volumes of Berkley Physics Course, three volumes of Sakurai, ten volumes of Addison-Wesley Modular Series on Solid State Devices, two volumes of Cohen-Tannoudji et al., three volumes of Edwards, three volumes of Carslaw, six volumes of Guillemin, three volumes of Tuttle, two volumes of Scott, two volumes of Budak, five volumes of Chen. It is curious to note that they are insisting me in the real sense of the term to verify all the entries of Gradshteyn-Ryzhik and three volumes of Bateman manuscript project for the last 40 years. It may be noted that academic output of a nice scholar is the response of a good quality RC coupled amplifier in the mid-band zone, whereas the same for a fine research worker is the Dirac's delta function. Incidentally, I can safely say that I belong to neither as a consequence of the academic surroundings which this life presents to me. I express my warm gratitude to H. L. Hartnagel, D. Bimberg, W. L. Freeman, and W. Schommers for various academic interactions spanning over the last three decades. I remember the sweet memories of P.N. Robson, I.M. Stephenson, V.S. Letokhov, J. Bodnar, and K.F. Brennan with true reverence for inspiring me with the ebullient idea that the publications of the research monographs from internationally reputed publishers containing innovative concepts is of prime importance to excel in creative research activity.

On 30 December 2006, I wrote a letter to Late P.T. Landsberg (popularly known as P.T.L among his scientific friends) for writing a book on Electron Statistics of nanostructured materials which can at least transform me in to a better scientist but P.T.L in turn requested me repeatedly to complete the proposed book at the earliest and often expressed his desire to write a foreword for this book. Incidentally, due to previous other heavy academic and related commitments I was unable to finish this present monograph and his wife Mrs. Sophia Landsberg in her letter of desperate sadness dated January 12, 2009, informed me that from 2008 onward due to Alzheimer's disease her husband had to give up scientific works. The disappearance of P.T.L. from my research scenario is a big shock to me, which I will have to bear till my own physical disappearance. I still remember his power-packed words that "The definition of Kamakhya Prasad Ghatak (K.P.G.) = M.Tech. + Ph.D. + D. Engg. + more than 300 research papers in nanoscience and technology in SCI Journals + more than 60 research papers and International Conferences of SPIE and MRS of USA + Ph.D. guide of more than three dozens of Ph.D. students + many research monographs form Springer-Verlag, Germany + HOD + Dean+ Senior Professor is a **big zero to P.T.L. if K.P.G. cannot live in a world full of new creative concepts and not merely repeating the past successes, since past success is a dead concept at least to P.T.L.**

On 21 December 1974, A. N. Chakravarti (an internationally recognized expert on Einstein Relation in general), my mentor in my first interaction with him, emphatically

energized me by making myself acquainted with the **famous Fermi-Dirac Integrals** and telling me that **I must master** *Semiconductor Statistics* (Pergamon Press, London, 1962) by **J. S. Blakemore** for my initiation in semiconductor physics. Later on, I got in touch with K. Seeger, the well-known author of the book *Semiconductor Physics* (Springer Series in Solid State Sciences, vol. 40, Springer-Verlag, Germany, 1982). The solid mathematical physicist Late P. N. Butcher has been a steady hidden force since 1983 before his sad demise with respect to our scripting the series in band structure dependent properties of nanostructured materials. Both P. T. L. and P. N. Butcher visited the Institute of Radio Physics and Electronics of the University of Calcutta, my ALMA MATER where I started my research as a M. Tech. student and later on as a faculty member. I formed permanent covalent bonds with J. S. Blakemore, K. Seeger, P. N. Butcher, and P.T. L through letters (pre-email era), and these four first class semiconductor physicist, in turn, shared with pleasure their vast creative knowledge of materials and related sciences with a novice like me.

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In this context, from the flashback of my memory I wish to offer my indebtedness to M. Mondal, the first member of my research team who in 1983 joined with me to complete his Ph.D. work under my guidance when R. K. Poddar, the then Vice-chancellor of the University of Calcutta selected me as a Lecturer (presently Assistant Professor) of the famous Department of Radio Physics and Electronics. In 1987, S. K. Sen, the then Vice-chancellor of Jadavpur University accepted me as the Reader (presently Associate Professor) in the Department of Electronics and Telecommunication Engineering and since then many young researchers (more than 12 in numbers consisting of B. Mitra, A. Ghoshal, D. Bhattacharya, A. R. Ghatak, and so on) around me created my research team and insisted me to work with them at the rate of 16 hours per day including holidays in different directionsof research for the purpose of my creative conversion from an ordinary engineer to a 360° research scientist, and consequently I enjoyed the high rate of research publications in different reputed international journals in various aspects of band structure-dependent properties of quantized structures. It is nice to note that these young talented researchers obtained their respective Ph. D degree under my direct supervision. Incidentally, in 1994, R. K. Basu, the then Vice-chancellor of the University of Calcutta selected me as a Professor in the Department of Electronic Science and another flood of research overwhelmed me in a new direction of materials science. The persons responsible for this change include S. Datta, S. Sengupta, A. Ali, and so on. The 11th and 12th names of this golden series are S. Bhattacharya and D. De,

respectively, who, in turn, formed permanent covalent bonds with me not only with respect to research (S. Bhattacharya and D. De are respectively the coauthors of seven and two monographs in different series of Springer) but also in all aspects of life in general.

It is interesting to note that after serving 18 years as a Professor in the Department of Electronic Science, in 2012, P. K. Bose, and the then Director of the National Institute of Technology, Agartala, requested me to join as a Professor and Departmental Head in Electronics and Communication Engineering. He being my life-long friend, I accepted his offer (and later on as a Dean), and more than 10 young scholars around me again directed my research in an altogether new direction. In 2015 the respected Director Professor S. Chakrabarti of Institute of Engineering and Management in Salt Lake City, Kolkata, has kindly offered me the position of Research Director and Senior Professor in his famous institute in the academic fag end of my life to complete my last run toward the creative knowledge temple with my new young research workers. I am grateful to him for his creative gesture. In my 40+ years of teaching life (I have the wide experience of teaching Physics, Mathematics, Applied Mechanics – from engineering statics up to nonlinear mechanics including indeterminate structures) and 70% of the courses of Electronics and Telecommunication and Electrical Engineering, respectively) and 40+ years of research life (mostly in Materials Science, Nano-science and Number Theory), I have finally realized that teaching without research is body without brain and research without teaching is body without blood **although my all-time hero, creatively prolific number-theorist Godfrey Harold Hardy in his classic book entitled *A Mathematician's Apology* (Cambridge University Press, 1990) tells us "I hate teaching."**

Incidentally, one young theoretician friend of mine often tells me that many works in theoretical semiconductor science are based on the following seven principles:

- Principles of placing the necessary and sufficient conditions of a proof in the band-gap regime.
- Principles of interchange of the summation and the integration processes and unconditioned convergences of the series and the integrals.
- Principles of random applications of one electron theory and superposition theorem in studying the properties of materials, although the many body effects are very important together with the fact that the nature is fundamentally nonlinear in nature.
- Principles of using the invariant band structure concept of materials even in the presence of strong external fields (light, electric, heavy doping, etc.) and the random applications of perturbation theory, which is in a sense quantum mechanical Taylor series without considering the related consequences.
- Principle of random applications of the binomial theorem without considering the important concept of branch cut.
- Principle of little discussion regarding the whole set of materials science comprising of different compounds having various band structures under different

physical conditions as compared with the simplified two-band model of Kane for III–V materials.
- Principle of using the Fermi's golden rule, the band structure, and the related features, which are valid for nondegenerate materials to materials having degenerate carrier concentrations directly.

Although my young friend is a purist in his conjecture, there are no doubt certain elements of truth inside his beautiful comments. I hope that our readers will present their intricate and advanced theories after paying due weightage of his aforementioned seven principles.

I offer special thanks to the members of my research team for placing their combined effort toward the development of this book in the DO-LOOP of a computer and critically reading the manuscript in its last phase before sending it to C. Ascheron, Ex-Executive Editor Physics, Springer-Verlag. Last but not the least; I am grateful forever to our lifelong time-tested friend S. Sanyal, Principal, Lake School for Girls, Kolkata, for not only motivating me at rather turbulent moments of my academic carrier but also instilling in me the concept that **the ratio of total accumulated knowledge in my chosen field of research to my own contribution in my topic of research tends to infinity at any time and is the definition of nonremovable pole in the transfer function of my life.**

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Kolkata, India
9 January 2019

K. P. Ghatak,
M. Mitra

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About the Authors

When Love is real, people don't need to impress, for Love in itself leaves a solid positive impression.

Professor Kamakhya Prasad Ghatak (h-index34, i10 index-168, maximum citation of a research paper 359 and total citations5295) is the first recipient of the Doctor of Engineering Degree of Jadavpur University, Kolkata, in 1991 since the inception of the university in 1955, and in the same year he received the Indian National Science Academy visiting fellowship award for IITKharagpur. He is the principal coauthor of more than 400 research papers in SCI journals, seven research monographs on various topics of nanotechnology from Springer-Verlag, Germany (Vol.170 in *Solid State Science*, Vols. 116, 137, and 167 in *Materials Science*, Vols. 255 and 260 in *Tracts in Modern Physics* (TMP), 1 in *Nanostructured Science and Technology* series) and vol. 1 in *Nanomaterials* series of DeGruyter, Germany. He is the solo author of Vols. 262 and 265 in TMP of the Springer-Verlag, Germany, and Vols. 7 and 8 in the *Series on the Foundations of Natural Science and Technology* of World Scientific. He is the Principal Editor of the two edited monographs in series in *Nanotechnology* of NOVA, USA. The score in Vidwan Portal Unit, Government of India, of Prof. Ghatak is 8.9 out of 10. Prof. Ghatak has successfully supervised more than 30 PhD students. AICTE, India, has selected the first R & D project in his life for the best project award in electronics and second best research project award considering all the branches of engineering for the year 2006, and he is the first recipient of the academic excellence award of the University of Engineering & Management, Kolkata, from the present Governor of West Bengal in its first convocation in 2017. He was Assistant Professor in the Department of Radiophysics and Electronics of the University of Calcutta from 1983 to 1987, Associate Professor in the Department of ETCE of Jadavpur University from 1987 to 1994, Professor and HOD of Electronic Science of the University of Calcutta from 1994 to 2012, HOD and Dean of the National Institute of Technology, Agartala from 2012 to 2014 and from January 2015 he has joined in the IEM UEM group, Kolkata, as Research Director and Senior Professor. He is the referee, Editor and Guest Editor of different reputed international journals. His present research interests are nanomaterials and genetic electronics, respectively. His brief CV has been enlisted in many biographical references of USA and UK.

Professor Madhuchhanda Mitra received her B.Tech, M.Tech, and Ph.D. (Tech) degrees in 1987, 1989, and 1998, respectively, from the University of Calcutta, Calcutta, India. She is a recipient of "Griffith Memorial Award" of the University of Calcutta. She is the principal co-author of 150 scientific research papers in international peer-reviewed journals. Her present research interests are nano-science and nanotechnology, identification of different biomarkers and biomedical signal processing which include feature extraction, compression, encryption and classification of electrocardiography (ECG) and photoplethysmography (PPG) signals. Presently, she is professor in the Department of Applied Physics, University of Calcutta, India, where she has been actively engaged in both teaching and research.

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Symbols

α	Band non-parabolicity parameter
a	The lattice constant
a_0, b_0	The widths of the barrier and the well for superlattice structures
A_0	The amplitude of the light wave
$\vec{A}$	The vector potential
$A(E, n_z)$	The area of the constant energy 2D wave vector space for ultrathin films
B	Quantizing magnetic field
B_2	The momentum matrix element
b	Bandwidth
c	Velocity of light
C_1	Conduction band deformation potential
C_2	A constant which describes the strain interaction between the conduction and valance bands
ΔC_{44}	Second-order elastic constant
ΔC_{456}	Third-order elastic constant
δ	Crystal field splitting constant
Δ_0	Interface width
$\Delta\left(\frac{1}{B}\right)$	Period of SdH oscillation
d_0	Superlattice period
$D_0(E)$	Density-of-states (DOS) function
$D_B(E)$	DOS function in magnetic quantization
$D_B(E, \lambda)$	DOS function under the presence of light waves
d_x, d_y, d_z	Nano thickness along the x, y and zdirections
$\Delta_{\parallel}$	Spin-orbit splitting constants parallel
$\Delta_{\perp}$	Spin-orbit splitting constants perpendicular to the C-axis
Δ	Isotropic spin-orbit splitting constant
d^3k	Differential volume of the k space
$\in$	Energy as measured from the center of the band gap
ε	Trace of the strain tensor
ε_0	Permittivity of free space
ε_∞	Semiconductor permittivity in the high frequency limit
ε_{sc}	Semiconductor permittivity
ΔE_g	Increased band gap
$\|e\|$	Magnitude of electron charge
E	Total energy of the carrier
E_0, ζ_0	Electric field
E_g	Band gap
E_i	Energy of the carrier in the ith band
E_{ki}	Kinetic energy of the carrier in the $i$thband
E_F	Fermi energy
E_{FB}	Fermi energy in the presence of magnetic quantization
E_n	Landau sub band energy
E_{Fs}	Fermi energy in the presence of size quantization
$\bar{E}_{Fn}$	Fermi energy for nipis
E_{FSL}	Fermi energy in superlattices
$\vec{\varepsilon}_s$	Polarization vector
E_{FQWSL}	Fermi energy in quantum wire superlattices with graded interfaces

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E_{F_L}	Fermi energy in the presence of light waves
$E_{F_{BL}}$	Fermi energy under quantizing magnetic field in the presence of light waves
E_{F2DL}	2D Fermi energy in the presence of light waves
E_{F1DL}	1D Fermi energy in the presence of light waves
E_{g0}	Un-perturbed band-gap
$Erfc$	Complementary error function
Erf	Error function
E_{F_h}	Fermi energy of HD materials
$\bar{E}_{hd}$	Electron energy within the band gap
F_s	Surface electric field
$F(V)$	Gaussian distribution of the impurity potential
$F_j(\eta)$	One parameter Fermi-Dirac integral of order j
f_0	Equilibrium Fermi-Dirac distribution function of the total carriers
f_{0i}	Equilibrium Fermi-Dirac distribution function of the carriers in the ith band
g_v	Valley degeneracy
G	Thermoelectric power under classically large magnetic field
G_0	Deformation potential constant
g^*	Magnitude of the band edge g-factor
h	Planck's constant
$\hat{H}$	Hamiltonian
$\hat{H}'$	Perturbed Hamiltonian
$H(E-E_n)$	Heaviside step function
$\hat{i}, \hat{j}$ and $\hat{k}$	Orthogonal triads
i	Imaginary unit
I	Light intensity
j_{ci}	Conduction current contributed by the carriers of the ith band
k	Magnitude of the wave vector of the carrier
k_B	Boltzmann's constant
λ	Wavelength of the light
$\bar{\lambda}_0$	Splitting of the two spin-states by the spin-orbit coupling and the crystalline field
$\bar{l}, \bar{m}, \bar{n}$	Matrix elements of the strain perturbation operator
L_x, L_z	Sample length along x and z directions
L_0	Superlattices period length
L_D	Debyescreening length
m_1	Effective carrier masses at the band-edge along x direction
m_2	Effective carrier masses at the band-edge along y direction
m_3	The effective carrier masses at the band-edge along z direction
m'_2	Effective-mass tensor component at the top of the valence band (for electrons) or at the bottom of the conduction band (for holes)
m_i^*	Effective mass of the $i$thcharge carrier in the ith band
$m_{\parallel}^*$	Longitudinal effective electron masses at the edge of the conduction band
$m_{\perp}^*$	Transverse effective electron masses at the edge of the conduction band
m_c	Isotropic effective electron masses at the edge of the conduction band
$m_{\perp,1}^*$, $m_{\parallel,1}^*$	Transverse and longitudinal effective electron masses at the edge of the conduction band for the first material in superlattice
m_r	Reduced mass
m_v	Effective mass of the heavy hole at the top of the valance band in the absence of any field
n	Landau quantum number

n_x,n_y, n_z	Size quantum numbers along the x, y and z directions
n_{1D},n_{2D}	1D and 2D carrier concentration
n_{2Ds}, n_{2Dw}	2D surface electron concentration under strong and weak electric field
$\bar{n}_{2Ds}$, $\bar{n}_{2Dw}$	Surface electron concentration under the strong and weak electric field quantum limit
n_i	Mini-band index for nipi structures
$N_{nipi}(E)$	DOS function for nipi structures
$N_{2DT}(E)$	2D DOS function
$N_{2D}(E,\lambda)$	2D DOS function in the presence of light waves
$N_{1D}(E,\lambda)$	1D DOS function in the presence of light waves
n_0	Total electron concentration
$\bar{n}_0$	Electron concentration in the electric quantum limit
n_i	Carrier concentration in the ith band
P	Isotropic momentum matrix element
P_n	Available noise power
$P_{\|}$	Momentum matrix elements parallel to the direction of crystal axis
$P_{\perp}$	Momentum matrix elements perpendicular to the direction of crystal axis
$\vec{r}$	Position vector
S_i	Zeros of the Airy function
$\vec{s}_0$	Momentum vector of the incident photon
t	Time scale
t_c	Tight binding parameter
T	Absolute temperature
$\tau_i(E)$	Relaxation time of the carriers in the ith band
$u_1(\vec{k},\vec{r}), u_2(\vec{k},\vec{r})$	Doubly degenerate wave functions
$V(E)$	Volume of κ space
V_0	Potential barrier encountered by the electron
$V(\vec{r})$	Crystal potential
x, y	Alloy compositions
z_t	Classical turning point
μ_i	Mobility of the carriers in the ith band
μ	Average mobility of the carriers
$\zeta(2r)$	Zeta function of order $2r$
$\Gamma(j+1)$	Complete Gamma function
η	Normalized Fermi energy
η_g	Impurity scattering potential
ω_0	Cyclotron resonance frequency
θ	Angle
μ_0	Bohr magnetron
ω	Angular frequency of light wave
$\uparrow',\downarrow'$	Spin up and down function

Part I: **Entropy in heavily doped quantum confined nonparabolic materials**

Knowledge is proud, he knows too much, but the wise is humble, he knows no more.

1 The entropy in quantum wells of heavily doped materials

If my only desire is to be desireless, then my consciousness is reversed.

1.1 Introduction

In recent years, with the advent of fine lithographical methods [1, 2], molecular beam epitaxy [3], organ metallic vapor-phase epitaxy [4], and other experimental techniques, the restriction of the motion of the carriers of bulk materials in one [quantum wells (QWs), doping superlattices, accumulation, and inversion layers], two (nanowires), and three (quantum dots, magneto-size quantized systems, magneto inversion layers, magneto accumulation layers, quantum dot superlattices, magneto QW superlattices, and magneto doping superlattices) dimensions has in the past few years attracted much attention not only for their potential in uncovering new phenomena in nanoscience but also for their interesting quantum device applications [5–8]. In QWs, the restriction of the motion of the carriers in the direction normal to the film (say, the z direction) may be viewed as carrier confinement in an infinitely deep 1D rectangular potential well, leading to quantization (known as quantum size effect (QSE)) of the wave vector of the carriers along the direction of the potential well, allowing 2D carrier transport parallel to the surface of the film representing new physical features not exhibited in bulk materials [9–13]. The low-dimensional heretostructures based on various materials are widely investigated because of the enhancement of carrier mobility [14].These properties make such structures suitable for applications in QWs lasers [15], hereto-junction field-effect transistors (FETs) [16, 17], high-speed digital networks [18–21], high-frequency microwave circuits [22], optical modulators [23], optical switching systems [24], and other devices. The constant energy 3D wave-vector space of bulk materials becomes 2D wave-vector surface in QWs due to dimensional quantization. Thus, the concept of reduction of symmetry of the wave-vector space and its consequence can unlock the physics of low-dimensional structures. In this chapter, we study the *entropy* in QWs of HD nonparabolic materials having different band structures in the presence of Gaussian band tails. At first, we shall investigate the *entropy* in QWs of HD nonlinear optical compounds, which are being used in nonlinear optics and light emitting diodes [25]. The quasi-cubic model can be used to investigate the symmetric properties of both the bands at the zone center of wave vector space of the same compound. Including the anisotropic crystal potential in the Hamiltonian, and special features of the nonlinear optical compounds, Kildal [26] formulated the electron dispersion law under the assumptions of isotropic momentum matrix element and the isotropic spin-orbit splitting constant, respectively, although the anisotropies in

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the two aforementioned band constants are the significant physical features of the said materials [27–29]. In Section 1.2.1, the *entropy* in QWs of HD nonlinear optical materials has been investigated on the basis of newly formulated HD dispersion relation of the said compound by considering the combined influence of the anisotropies of the said energy band constants together with the inclusion of the crystal field splitting, respectively, within the framework of $\vec{k}\cdot\vec{p}$ formalism. The III–V compounds find applications in infrared detectors [30], quantum dot light emitting diodes [31], quantum cascade lasers [32], QWs wires [33], optoelectronic sensors [34], high electron mobility transistors [35], etc. The electron energy spectrum of III–V materials can be described by the three- and two-band models of Kane [36, 37], together with the models of Stillman et al. [38], Newson and Kurobe [39] and, Palik et al. [40], respectively. In this context it may be noted that the ternary and quaternary compounds enjoy the singular position in the entire spectrum of optoelectronic materials. The ternary alloy $Hg_{1-x}Cd_xTe$ is a classic narrow gap compound. The band gap of this ternary alloy can be varied to cover the spectral range from 0.8 to over 30μm [41] by adjusting the alloy composition. $Hg_{1-x}Cd_xTe$ finds extensive applications in infrared detector materials and photovoltaic detector arrays in the 8–12μm wave bands [42]. The above uses have generated the $Hg_{1-x}Cd_xTe$ technology for the experimental realization of high-mobility single crystal with specially prepared surfaces. The same compound has emerged to be the optimum choice for illuminating the narrow sub-band physics because the relevant material constants can easily be experimentally measured [43]. Besides, the quaternary alloy $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP, also finds wide use in the fabrication of avalanche photo-detectors [44], hereto-junction lasers [45], light emitting diodes [46] and avalanche photodiodes [47], field effect transistors, detectors, switches, modulators, solar cells, filters, and new types of integrated optical devices are made from the quaternary systems [48]. It may be noted that all types of band models as discussed for III–V materials are also applicable for ternary and quaternary compounds. In Section 1.2.2, the ***Entropy*** in QWs of HD III–V, ternary and quaternary materials has been studied in accordance with the corresponding HD formulation of the band structure and the simplified results for wide gap materials having parabolic energy bands under certain limiting conditions have further been demonstrated as a special case in the absence of heavy doping and thus confirming the compatibility test. The II–VI materials are being used in nano-ribbons, blue green diode lasers, photosensitive thin films, infrared detectors, ultra-high-speed bipolar transistors, fiber optic communications, microwave devices, solar cells, semiconductor gamma-ray detector arrays, semiconductor detector gamma camera and allow for a greater density of data storage on optically addressed compact discs [49–56]. The carrier energy spectra in II–VI compounds are defined by the Hopfield model [57] where the splitting of the two-spin states by the spin-orbit coupling and the crystalline field has been taken into account. Section 1.2.3 contains the investigation of the ***Entropy*** in QWs of HD II–VI compounds.

Lead Chalcogenides (PbTe, PbSe, and PbS) are IV–VI nonparabolic materials whose studies over several decades have been motivated by their importance in infrared IR detectors, lasers, light-emitting devices, photo-voltaic, and high temperature thermo-electrics [58–62]. PbTe, in particular, is the end compound of several ternary and quaternary high performance high temperature thermoelectric materials [63–67]. It has been used not only as bulk but also as films [68–71], QWs [72] superlattices [73, 74] nanowires [75] and colloidal and embedded nano-crystals [76, 77, 78, 79], and PbTe films doped with various impurities have also been investigated [80–87] These studies revealed some of the interesting features that had been seen in bulk PbTe, such as Fermi-level pinning and, in the case of superconductivity [88]. In Section 1.2.4, the 2D ***Entropy*** in QWs of HD IV–VI materials has been studied taking PbTe, PbSe, and PbS as examples. The stressed materials are being investigated for strained silicon transistors, quantum cascade lasers, semiconductor strain gages, thermal detectors, and strained-layer structures [89–92]. The ***Entropy*** in QWs of HD stressed compounds (taking stressed n-InSb as an example) has been investigated in Section 1.2.5 The vacuum deposited Tellurium (Te) has been used as the semiconductor layer in thin-film transistors (TFT) [93] which is being used in CO_2 laser detectors [94], electronic imaging, strain sensitive devices [95, 96], and multichannel Bragg cell [97]. Section 1.2.6 contains the investigation of ***Entropy*** in QWs of HD Tellurium. The n-Gallium Phosphide (n-GaP) is being used in quantum dot light emitting diode [98], high efficiency yellow solid state lamps, light sources, high peak current pulse for high gain tubes. The green and yellow light emitting diodes made of nitrogen-doped n-GaP possess a longer device life at high drive currents [99–101]. In Section 1.2.7, the ***Entropy*** in QWs of HD n-GaP has been studied. The Platinum Antimonide ($PtSb_2$) finds application in device miniaturization, colloidal nanoparticle synthesis, sensors and detector materials and thermo-photovoltaic devices [102–104]. Section 1.2.8 explores the ***Entropy*** in QWs of HD $PtSb_2$. Bismuth telluride (Bi_2Te_3) was first identified as a material for thermoelectric refrigeration in 1954 [105] and its physical properties were later improved by the addition of bismuth selenide and antimony telluride to form solid solutions. The alloys of $Bi_2Te_3$are useful compounds for the thermoelectric industry and have been investigated in the literature [106–110]. In Section 1.2.9, the ***Entropy*** in QWs of HD Bi_2Te_3 has been considered. The usefulness of elemental semiconductor Germanium is already well known since the inception of transistor technology and, it is also being used in memory circuits, single photon detectors, single photon avalanche diode, ultrafast optical switch, THz lasers and THz spectrometers [111–114]. In Section 1.2.10, the ***Entropy*** has been studied in QWs of HD Ge. Gallium Antimonide (GaSb) finds applications in the fiber optic transmission window, hereto-junctions, and QWs. A complementary hereto-junction field effect transistor in which the channels for the p-FET device and the n-FET device forming the complementary FET are formed from GaSb. The band gap energy of GaSb makes it suitable for low power operation [115–120]. In Section 1.2.11, the ***Entropy*** in QWs of HD GaSb has

been studied. The II–V materials have been studied in photovoltaic cells constructed of single crystal semiconductor materials in contact with electrolyte solutions. Cadmium selenide shows an open-circuit voltage of 0.8V and power conservation coefficients near 6 percent for 720-nm light [121]. They are also used in ultrasonic amplification [122]. The development of an evaporated thin film transistor using cadmium selenide as the semiconductor has been reported by Weimer [123, 124]. The ***Entropy*** in HD QWs of II–V materials has been presented in Section 1.2.12. In Section 1.2.13, the ***Entropy*** in HDQWs of $Pb_{1-x}Ga_xTe$ has been investigated [125]. The diphosphides finds prominent role in biochemistry where the folding and structural stabilization of many important extra-cellular peptide and protein molecules, including hormones, enzymes, growth factors, toxins, and immunoglobulin are concerned [126]. Besides, artificial introduction of extra diphosphides into peptides or proteins can improve biological activity [127] or confer thermal stability [128]. The asymmetric diphosphide bond formation in peptides containing a free thiol group takes place over a wide pH range in aqueous buffers and can be crucially monitored by spectro-photometric titration of the released 3-nitro-2-pyridinethiol [129–134]. In Section 1.2.14, the ***Entropy*** in HD QWs of zinc and cadmium diphosphides has been investigated. Section 1.3 contains the result and discussions pertaining to this chapter. The last Section 1.4 contains 25 open research problems.

1.2 Theoretical background

1.2.1 Entropy in quantum wells (QWs) of HD nonlinear optical materials

The form of **k.p** matrix for nonlinear optical compounds can be expressed extending Bodnar [27] as

$$\bar{H} = \begin{bmatrix} \bar{H}_1 & \bar{H}_2 \\ \bar{H}_2^{+} & \bar{H}_1 \end{bmatrix} \tag{1.1}$$

where,

$$\bar{H}_1 = \begin{bmatrix} \bar{E}_{g_0} & 0 & \bar{P}_{||}\bar{k}_z & 0 \\ 0 & (-2\Delta_{||}/3) & (\sqrt{2}\Delta_{\perp}/3) & 0 \\ \bar{P}_{||}\bar{k}_z & (\sqrt{2}\Delta_{\perp}/3) & -\left(\delta+\frac{1}{3}\Delta_{||}\right) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \ \bar{H} = \begin{bmatrix} 0 & -\bar{f}_{,+} & 0 & \bar{f}_{,-} \\ \bar{f}_{,+} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \bar{f}_{,+} & 0 & 0 & 0 \end{bmatrix}$$

in which $\bar{E}_{g_0}$ is the band gap in the absence of any field, $\bar{P}_{||}$ and $\bar{P}_{\perp}$ are the momentum matrix elements parallel and perpendicular to the direction of crystal axis axis, respectively, δ is the crystal field splitting constant, $\Delta_{||}$ *and* $\Delta_{\perp}$ are the spin-orbit splitting constants parallel and perpendicular to the *C*-axis, respectively,

$\bar{f}_{,\pm} \equiv \left(\bar{P}_{\perp}/\sqrt{2}\right)\left(\bar{k}_x \pm i\bar{k}_y\right)$ and $i = \sqrt{-1}$. Thus, neglecting the contribution of the higher bands and the free electron term, the diagonalization of the above matrix leads to the dispersion relation of the conduction electrons in bulk specimens of nonlinear optical materials as

$$\gamma(\bar{E}) = \bar{f}_1(\bar{E})\bar{k}_s^2 + \bar{f}_2(\bar{E})\bar{k}_z^2 \tag{1.2}$$

where

$$\gamma(\bar{E}) = \bar{E}(\bar{E}+\bar{E}_{g_0})[(\bar{E}+\bar{E}_{g_0})(\bar{E}+\bar{E}_{g_0}+\Delta_{||}) + \delta(\bar{E}+\bar{E}_{g_0}+\frac{2}{3}\Delta_{||}) + \frac{2}{3}(\Delta_{||}^2 - \Delta_{\perp}^2)]$$

$\bar{E}$ is the total energy of the electron as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization, $\bar{k}_s^2 = \bar{k}_x^2 + \bar{k}_y^2$,

$$f_1(\bar{E}) = \frac{\hbar^2\bar{E}_{g_0}(\bar{E}_{g_0}+\Delta_{\perp})}{[2\bar{m}_{\perp}^{*}(\bar{E}_{g_0}+\frac{2}{3}\Delta_{\perp})]}\left[\delta\left(\bar{E}+\bar{E}_{g_0}+\frac{1}{3}\Delta_{||}\right) + (\bar{E}+\bar{E}_{g_0})\left(\bar{E}+\bar{E}_{g_0}+\frac{2}{3}\Delta_{||}\right) + \frac{1}{9}(\Delta_{||}^2 - \Delta_{\perp}^2)\right],$$

$$f_2(\bar{E}) = \frac{\hbar^2 E_{g_0}(\bar{E}_{g_0}+\Delta_{||})}{[2\bar{m}_{||}^{*}(\bar{E}_{g_0}+\frac{2}{3}\Delta_{\perp})]}\left[(\bar{E}+\bar{E}_{g_0})\left(\bar{E}+\bar{E}_{g_0}+\frac{2}{3}\Delta_{||}\right)\right],\ \hbar = \frac{h}{2\pi}$$

h is Planck's constant and $\bar{m}^{*}_{||}$ *and* $\bar{m}^{*}_{\perp}$ are the longitudinal and transverse effective electron masses at the edge of the conduction band, respectively.

Thus the generalized unperturbed electron energy spectrum for the bulk specimens of the nonlinear optical materials in the absence of band tails can be expressed following (1.2) as

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{||}^{*}} + \left(\frac{\bar{b}_{||}}{\bar{b}_{\perp}}\frac{\bar{c}_{\perp}}{\bar{c}_{||}}\right)\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^{*}} = \left\{\frac{\bar{E}(\alpha\bar{E}+1)(\bar{b}_{||}\bar{E}+1)}{(\bar{c}_{||}\bar{E}+1)} + \frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}\left[\delta\bar{E} + \frac{2}{9}(\Delta_{||}^2 - \Delta_{\perp}^2)\right]\right.$$
$$\left. - \left(\frac{2}{9}\right)\frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}\frac{(\Delta_{||}^2 - \Delta_{\perp}^2)}{(\bar{c}_{||}\bar{E}+1)}\right\} - \left(\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^{*}}\right)\left\{\left(\frac{\bar{b}_{||}}{\bar{b}_{\perp}}\frac{\bar{c}_{\perp}}{\bar{c}_{||}}\right)\left[\left(\frac{\delta}{2} + \frac{\Delta_{||}^2 - \Delta_{\perp}^2}{6\Delta_{||}}\right)\frac{\alpha}{\alpha\bar{E}+1}\right.\right.$$
$$\left.\left. + \left(\frac{\delta}{2} - \left\{\frac{\Delta_{||}^2 - \Delta_{\perp}^2}{6\Delta_{||}}\right\}\right)\frac{\bar{c}_{||}}{\bar{c}_{||}\bar{E}+1}\right]\right\} \tag{1.3}$$

where

$$\bar{b}_{||} \equiv (\bar{E}_{g_0}+\Delta_{||})^{-1}, \bar{c}_{\perp} \equiv \left(\bar{E}_{g_0}+\frac{2}{3}\Delta_{\perp}\right)^{-1}, \bar{b}_{\perp} \equiv (\bar{E}_{g_0}+\Delta_{\perp})^{-1},$$
$$\bar{c}_{||} = \left(\bar{E}_{g_0}+\frac{2}{3}\Delta_{||}\right)^{-1} \textit{ and } \alpha = (\bar{E}_{g_0})^{-1}.$$

The Gaussian distribution $\bar{F}(\bar{V})$ of the impurity potential is given by [131]

$$\bar{F}(\bar{V}) = (\pi\eta_g^2)^{1/2} \exp(-\bar{V}^2/\eta_g^2) \tag{1.4}$$

where η_g is the impurity scattering potential. It appears from (1.4) that the variance parameter η_g is not equal to zero, but the mean value is zero. Further, the impurities are assumed to be uncorrelated and the band mixing effect has been neglected in this simplified theoretical formalism.

Using the (1.3) and (1.4), we get

$$\begin{aligned}
&\left[\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{||}^*}\int_{-\infty}^{\bar{E}}\bar{F}(\bar{V})d\bar{V}\right] + \left[\left(\frac{\bar{b}_{||}}{\bar{b}_\perp}\frac{\bar{c}_\perp}{\bar{c}_{||}}\right)\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^*}\int_{-\infty}^{\bar{E}}\bar{F}(\bar{V})d\bar{V}\right] = \\
&\left\{\int_{-\infty}^{\bar{E}}\frac{(\bar{E}-\bar{V})[\alpha(\bar{E}-\bar{V})+1][\bar{b}_{||}(\bar{E}-\bar{V})+1}{[\bar{c}_{||}(\bar{E}-\bar{V})+1]}\bar{F}(\bar{V})d\bar{V} + \frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}\right. \\
&\left[\delta\int_{-\infty}^{\bar{E}}(\bar{E}-\bar{V})\bar{F}(\bar{V})d\bar{V} + \frac{2}{9}(\Delta_{||}^2-\Delta_\perp^2)\int_{-\infty}^{\bar{E}}\bar{F}(\bar{V})d\bar{V}\right] - \left(\frac{2}{9}\right)\frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}(\Delta_{||}^2-\Delta_\perp^2) \\
&\left.\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})d\bar{V}}{[\bar{c}_{||}(\bar{E}-\bar{V})+1]}\right\} - + \frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}\left[\delta\int_{-\infty}^{\bar{E}}(\bar{E}-\bar{V})\bar{F}(\bar{V})d\bar{V} + \frac{2}{9}(\Delta_{||}^2-\Delta_\perp^2)\right. \\
&\left.\int_{-\infty}^{\bar{E}}\bar{F}(\bar{V})d\bar{V}\right] - \left(\frac{2}{9}\right)\frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}(\Delta_{||}^2-\Delta_\perp^2)\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})d\bar{V}}{[\bar{c}_{||}(\bar{E}-\bar{V})+1]}\Bigg\} - \left(\frac{\bar{\hbar}^2\bar{k}_s^2}{2\bar{m}_\perp^*}\right) \\
&\left\{\left(\frac{\bar{b}_{||}}{\bar{b}_{||_\perp}}\frac{\bar{c}_\perp}{\bar{c}_{||}}\right)\left[\left(\frac{\delta}{2}+\frac{\Delta_{||}^2-\Delta_\perp^2}{6\Delta_{||}}\right)\alpha\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})d\bar{V}}{[\alpha(\bar{E}-\bar{V})+1]}\right.\right. \\
&\left.\left.+\left(\frac{\delta}{2}+\frac{\Delta_{||}^2-\Delta_\perp^2}{6\Delta_{||}}\right)\bar{c}_{||}\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})d\bar{V}}{[\bar{c}_{||}(\bar{E}-\bar{V})+1]}\right]\right\}
\end{aligned} \tag{1.5}$$

The (1.5) can be written as

$$\begin{aligned}
&\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{||}^*}\bar{I}(1) + \left(\frac{\bar{b}_{||}}{\bar{b}_\perp}\frac{\bar{c}_1}{\bar{c}_{||}}\right)\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^*}\bar{I}(1) = \\
&= \left\{\bar{I}_3(\bar{c}_{||}) + \frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}\left[\delta\bar{I}(4) + \frac{2}{9}(\Delta_{||}^2-\Delta_\perp^2)\bar{I}(1)\right] - \left(\frac{2}{9}\right)\frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}(\Delta_{||}^2-\Delta_\perp^2)\bar{I}_6(\bar{c}_{||})\right\} \\
&- \left(\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^*}\right)\left\{\left(\frac{\bar{b}_{||}}{\bar{b}_\perp}\frac{\bar{c}_1}{\bar{c}_{||}}\right)\left[\left(\frac{\delta}{2}+\frac{\Delta_{||}^2-\Delta_\perp^2}{6\Delta_{||}}\right)\alpha\bar{I}(\alpha) + \left(\frac{\delta}{2}\left\{\frac{\Delta_{||}^2-\Delta_\perp^2}{6\Delta_{||}}\right\}\right)\bar{c}_{||}\bar{I}(\bar{c}_{||})\right]\right\}
\end{aligned} \tag{1.6}$$

Let us substitute

$$\bar{I}(1) = \int_{-\infty}^{\bar{E}}\bar{F}(\bar{V})d\bar{V} \tag{1.7}$$

$$\bar{I}_3(\bar{c}_{||}) = \int_{-\infty}^{\bar{E}} \frac{(\bar{E}-\bar{V})[\alpha(\bar{E}-\bar{V})+1][\bar{b}_{||}(\bar{E}-\bar{V})+1]}{[\bar{c}_{||}(\bar{E}-\bar{V})+1]}\bar{F}(\bar{V})\bar{d}\bar{V}$$

$$\bar{I}_3(\bar{c}_{||}) = \int_{-\infty}^{\bar{E}} \frac{(\bar{E}-\bar{V})[\alpha(\bar{E}-\bar{V})+1][\bar{b}_{||}(\bar{E}-\bar{V})+1]}{[c_{||}(E-V)+1]}\bar{F}(\bar{V})\bar{d}\bar{V} \tag{1.8}$$

$$\bar{I}_3(\bar{c}_{||}) = \int_{-\infty}^{\bar{E}} \frac{(\bar{E}-\bar{V})[\alpha(\bar{E}-\bar{V})+1][\bar{b}_{||}(\bar{E}-\bar{V})+1]}{[\bar{c}_{||}(\bar{E}-\bar{V})+1]}\bar{F}(\bar{V})\bar{d}\bar{V}$$

$$\bar{I}(4) = \int_{-\infty}^{\bar{E}} (\bar{E}-\bar{V})\bar{F}(\bar{V})\bar{d}\bar{V} \tag{1.9}$$

$$\bar{I}(\alpha) = \int_{-\infty}^{\bar{E}} \frac{\bar{F}(\bar{V})\bar{d}\bar{V}}{[\alpha(\bar{E}-\bar{V})+1]} \tag{1.10}$$

Substituting $\bar{E}-\bar{V} \equiv \bar{x}$ and, $\frac{\bar{x}}{\eta_g} \equiv \bar{t}_0$ we get from (1.7)

$$\begin{aligned} \bar{I}(1) &= (\exp\left(-\frac{\bar{E}^2}{\eta_g^2}\right)/\sqrt{\pi}) \int_0^{\infty} \exp\left[-\bar{t}_0^2 + \left(\frac{2\bar{E}\bar{t}_0}{\eta_g}\right)\right] d\bar{t}_0 \\ \bar{I}(1) &= \left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right] \end{aligned} \tag{1.11}$$

where $Erf(\bar{E}/\eta_g)$s the error function of $((\bar{E}/\eta_g))$.

From (1.9), we can write

$$\begin{aligned} \bar{I}(4) = \left(1/\eta_g\sqrt{\pi}\right) \int_{-\infty}^{\bar{E}} (\bar{E}-\bar{V}) \exp(-\bar{V}^2/\eta_g^2)\bar{d}\bar{V} = \frac{\bar{E}}{2}[1+Erf(\bar{E}/\eta_g)] \\ -\left\{\frac{1}{\sqrt{\pi\eta_g^2}} \int_{-\infty}^{\bar{E}} \bar{V} \exp(-\bar{V}^2/\eta_g^2)\bar{d}\bar{V}\right\} \end{aligned} \tag{1.12}$$

After computing this simple integration, we obtain

Thus,

$$\bar{I}(4) = \eta_g \exp(-\bar{E}^2/\eta_g^2)(2\sqrt{\pi}) + \frac{\bar{E}}{2}(1+Erf(\bar{E}/\eta_g)) = \gamma_0(\bar{E},\eta_g) \tag{1.13}$$

From (1.10), we can write

$$\bar{I}(\alpha) = \frac{1}{\sqrt{\pi\eta_g^2}} \int_{-\infty}^{\bar{E}} \frac{\exp(-\bar{V}^2/\eta_g^2)\bar{d}\bar{V}}{[\alpha(\bar{E}-\bar{V})+1]} \tag{1.14}$$

When, $\bar{V} \to \pm\infty$, $\frac{1}{[\alpha(\bar{E}-\bar{V})+1]} \to 0$ and; $\exp(-\bar{V}^2/\eta_g^2) \to 0$

Thus (1.14) can be expressed as

$$\bar{I}(\alpha) = (1/\alpha\eta_g\sqrt{\pi}) \int_{-\infty}^{\infty} \exp(-\bar{t}^2)(\bar{u}-\bar{t})^{-1}\bar{dt} \tag{1.15}$$

where,

$$\frac{\bar{V}}{\eta_g} = \bar{t} \text{ and } \bar{u} \equiv \left(\frac{1+\alpha E}{\alpha\eta}\right)$$

It is well known that [123, 124]

$$\bar{W}(\bar{Z}) = (i/\pi) \int_{-\infty}^{\infty} (\bar{Z}-\bar{t})^{-1} \exp(-\bar{t}^2)\bar{dt} \tag{1.16}$$

In which $i = \sqrt{-1}$ and Z, in general, is a complex number.

We also know [123, 124],

$$\bar{W}(\bar{Z}) = (i/\pi) \exp(-\bar{Z}^2) Erfc(-i\bar{Z}) \tag{1.17}$$

where

$$Erfc(\bar{Z}) \equiv 1 - Erf(\bar{Z}).$$

Thus, $Erfc(-i\bar{u}) = 1 - Erf(-i\bar{u})$

Since, $Erf(-i\bar{u}) = -Erf(i\bar{u})$

Thus,

$$\bar{I}(\alpha) = [-i\sqrt{\pi}/\alpha\eta_g] \exp(-\bar{u}^2)[1 + Erf(i\bar{u})] \tag{1.18}$$

We also know that [123, 124]

$$Erf(\bar{x}+i\bar{y}) = Erf(\bar{x}) + \left(\frac{e^{-x^2}}{2\pi\bar{x}}\right)\left[(1-\cos(2xy)) + i\sin(2xy)\right.$$
$$\left. + \frac{2}{\pi}e^{-x^2}\sum_{p=1}^{\infty}\frac{\exp(-\bar{p}^2/4)}{(\bar{p}^2+4\bar{x}^2)}\right][\bar{f}_p(\bar{x},\bar{y}) + i\bar{g}_p(\bar{x},\bar{y}) + \varepsilon(\bar{x},\bar{y})] \tag{1.19}$$

where

$$\bar{f}_p(\bar{x},\bar{y}) = [2x - 2x\cosh(\bar{p}\bar{y})\cos(2\bar{x}\,\bar{y}) + \bar{p}\sinh(\bar{p}\bar{y})\sin(2\bar{x}\,\bar{y})],$$

$$\bar{g}_p(\bar{x},\bar{y}) \equiv [2\bar{x}\cosh(\bar{p}\,\bar{y})\sin(2\bar{x}\,\bar{y}) + p\sinh(\bar{p}\,\bar{y})\cos(2\bar{x}\,\bar{y})] \left|\varepsilon(\bar{x},\bar{y}))\right| \approx 10^{-15}\left|Erf(\bar{x}+i\bar{y})\right|$$

Substituting $\bar{x} = 0$ and $\bar{y} = \bar{u}$ in (1.19), we obtain,

$$Erf(i\bar{u}) = \left(\frac{2i}{\pi}\right)\sum_{\bar{p}=1}^{\infty}\left\{\frac{\exp(-\bar{p}^2/4)}{\bar{p}}\sinh(\bar{p}\ \bar{u})\right\} \tag{1.20}$$

Therefore, we can write

$$\bar{I}(\alpha) = \bar{C}_{21}(\alpha, \bar{E}, \eta_g) - i\bar{D}_{21}(\alpha, \bar{E}, \eta_g) \tag{1.21}$$

where,

$$\bar{C}_{21}(\alpha, \bar{E}, \eta_g) = \left[\frac{2}{\alpha\eta_g\sqrt{\pi}}\right] \exp(-\bar{u}^2) \left[\sum_{\bar{p}=1}^{\infty} \left\{ \frac{\exp(-\bar{p}^2/4)}{\bar{p}} \sinh(\bar{p}\,\bar{u}) \right\}\right] \text{ and}$$

$$\bar{D}_{21}(\alpha, \bar{E}, \eta_g) = \left[\frac{\sqrt{\pi}}{\alpha\eta_g} \exp(-\bar{u}^2)\right]$$

The (1.21) consists of both real and imaginary parts and therefore, $\bar{I}_3(\alpha)$ ***is complex, which can also be proved by using the method of analytic continuation of the subject Complex Analysis.***

The integral $\bar{I}_3(\bar{c}_{||})$ in (1.8) can be written as

$$\bar{I}_3(\bar{c}_{||}) = \left(\frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}\right)\bar{I}(5) + \left(\frac{\alpha\bar{c}_{||} + b_{||}\bar{c}_{||} - \alpha b_{||}}{\bar{c}_{||}^2}\right)\bar{I}(4) + \frac{1}{\bar{c}_{||}}\left(1 - \frac{\alpha}{\bar{c}_{||}}\right)\left(1 - \frac{\bar{c}_{||}}{\bar{c}_{||}}\right)\bar{I}(1)$$
$$- \left\{\frac{1}{\bar{c}_{||}}\left(1 - \frac{\alpha}{\bar{c}_{||}}\right)\left(1 - \frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\bar{I}(\bar{c}_{||})\right\} \tag{1.22}$$

where

$$\bar{I}(5) = \int_{-\infty}^{\bar{E}} (\bar{E} - \bar{V})^2 \bar{F}(\bar{V}) d\bar{V} \tag{1.23}$$

From (1.23) we can write

$$\bar{I}(5) = \frac{1}{\sqrt{\pi\eta_g^2}}\left[\bar{E}^2 \int_{-\infty}^{\bar{E}} \exp\left(\frac{-\bar{V}^2}{\eta_g^2}\right) d\bar{V} - 2\bar{E}\int_{-\infty}^{\bar{E}} \bar{V}\exp\left(\frac{-\bar{V}^2}{\eta_g^2}\right) d\bar{V}\right.$$
$$\left. + \int_{-\infty}^{\bar{E}} \bar{V}^2 \exp\left(\frac{-\bar{V}^2}{\eta_g^2}\right) d\bar{V}\right]$$

The evaluations of the component integrals lead us to write

$$\bar{I}(5) = \frac{\eta_g\bar{E}}{2\sqrt{\pi}} \exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right) + \frac{1}{4}(\eta_g^2 + 2\bar{E}^2)\left[1 + Erf\left(\frac{\bar{E}}{\eta_g}\right)\right] = \theta_0(\bar{E}, \eta_g) \tag{1.24}$$

Thus combining the aforementioned equations, $\bar{I}_3(\bar{c}_{||})$ can be expressed as

$$\bar{I}_3(\bar{c}_{||}) = \bar{A}_{21}(\bar{E}, \eta_g) + \bar{i}\bar{B}_{21}(\bar{E}, \eta_g) \tag{1.25}$$

where,

$$\bar{A}_{21}(\bar{E},\eta_g)=\left[\frac{\alpha\bar{b}_{||}}{\bar{c}_{||}}\left[\frac{\eta_g\bar{E}}{2\sqrt{\pi}}\exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)-\frac{1}{4}(\eta_g^2+2\bar{E}^2)\left\{1+Erf\left(\frac{\bar{E}}{\eta_g}\right)\right\}\right]\right.$$
$$+\left[\frac{\alpha\bar{c}_{||}+\bar{b}_{||}\bar{c}_{||}-\alpha\bar{b}_{||}}{\bar{c}_{||}^2}\right]\left\{\frac{\bar{E}}{2}[1+Erf(\bar{E}/\eta)]+\frac{\eta\exp(-\bar{E}^2/\eta_g^2)}{2\sqrt{\pi}}\right\}$$
$$+\frac{1}{\bar{c}_{||}}\left(1-\frac{\alpha}{\bar{c}_{||}}\right)\left(1-\frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\frac{1}{2}[1+Erf(\bar{E}/\eta)]$$
$$-\left\{\frac{2}{\bar{c}_{||}^2\eta_g\sqrt{\pi}}\left(1-\frac{\alpha}{\bar{c}_{||}}\right)\left(1-\frac{\bar{b}_{||}}{\bar{c}_{\|\|}}\right)\exp(-\bar{u}_1^2)\right\}$$
$$\left.\left[\sum_{p=1}^{\infty}\left\{\frac{\exp(-p^2/4)}{p}\sinh(\bar{p}\bar{u}_1)\right\}\right]\bar{u}_1\equiv\left[\frac{1+\bar{c}_{||}\bar{E}}{\bar{c}_{||}\eta_g}\right]\right.$$

and

$$\bar{B}_{21}(\bar{E},\eta_g)\equiv\frac{\sqrt{\pi}}{\bar{c}_{||}^2\eta_g}\left(1-\frac{\alpha}{\bar{c}_{||}}\right)\left(1-\frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\exp(-\bar{u}_1^2)$$

Therefore, the combination of all the appropriate integrals together with algebraic manipulations leads to the expression of the dispersion relation of the conduction electrons of HD nonlinear optical materials forming Gaussian band tails as

$$\frac{h^2\bar{k}_z^2}{2\bar{m}_{||}^*\bar{T}_{21}(\bar{E},h_g)}+\frac{h^2\bar{k}_s^2}{2\bar{m}_{\perp}^*\bar{T}_{22}(\bar{E},h_g)}=1 \tag{1.26}$$

where, $\bar{T}_{21}(\bar{E},h_g)$ and $\bar{T}_{22}(\bar{E},h_g)$ have both real and complex parts and are given by

$$\bar{T}_{21}(\bar{E},h_g)=[\bar{T}_{27}(\bar{E},h_g)+i\bar{T}_{28}(\bar{E},h_g)],\ \bar{T}_{27}(\bar{E},h_g)=\left[\frac{\bar{T}_{23}(\bar{E},h_g)}{\bar{T}_5(\bar{E},h_g)}\right]$$

$$\bar{T}_{23}(\bar{E},h_g)\equiv\left[\bar{A}_{21}(\bar{E},h_g)+\frac{a\bar{b}_{||}}{\bar{c}_{||}}\left[\mathrm{dg}_0(\bar{E},h_g)+\frac{1}{9}(\mathrm{D}_{||}^2-\mathrm{D}_{\perp}^2)[1+Erf(\bar{E}/h_g)\right]\right]$$
$$-\left\{\frac{2}{9}\left(\frac{a\bar{b}_{||}}{\bar{c}_{||}}\right)(\mathrm{D}_{||}^2-\mathrm{D}_{\perp}^2)\bar{G}_{21}(\bar{c}_{||},\bar{E},h_g)\right\}\Bigg],$$

$$\bar{G}_{21}(\bar{E},h_g)\equiv\frac{2}{\bar{c}_{||}h_g\sqrt{p}}\exp(-u_1^2)\sum_{\bar{p}=1}^{\infty}\left\{\frac{\exp(-\bar{p}^2/4)}{\bar{p}}\sinh(\bar{p}\bar{u}_1)\right\},$$

$$\bar{T}_5(\bar{E},h_g)\equiv\frac{1}{2}[1+Erf(\bar{E}/h_g)],$$

$$\bar{T}_{28}(\bar{E},h_g)\equiv\left[\frac{\bar{T}_{24}(\bar{E},h_g)}{\bar{T}_5(\bar{E},h_g)}\right],\bar{T}_{24}(\bar{E},h_g)\equiv\left[\bar{B}_{21}(\bar{E},h_g)+\frac{2}{9}\frac{a\bar{b}_{||}}{\bar{c}_{||}}(\mathrm{D}_{||}^2-\mathrm{D}_{\perp}^2)\bar{H}_{21}(\bar{c}_{||},\bar{E},h_g)\right]$$

$$\bar{H}_{21}(\bar{c}_{||},\bar{E},h_g) \equiv \left[\frac{\sqrt{p}}{h_g\bar{c}_{||}}\exp(-\bar{u}_1^2)\right], \bar{T}_{22}(\bar{E},h_g) \equiv [\bar{T}_{29}(\bar{E},h_g)+i\bar{T}_{30}(\bar{E},h_g)],$$

$$\bar{T}_{29}(\bar{E},h_g) \equiv \frac{\bar{T}_3(\bar{E},h_g)\bar{T}_{25}(\bar{E},h_g)-\bar{T}_{24}(\bar{E},h_g)\bar{T}_{26}(\bar{E},h_g)}{[\bar{T}_{25}(\bar{E},h_g)^2+\bar{T}_{26}(\bar{E},h_g)^2]}$$

$$\bar{T}_{25}(\bar{E},h_g) \equiv \left[\left(\frac{\bar{b}_{||}}{\bar{b}_\perp}\frac{\bar{c}_\perp}{\bar{c}_{||}}\right)\frac{1}{2}\left[1+Erf\left(\frac{\bar{E}}{h_g}\right)\right]+\left(\frac{\bar{b}_{||}}{\bar{b}_\perp}\frac{\bar{c}_{||}}{\bar{c}_\perp}\right)\left(\frac{d}{2}+\left[\frac{D_{||}^2-D_\perp^2}{6D_{||}}\right]\right)a_{||}\bar{C}_{21}(a_{||},\bar{E},h_g)\right.$$
$$\left.+\left(\frac{\bar{b}_{||}\bar{c}_\perp}{\bar{b}_\perp}\right)\left(\frac{d}{2}-\left[\frac{D_{||}^2-D_\perp^2}{6D_{||}}\right]\right)\bar{G}_{21}(a_{||},\bar{E},h_g)\right],$$

$$\bar{C}_{21}(a_{||},\bar{E},h_g) \equiv \left[\frac{2}{a\sqrt{p}h_g}\exp(-\bar{u}^2)\left[\sum_{p=1}^{\infty}\frac{\exp(-p^2/4)}{p}\sinh(\bar{p}\,\bar{u})\right]\right],$$

$$T_{26}(\bar{E},h_g) \equiv \left(\frac{\bar{b}_{||}}{\bar{b}_\perp}\frac{\bar{c}_\perp}{\bar{c}_{||}}\right)\left(\frac{d}{2}-\left[\frac{D_{||}^2-D_\perp^2}{6D_{||}}\right]\right)a\bar{D}_{21}(a_{||},\bar{E},h_g)$$
$$+\frac{\bar{b}_{||}\bar{c}_\perp}{\bar{b}_\perp}\left(\frac{d}{2}-\left[\frac{D_{||}^2-D_\perp^2}{6D_{||}}\right]\right)\bar{H}_{21}(\bar{c}_{||},\bar{E},h_g),$$

and

$$\eta_g = h_g,\ D_{||} = \Delta_{11},\ D_\perp = \Delta_\perp$$

$$\bar{T}_{30}(\bar{E},h_g) \equiv \frac{\bar{T}_{24}(\bar{E},h_g)\bar{T}_{25}(\bar{E},h_g)+\bar{T}_{23}(\bar{E},h_g)\bar{T}_{26}(\bar{E},h_g)}{[(\bar{T}_{25}(\bar{E},h_g))^2+(\bar{T}_{26}(\bar{E},h_g))^2]}$$

From (1.26), it appears that the energy spectrum in HD nonlinear optical materials is complex. The complex nature of the electron dispersion law in HD materials occurs from the existence of the essential poles in the corresponding electron energy spectrum in the absence of band tails. It may be noted that the complex band structures have already been studied for bulk materials and superlattices without heavy doping [135] and bear no relationship with the complex electron dispersion law as indicated by (1.26). The physical picture behind the formulation of the complex energy spectrum in HDS is the interaction of the impurity atoms in the tails with the splitting constants of the valance bands. More is the interaction; more is the prominence of the complex part than the other case. In the absence of band tails, $\eta_g \to 0$, and there is no interaction of the impurity atoms in the tails with the spin orbit constants. As a result, there exist no complex energy spectrum and (1.26) gets converted into (1.2) when $\eta_g \to 0$. Besides, the complex spectra are not related to same evanescent modes in the band tails and the conduction bands.

It is interesting to note that the single important concept in the whole spectra of materials and allied sciences is the effective electron mass which is in disguise in the apparently simple (1.26), and can, briefly be described as follows:

Effective Electron Mass (EEM): The effective mass of the carriers in materials, being connected with the mobility, is known to be one of the most important physical quantities, used for the analysis of electron devices under different operating conditions [136]. The carrier degeneracy in materials influences the effective mass when it is energy dependent. Under degenerate conditions, only the electrons at the Fermi surface of n-type materials participate in the conduction process and hence, the effective mass of the electrons corresponding to the Fermi level (EEM) would be of interest in electron transport under such conditions. The Fermi energy is again determined by the electron energy spectrum and the carrier statistics and therefore, these two features would determine the dependence of the effective electron mass in degenerate n-type materials under the degree of carrier degeneracy. In recent years, various energy wave vector dispersion relations have been proposed [137–139] which have created the interest in studying the effective mass in such materials under external conditions. It has, therefore, different values in different materials and varies with electron concentration, with the magnitude of the reciprocal quantizing magnetic field undermagnetic quantization, with the quantizing electric field as in inversion layers, with the nano-thickness as in UFs and nano wires and with superlattice period as in the quantum confined superlattices of small gap materials with graded interfaces having various carrier energy spectra [140–156].

The transverse and the longitudinal EEMs at the Fermi energy $\bar{E}_{F_n}$ of HDS in the presence of band tails as measured from the edge of the conduction band in the vertically upward direction in the absence of band tails of HD nonlinear optical materials can, respectively, be expressed as

$$\bar{m}_{\perp}^{*} = m_{\perp}^{*}\{\bar{T}_{29}(\bar{E},\eta_g)\}'\Big|_{\bar{E}=\bar{E}_{F_n}} \quad (1.27)$$

and

$$m_{||}^{*} = m_{||}^{*}\{\bar{T}_{27}(\bar{E},\eta_g)\}'\Big|_{\bar{E}=\bar{E}_{F_n}} \quad (1.28)$$

where the primes denote the differentiations of the differentiable functions with respect to Fermi energy in the appropriate case.

In the absence of band tails $\eta_g \to 0$ and we get

$$\bar{m}_{\perp}^{*}(\bar{E}_F,\bar{O}) = \frac{\hbar^2}{2}\left[\frac{\psi_2(\bar{E})\{\psi_1(\bar{E})\}' - \psi_1(\bar{E})\{\psi_2(\bar{E})\}'}{\{\psi_2(\bar{E})\}}\right]_{\bar{E}=\bar{E}_F} \quad (1.29)$$

and

$$m_{||}^{*}(\bar{E}_F,\bar{O}) = \frac{\hbar^2}{2}\left[\frac{\psi_3(\bar{E})\{\psi_1(\bar{E})\}' - \{\psi_1(\bar{E})\}\{\psi_3(\bar{E})\}'}{\{\psi_3(\bar{E})\}}\right]_{\bar{E}=\bar{E}_F} \quad (1.30)$$

where $\bar{E}_F$ is the Fermi energy as measured from the edge of the conduction band in the vertically upward direction in the absence of band tails $\psi_1(\bar{E}) = \gamma(\bar{E}), \psi_2(\bar{E}) = \bar{f}_1(\bar{E})$, *and* $\psi_3(\bar{E}) = \bar{f}_2(\bar{E})$,

Comparing the aforementioned equations, one can infer that **the effective masses exist in the forbidden zone, which is impossible without the effect of band tailing. For materials, in the absence of band tails the effective mass in the band gap is infinity.**

The DOS function is given by

$$\bar{N}_{HD}(\bar{E}, \eta_g) = \frac{2\bar{g}_v \bar{m}^*_{\perp} \sqrt{2m^*_{||}}}{3\pi^2\hbar^3} \bar{R}_{11}(\bar{E}, \eta_g) \cos[\psi_{11}(\bar{E}, \eta_g)] \tag{1.31a}$$

where, $\bar{g}_v$ is the valley degeneracy,

$$\begin{aligned}\bar{R}_{11}(\bar{E}, \eta_g) \equiv \Bigg[\Bigg[\{\bar{T}_{29}(\bar{E}, \eta_g)\}' \sqrt{\bar{x}(\bar{E}, \eta_g)} + \frac{\bar{T}_{29}(\bar{E}, \eta_g)\{\bar{x}(\bar{E}, \eta_g)\}'}{2\sqrt{\bar{x}(\bar{E}, \eta_g)}} \\ - \{\bar{T}_{30}(\bar{E}, \eta_g)\}' \sqrt{\bar{y}(\bar{E}, \eta_g)} \frac{\bar{T}_{30}(\bar{E}, \eta_g)\{y(\bar{E}, \eta_g)\}'}{2\sqrt{\bar{y}(\bar{E}, \eta_g)}}\Bigg]^2 \\ + \Bigg[\{\bar{T}_{29}(\bar{E}, \eta_g)\}' \sqrt{\bar{y}(\bar{E}, \eta_g)} + \frac{\bar{T}_{29}(\bar{E}, \eta_g)\{\bar{y}(\bar{E}, \eta_g)\}'}{2\sqrt{\bar{y}(\bar{E}, \eta_g)}} \\ + \{\bar{T}_{30}(\bar{E}, \eta_g)\}' \sqrt{x(\bar{E}, \eta_g)} \frac{\bar{T}_{30}(\bar{E}, \eta_g)\{\bar{x}(\bar{E}, \eta_g)\}'}{2\sqrt{\bar{x}(\bar{E}, \eta_g)}}\Bigg]^2\Bigg]^{1/2},\end{aligned}$$

$$\bar{x}(\bar{E}, \eta_g) \equiv \frac{1}{2}\left[\bar{T}_{27}(\bar{E}, \eta_g) + \sqrt{\{\bar{T}_{27}(\bar{E}, \eta_g)\}^2 + \{\bar{T}_{28}(\bar{E}, \eta_g)\}^2}\right],$$

$$\bar{y}(\bar{E}, \eta_g) \equiv \frac{1}{2}\left[\sqrt{\{\bar{T}_{27}(\bar{E}, \eta_g)\}^2 + \{\bar{T}_{28}(\bar{E}, \eta_g)\}^2} - \bar{T}_{27}(\bar{E}, \eta_g)\right]$$

and

$$\begin{aligned}\psi_{11}(\bar{E}, \eta_g) \equiv \tan^{-1}\Bigg[\Bigg[\{\bar{T}_{29}(\bar{E}, \eta_g)\}' \sqrt{y(\bar{E}, \eta_g)} + \frac{\bar{T}_{29}(\bar{E}, \eta_g)}{2\sqrt{\bar{y}(\bar{E}, \eta_g)}} + \{\bar{T}_{30}(\bar{E}, \eta_g)\}' \sqrt{\bar{x}(\bar{E}, \eta_g)} \\ + \frac{\bar{T}_{30}\{\bar{x}(\bar{E}, \eta_g)\}'}{2\sqrt{\bar{x}(\bar{E}, \eta_g)}}\Bigg]\Bigg[\{\{\bar{T}_{29}(\bar{E}, \eta_g)\}'\} \sqrt{\bar{x}(\bar{E}, \eta_g)} + \frac{\bar{T}_{29}(\bar{E}, \eta_g)\{\bar{x}(\bar{E}, \eta_g)\}'}{2\sqrt{\bar{x}(\bar{E}, \eta_g)}} \\ - \{\bar{T}_{30}(\bar{E}, \eta_g)\}' \sqrt{\bar{y}(\bar{E}, \eta_g)} + \frac{\bar{T}_{30}\{\bar{t}(\bar{E}, \eta_g)\}'}{2\sqrt{\bar{y}(\bar{E}, \eta_g)}}\Bigg]^{-1}\Bigg]\end{aligned}$$

The oscillatory nature of the DOS for HD nonlinear optical materials is apparent from (1.31a). For, $\psi_{11}(\bar{E}, \eta_g) \geq \pi$, the cosine function becomes negative leading to the negative values of the DOS. The electrons cannot exist for the negative values of the DOS and therefore, this region is forbidden for electrons, which indicates that in the band tail, **there appears a new forbidden zone in addition to the normal band gap of the semiconductor.**

The use of (1.31a) leads to the expression of the electron concentration as

$$\bar{n}_0 = \frac{2\bar{g}_v \bar{m}_{\perp}^{*}\sqrt{2\bar{m}^{*}}}{3\pi^2\hbar^3}\left[\bar{I}_{11}(\bar{E}_{F_h}, \eta_g) + \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{I}_{11}(\bar{E}_{F_h}, \eta_g)]\right] \tag{1.31b}$$

where,

$$\bar{I}_{11}(\bar{E}_{F_h}, \eta_g) \equiv [\bar{T}_{29}(\bar{E}_{F_h}, \eta_g)\sqrt{\bar{x}(\bar{E}_{F_h}, \eta_g)} - \bar{T}_{30}(\bar{E}_{F_h}, \eta_g)\sqrt{y(\bar{E}_{F_h}, \eta_g)}$$

$$\bar{L}(\bar{r}) = 2(\bar{k}_B\bar{T})^{2r}(1-2^{1-2r})\xi(2\bar{r})\frac{\partial^{2r}}{\partial\bar{E}_{Fs}^{2r}} \tag{1.31c}$$

$\bar{r}$ is the set of real positive integers whose upper s and $\xi(2\bar{r})$ is the Zeta function of order $2\bar{r}$ [133, 134].

The entropy per unit volume which can be written as

$$\overline{S_0} = -\frac{\partial\Omega}{\partial\bar{T}}\Big|_{\bar{E}=\bar{E}_F} \tag{1.31d}$$

in which Ω is the thermodynamic potential which, in turn, can be expressed in accordance with the Fermi–Dirac statistics as

$$\Omega = -\bar{k}_B\bar{T}\sum \ln\left|1+\exp\left[\frac{\bar{E}_F - \bar{E}_{\delta_0}}{\bar{k}_B\bar{T}}\right]\right| \tag{1.31e}$$

where the summation is carried out over all the possible δ_0 states and $\bar{k}_B$ is Boltzmann constant.

Thus, combining 1.31d and1.31e, the magnitude of the entropy for HD systems can be written in a simplified form as

$$\bar{S}_0 = (\pi^2\bar{k}_B^2\bar{T}/3)\left(\frac{\partial\bar{n}_0}{\partial(\bar{E}_F - \bar{E}_{hd}}\right) \tag{1.31f}$$

where $\bar{E}_{hd}$ is the electron energy within the band gap, as measured from $\bar{k}=0$ and should be obtained from the dispersion relation of the HD materials under the conditions $\bar{E}-\bar{E}_{hd}$ when $\bar{k}=0$. It should be noted that being a thermodynamic relation and temperature induced phenomena, the entropy as expressed by (1.31f), in general, is valid for electronic materials having arbitrary dispersion relations and their nanostructures. In addition to bulk materials in the presence of strong magnetic

field, (1.31f) is valid under one-, two- and three-dimensional quantum confinement of the charge carriers (such as quantum wells in ultrathin films, nipi structures, inversion and accumulation layers, quantum well superlattices, carbon nanotubes, quantum wires, quantum wire superlattices, quantum dots, magneto inversion and accumulation layers, quantum dot superlattices, magneto nipis, quantum well superlattices under magnetic quantization, ultrathin films under magnetic quantization, etc.). The formulation of $\bar{S}_0$ requires the relation between electron statistics and the corresponding Fermi energy, which is basically the band structure-dependent quantity and changes under different physical conditions. It is worth remarking to note that the number $(\pi^2/3)$ has occurred as a consequence of mathematical analysis and is not connected with the well- known Lorenz number. For quantum wells in ultrathin films, nipi structures, inversion and accumulation layers, quantum well superlattices, magneto inversion and accumulation layers, magneto nipis, quantum well superlattices under magnetic quantization and magneto size quantization, the carrier concentration is measured per unit area whereas, for quantum wires, quantum wires under magnetic field, quantum wire superlattices and such allied systems, the same can be measured per unit length. Besides, for bulk materials under strong magnetic field, quantum dots, quantum dots under magnetic field, quantum dot superlattices and quantum dot superlattices under magnetic field, the carrier concentration is expressed per unit volume.

For HD nonlinear materials, $\bar{E}_{hd}$ is the smallest negative root of the equation

$$[\bar{T}_{27}(\bar{E}_{hd},\eta_g)\bar{T}_{29}(\bar{E}_{hd},\eta_g)-\bar{T}_{28}(\bar{E}_{hd},\eta_g)\bar{T}_{30}(\bar{E}_{hd},\eta_g)]=0 \tag{1.31g}$$

Therefore, the entropy can be numerically evaluated by using (1.31b), (1.31f), (1.31g) and the allied definitions.

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (1.26) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{||}\bar{T}_{21}(\bar{E},\eta_g)}+\frac{\hbar^2\bar{k}_s^2}{2\bar{m}^*_{\perp}\bar{T}_{22}(\bar{E},\eta_g)}=1 \tag{1.32}$$

where, $\bar{n}_z(=1,\ 2,\ 3)$ and $\bar{d}_z$ are the size quantum number and the nano-thickness along the z-direction, respectively.

The general expression of the total 2D DOS $(\bar{N}_{2DT}(\bar{E}))$ can, in general, be expressed as

$$\bar{N}_{2DT}(\bar{E})=\frac{2\bar{g}_v}{(2\pi)^2}\sum_{n_z=1}^{n_{z\max}}\frac{\partial\bar{A}(\bar{E},\bar{n}_z)}{\partial\bar{E}}\bar{H}(\bar{E}-\bar{E}_{n_z}) \tag{1.33}$$

where $\bar{A}(\bar{E},\bar{n}_z)$ is the area of the constant energy 2D Wave vector space and in this case it is for QWs $\bar{H}(\bar{E}-\bar{E}_{n_z})$ is the Heaviside step function and $\bar{E}_{n_z}$ is the corresponding

sub-band energy. Using (1.32) and (1.33), the expression of the $\bar{N}_{2DT}(\bar{E})$ for QWs of HD nonlinear optical materials can be written as

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_{\perp}^{*}\bar{g}_{v}}{\pi\hbar^{2}} \sum_{\bar{n}_{z}=1}^{\bar{n}_{z\max}} \bar{T}_{1D}{}'(\bar{E}, \eta_{g}, \bar{n}_{z})\bar{H}(\bar{E} - \bar{E}_{n_{z}D_{1}}) \tag{1.34}$$

where,

$$\bar{T}_{1D}(\bar{E}, \eta_{g}, \bar{n}_{z}) = \left[1 - \frac{\hbar^{2}(\bar{n}_{z}\pi/\bar{d}_{z})^{2}}{2\bar{m}_{||}^{*}\bar{T}_{21}(\bar{E}, \eta_{g})}\right]\bar{T}_{22}(\bar{E}, \eta_{g}),$$

$\bar{H}(\bar{E} - \bar{E}_{n_{z}})$ is the Heaviside step function and $\bar{E}_{n_{z}D_{1}}$ is the corresponding sub-band energy which in this case is given by the following equation

$$\frac{\hbar^{2}(\bar{n}_{z}\pi/\bar{d}_{z})^{2}}{2\bar{m}_{||}^{*}\bar{T}_{21}(\bar{E}_{n_{z}D_{1}}, \eta_{g})} = 1 \tag{1.35}$$

Thus we observe that both the total DOS and sub-band energies of QWs of HD nonlinear optical materials are complex due to the presence of the pole in energy axis of the corresponding materials in the absence of band tails.

EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1HD}, \eta_{g}, \bar{n}_{z}) = \bar{m}_{\perp}^{*}[\text{Real part of } \bar{T}'_{1D}(\bar{E}_{F1HD}, \eta_{g}, \bar{n}_{z})] \tag{1.36}$$

where $\bar{E}_{F1HD}$ is the Fermi energy in the presence of size quantization of the QWs of HD nonlinear optical materials as measured from the edge of the conduction band in the vertically upward direction in the absence of any perturbation.

Thus, we observe that EEM is the function of size quantum number and the Fermi energy due to the combined influence of the crystal filed splitting constant and the anisotropic spin-orbit splitting constants, respectively. Besides it is a function of η_{g} due to which EEM exists in the band gap, which is otherwise impossible.

Combining (1.34) with the Fermi–Dirac occupation probability factor, integrating between$\bar{E}_{n_{z}D1}$ to infinity and applying the generalized Summerfield's lemma [152–153], the 2D carrier statistics in this case assumes the form

$$\bar{n}_{2D} = \frac{\bar{m}_{\perp}^{*}\bar{g}_{v}}{\pi\hbar^{2}} \sum_{\bar{n}_{z}=1}^{\bar{n}_{\max}} [\text{Real part of } [\bar{T}_{1D}(\bar{E}_{F1HD}, \eta_{g,}\bar{n}_{z}) + \bar{T}_{2D}(\bar{E}_{F1HD}, \eta_{g}, \bar{n}_{z})]] \tag{1.37}$$

where,

$$\bar{T}_{2D}(\bar{E}_{F1HD}, \eta_{g}, \bar{n}_{z}) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{T}_{1D}(\bar{E}_{F1HD}, \eta_{g}, \bar{n}_{z})], \tag{1.38}$$

Therefore combining (1.37) and (1.31f) we can study the entropy in this case.

In the absence of heavy doping, the 2D dispersion relation EEM in the x–y plane at the Fermi level, the total 2D DOS and the electron concentration for QWs of nonlinear optical materials in the absence of band tails can, respectively, be written as

$$\psi_1(\bar{E}) = \psi_2(\bar{E})\bar{k}_s^2 + \psi_3(\bar{E})(\bar{n}_z\pi/\bar{d}_z)^2$$

$$\bar{m}^*(\bar{E}_{Fs}, \bar{n}_z) = \left(\frac{\hbar^2}{2}\right)[\psi_2(\bar{E}_{Fs})]^2\left[\psi_2(\bar{E}_{Fs})\left\{\{\psi_1(\bar{E}_{Fs})\}' - \{\psi_3(\bar{E}_{Fs})\}'\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right\}\right. \tag{1.39}$$

$$\left. - \left\{\psi_1(\bar{E}_{Fs}) - \psi_3(\bar{E}_{Fs})\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right\}\{\psi_2(\bar{E}_{Fs})\}'\right]$$

$$\bar{N}_{2DT}(\bar{E}) = \left(\frac{\bar{g}_v}{2\pi}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\psi_2(\bar{E})]^2\left[\psi_2(\bar{E})\left\{\{\psi_1(\bar{E}_{Fs})\}' - \{\psi_3(\bar{E})\}'\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right\}\right. \tag{1.40}$$

$$\left. - \{\psi_1(\bar{E}) - \psi_3(\bar{E})(\frac{\bar{n}_z\pi}{\bar{d}_z})^2\}\{\psi_2(\bar{E})\}'\right]\bar{H}(\bar{E} - \bar{E}_{n_{z_1}}) \tag{1.41}$$

$$\psi_1(\bar{E}_{n_{z_1}}) = \psi_2(\bar{E}_{n_{z_1}})\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \tag{1.42a}$$

$$\bar{n}_{2D} = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{T}_{51}(\bar{E}_{Fs}, \bar{n}_z) + \bar{T}_{52}(\bar{E}_{Fs}, \bar{n}_z)] \tag{1.42b}$$

where $\psi_1(\bar{E}) = \gamma(\bar{E}), \psi_2(\bar{E}) = \bar{f}_1(\bar{E}), \psi_3(\bar{E}) = \bar{f}_2(\bar{E})$, $\bar{E}_{n_{z_1}}$ are the sub-band energies, $\bar{E}_{Fs}$ is the Fermi energy in the 2D sized quantized material in thepresence of size quantization and in the absence of heavy doping as measured from the edgeof the conduction band in the vertically upward direction in the absence of any quantization,

$$\bar{T}_{51}(\bar{E}_{Fs}, \bar{n}_z) \equiv \left[\frac{\psi_1(\bar{E}_{Fs}) - \psi_3(\bar{E}_{Fs})(\bar{n}_z\pi/\bar{d}_z)^2}{\psi_2(\bar{E}_{Fs})}\right]$$

and

$$\bar{T}_{52}(\bar{E}_{Fs}, \bar{n}_z) \equiv \sum_{r=1}^{s}\bar{L}(\bar{r})[\,\bar{T}_{51}(\bar{E}_{Fs}, \bar{n}_z)] \tag{1.43}$$

In the absence of band tails, the entropy can be written as

$$\bar{S}_0 = (\pi^2\bar{k}_B^2\bar{T}/3)\left(\frac{\partial\bar{n}_0}{\partial\bar{E}_F}\right) \tag{1.44}$$

Thus, using (1.43) and (1.44), we can study the entropy in this case.

In the absence of heavy doping, the DOS for bulk specimens of nonlinear optical materials is given by

$$\bar{D}_0(\bar{E}) = \bar{g}_v(3\pi^2)^{-1}\psi_4(\bar{E}) \tag{1.45}$$

where,

$$\psi_4(\bar{E}) \equiv \left[\frac{3}{2}\frac{\sqrt{\psi_1(\bar{E})}[\psi_1(\bar{E})]'}{\psi_2(\bar{E})\sqrt{\psi_3(\bar{E})}} - \frac{[\psi_2(\bar{E})]'[\psi_1(\bar{E})]^{3/2}}{[\psi_2(\bar{E})]^2\sqrt{\psi_3(\bar{E})}} - \frac{1}{2}\frac{[\psi_3(\bar{E})]'[\psi_1(\bar{E})]^{3/2}}{\psi_2(E)[\psi_3(\bar{E})]^{3/2}}\right],$$

$$[\psi_1(\bar{E})]' \equiv [(2\bar{E}+\bar{E}_g)\psi_1(\bar{E})[\bar{E}(\bar{E}+\bar{E}_g)]^{-1} + \bar{E}(\bar{E}+\bar{E}_g)(2\bar{E}+2\bar{E}_g+\delta+\Delta_{||})],$$

$$[\psi_2(\bar{E})]' \equiv \left[2\bar{m}^*_{\perp}\left(\bar{E}_g+\frac{2}{3}\Delta_{\perp}\right)\right]^{-1}[\hbar^2\bar{E}_g(\bar{E}_g+\Delta_{\perp})]\left[\delta+2\bar{E}+2\bar{E}_g+\frac{2}{3}\Delta_{||}\right]$$

and

$$[\psi_3(\bar{E})]' \equiv \left[2\bar{m}^*_{\perp}\left(\bar{E}_g+\frac{2}{3}\Delta_{||}\right)\right]^{-1}[\hbar^2\bar{E}_g(\bar{E}_g+\Delta_{||})]\left[2\bar{E}+2\bar{E}_g+\frac{2}{3}\Delta_{||}\right]$$

Combining (1.45) with the Fermi–Dirac occupation probability factor and using the generalized Summerfield's lemma[153], the electron concentration can be written as

$$\bar{n}_0 = \bar{g}_v(3\pi^2)^{-1}[\bar{M}(\bar{E}_F) + \bar{N}(\bar{E}_F)] \tag{1.46}$$

where,

$$\bar{M}(\bar{E}_F) \equiv \left[\frac{[\psi_1(\bar{E}_F)]^{\frac{3}{2}}}{\psi_2(\bar{E}_F)\sqrt{\psi_3(\bar{E}_F)}}\right],$$

$\bar{E}_F$ is the Fermi energy of the bulk specimen in the absence of band tails as measured from the edge of the conduction band in the vertically upward direction and

$$\bar{N}(\bar{E}_F) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})\bar{M}(\bar{E}_F) \tag{1.47}$$

Thus, using (1.46a) and (1.44), we can study the entropy in this case.

1.2.2 Entropy in quantum wells (QWs) of HD III–V materials

The dispersion relation of the conduction electrons of III–V compounds are described by the models of Kane (both three and two bands) [36, 37], Stillman et al. [38, 39] and Palik et al. [40], respectively. For the purpose of complete and coherent presentation and relative comparison, the entropy in QWs of HD III–V materials have also been investigated in accordance with the aforementioned different dispersion relations as follows:

(a) The Three-Band Model of Kane

Under the conditions $\delta = 0, \Delta_{||} = \Delta_{\perp} = \Delta$ (isotropic spin orbit splitting constant) and $\bar{m}^*_{||} = \bar{m}^*_{\perp} = \bar{m}_c$ (isotropic effective electron mass at the edge of the conduction band), (1.2) gets simplified as

$$\frac{\hbar^2 \bar{k}^2}{2\bar{m}_c} = \bar{I}_{11}(\bar{E}), \bar{I}_{11}(\bar{E}) \equiv \frac{\bar{E}(\bar{E}+\bar{E}_{g_0})(\bar{E}+\bar{E}_{g_0}+\Delta)(\bar{E}_{g_0}+\frac{2}{3}\Delta)}{\bar{E}_{g_0}(\bar{E}_{g_0}+\Delta)(\bar{E}+\bar{E}_{g_0}+\frac{2}{3}\Delta)} \tag{1.48}$$

which is known as the three-band model of Kane [36] and is often used to investigate the physical properties of III–V materials.

Under the said conditions, the HD electron dispersion law in this case can be written from (1.26) as

$$\frac{\hbar^2 \bar{k}^2}{2\bar{m}_c} = \bar{T}_{31}(\bar{E}, \eta_g) + i\bar{T}_{32}(\bar{E}, \eta_g) \tag{1.49}$$

where,

$$\begin{aligned}\bar{T}_{31}(\bar{E}, \eta_g) \equiv \left(\frac{2}{1+Erf(\bar{E}/\eta_g)}\right) \Bigg[& \frac{\bar{a}\bar{b}}{\bar{c}}\theta_0(\bar{E}, \eta_g) \\ & + \left[\frac{\alpha\bar{c}+\bar{b}\bar{c}-\alpha\bar{b}}{\bar{c}^2}\right]\gamma_0(\bar{E}, \eta_g) + \frac{1}{\bar{c}}\left(1-\frac{\alpha}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)\frac{1}{2}\left[1+Erf\left(\frac{\bar{E}}{\eta_g}\right)\right] \\ & - \frac{1}{\bar{c}}\left(1-\frac{\alpha}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)\frac{2}{c\eta_g\sqrt{\pi}}\exp(-\bar{u}_2^2)\left[\sum_{\bar{p}=1}^{\infty}\frac{\exp(-\bar{p}^2/4)}{\bar{p}}\sinh(\bar{p}\bar{u}_2)\right]\Bigg],\end{aligned}$$

$$\bar{b} \equiv (\bar{E}_g + \Delta)^{-1}, \bar{c} \equiv \left(\bar{E}_g + \frac{2}{3}\Delta\right)^{-1}$$

$$\bar{u}_2 \equiv \frac{1+\bar{c}E}{\bar{c}\eta_g} \text{ and } \bar{T}_{32}(\bar{E}, \eta_g) \equiv \left(\frac{2}{1+Erf(\bar{E}/\eta_g)}\right)\frac{1}{\bar{c}}\left(1-\frac{\alpha}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)\frac{\sqrt{\pi}}{c\eta_g}\frac{\sqrt{\pi}}{c\eta_g}\exp(-\bar{u}_2^2)$$

Thus, the complex energy spectrum occurs due to the term $\bar{T}_{32}(\bar{E}, \eta_g)$ and this imaginary band is quite different from the forbidden energy band.

EEM at the Fermi level is given by

$$\bar{m}^*(\bar{E}_{Fs}, \eta_g) = \bar{m}_c\{\bar{T}_{31}(\bar{E}, \eta_g)\}'\Big|_{\bar{E}=\bar{E}_{Fs}} \tag{1.50}$$

Thus, EEM in HD III–V, ternary and quaternary materials exists in the band gap, which is the new attribute of the theory of band tailing.

In the absence of band tails, $\eta_g \to 0$ and EEM assumes the form

$$\bar{m}^*(\bar{E}_F) = \bar{m}_c\{\bar{I}_{11}(\bar{E})\}'\Big|_{\bar{E}=\bar{E}_F} \tag{1.51}$$

The DOS function in this case can be written as

$$\bar{N}_{HD}(\bar{E},\eta_g)=\frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\bar{R}_{21}(\bar{E},\eta_g)\cos[\vartheta_{21}(\bar{E},\eta_g)] \tag{1.52}$$

where,

$$\bar{R}_{21}(\bar{E},\eta_g)\equiv\left[\frac{[\{\alpha_{11}(\bar{E},\eta_g)\}']^2}{4\alpha_{11}(\bar{E},\eta_g)}+\frac{[\{\beta_{11}(\bar{E},\eta_g)\}']^2}{4\beta_{11}(\bar{E},\eta_g)}\right]^{1/2}$$

$$\alpha_{11}(\bar{E},\eta_g)\equiv\frac{1}{2}\left[\bar{T}_{33}(\bar{E},\eta_g)+\sqrt{\{\bar{T}_{33}(\bar{E},\eta_g)\}^2+\{\bar{T}_{34}(\bar{E},\eta_g)\}^2}\right],$$

$$\bar{T}_{33}(\bar{E},\eta_g)\equiv\left[\{\bar{T}_{31}(\bar{E},\eta_g)\}^3-3\bar{T}_{31}(\bar{E},\eta_g)\{\bar{T}_{32}(\bar{E},\eta_g)\}^2\right],$$

$$\bar{T}_{34}(\bar{E},\eta_g)\equiv\left[3\bar{T}_{32}(\bar{E},\eta_g)\{\bar{T}_{31}(\bar{E},\eta_g)\}^2-\{\bar{T}_{32}(\bar{E},\eta_g)\}^3\right],$$

$$\beta_{11}(\bar{E},\eta_g)\equiv\frac{1}{2}\left[\sqrt{\{\bar{T}_{33}(\bar{E},\eta_g)\}^2+\{\bar{T}_{34}(\bar{E},\eta_g)\}^2}-\bar{T}_{33}(\bar{E},\eta_g)\right]$$

and

$$\vartheta_{21}(\bar{E},\eta_g)\equiv\tan^{-1}\left[\frac{\{\beta_{11}(\bar{E},\eta_g)\}'}{\{\alpha_{11}(\bar{E},\eta_g)\}'}+\sqrt{\frac{\alpha_{11}(\bar{E},\eta_g)}{\beta_{11}(\bar{E},\eta_g)}}\right]$$

Thus, the oscillatory DOS function becomes negative for $\vartheta_{21}(\bar{E},\eta_g)\geq\pi$ and a new forbidden zone will appear in addition to the normal band gap.

The electron concentration can be expressed as

$$\bar{n}_0=\frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\left[\bar{I}_{111e}(\bar{E}_{F_h},\eta_s)+\sum_{\bar{r}=1}^{\bar{s}}l(r)[\bar{I}_{111e}(\bar{E}_{F_h},\eta_s)]\right] \tag{1.53}$$

where

$$\bar{T}_{111e}(\bar{E}_{F_h},\eta_g)=\{\gamma_2(\bar{E}_{F_h},\eta_g)\}^{3/2}$$

In this case, $\bar{E}_{hd}$ is given by

$$\bar{T}_{31}(\bar{E}_{hd},\eta_g)=0 \tag{1.54}$$

The numerical evaluation of the *entropy* has been done by using (1.53), (1.31f), (1.54) and the allied definitions.

For dimensional quantization along *z*-direction, the dispersion relation of the 2D electrons in this case can be written following (1.49) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{k}_s)^2}{2\bar{m}_c} = \bar{T}_{31}(\bar{E},\eta_g) + i\bar{T}_{32}(\bar{E},\eta_g) \tag{1.55}$$

The expression of the $\bar{N}_{2DT}(\bar{E})$ in this case assumes the form

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{T}'_{5D}(\bar{E},\eta_g,\bar{n}_z)\bar{H}(\bar{E}-\bar{E}_{n_zD5}) \tag{1.56}$$

where

$$\bar{T}_{5D}(\bar{E},\eta_g,\bar{n}_z) = [\bar{T}_{31}(\bar{E},\eta_g) + i\bar{T}_{32}(\bar{E},\eta_g) - \hbar^2(\bar{n}_z\pi/\bar{d}_z)^2(2\bar{m}_c)^{-1}]$$

and the sub-band energies $\bar{E}_{n_zD5}$ in this case given by

$$\{\hbar^2(\bar{n}_z/\bar{d}_z)^2\}(2\bar{m}_c)^{-1} = \bar{T}_{31}(\bar{E}_{n_zD5},\eta_g) \tag{1.57}$$

Thus, we observe that both the total DOS in QWs of HD III–V compounds and the sub-band energies are complex due to the presence of the pole in energy axis of the corresponding materials in the absence of band tails.

EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \bar{m}_c[\bar{T}'_{31}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)] \tag{1.58}$$

Therefore, under the same conditions as used in obtaining (1.48) from (1.2), the 2D carrier statistics in this case can be written by using the same conditions from (1.37) as

$$\bar{n}_{2D} = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{zz_{\max}}} [\mathrm{Real\ part\ of}[\bar{T}_{5D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) + \bar{T}_{6D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)]] \tag{1.59}$$

where

$$\bar{T}_{6D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \sum_{r=1}^{s}\bar{L}(\bar{r})[\bar{T}_{5D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)]$$

Therefore, combining (1.31f) and (1.59) we can study the *entropy* in this case.

In the absence of band tails, the 2D dispersion relation, EEM in the x–y plane at the Fermi level, the total 2D DOS, the sub-band energy and the electron concentration for QWs of III–V materials assume the following forms

$$\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_c} + \frac{\hbar^2}{2\bar{m}_c}(\bar{n}_z\pi/\bar{d}_x)^2 = \bar{I}_{11}(\bar{E}) \tag{1.60}$$

$$\bar{m}^*(\bar{E}_{Fs}) = \bar{m}_c\{\bar{I}_{11}(\bar{E}_{Fs})\}' \tag{1.61}$$

$$\bar{N}_{2DT}(\bar{E}) = \left(\frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2}\right) \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \{[\bar{I}_{11}(\bar{E})]' \bar{H}(\bar{E} - \bar{E}_{n_{z_2}})\} \tag{1.62}$$

where the sub-band energies $\bar{E}_{n_{z_2}}$ can be expressed as

$$\bar{I}_{11}(\bar{E}_{N_{Z_2}}) = \frac{\hbar^2}{2\bar{m}_c}(\bar{n}_z\pi/\bar{d}_z)^2 \tag{1.63}$$

$$\bar{n}_{2D} = \left(\frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2}\right) \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{T}_{53}(\bar{E}_{Fs}, \bar{n}_z) + \bar{T}_{54}(\bar{E}_{Fs}, \bar{n}_z)] \tag{1.64}$$

where

$$\bar{T}_{55}(\bar{E}_{Fs}, \bar{n}_z) \equiv \left[\bar{I}_{11}(\bar{E}_{Fs}) - \frac{\hbar^2}{2\bar{m}_c}(\bar{n}_z\pi/\bar{d}_z)^2\right]$$

and

$$\bar{T}_{54}(\bar{E}_{Fs}, \bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) \bar{T}_{53}(\bar{E}_{Fs}, \bar{n}_z) \tag{1.65}$$

It is worth noting that the EEM in this case is a function of Fermi energy alone and is independent of size quantum number.

Thus, using (1.64) and (1.44), we can study the entropy in this case.

In the absence of band tails, the DOS function and the electron concentration, in bulk III–V, ternary, and quaternary materials in accordance with the unperturbed three-band model of Kane assume the following forms.

$$\bar{D}_0(\bar{E}) = 4\pi g_v \left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2} \sqrt{\bar{I}_{11}(\bar{E})}[\bar{I}'_{11}(\bar{E})] \tag{1.66}$$

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2} [\bar{M}_1(\bar{E}_F) + \bar{N}_1(\bar{E}_F)] \tag{1.67}$$

where

$$\bar{I}'_{11}(\bar{E}) \equiv \bar{I}_{11}(\bar{E})\left[\frac{1}{\bar{E}} + \frac{1}{\bar{E}+\bar{E}_g} + \frac{1}{\bar{E}+\bar{E}_g+\Delta} - \frac{1}{\bar{E}+\bar{E}_g+\frac{2}{3}\Delta}\right], \bar{M}_1(\bar{E}_F) \equiv [\bar{I}_{11}(\bar{E})]^{3/2},$$

and

$$\bar{N}_1(\bar{E}_F) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) \bar{M}_1(\bar{E}_F) \tag{1.68}$$

Thus using (1.44) and (1.67) we can study the entropy in this case

Under the inequalities $\Delta > > \bar{E}_{g_0}$ or $\Delta < < \bar{E}_{g_0}$, (1.48) can be expressed as

$$\bar{E}(1+\alpha\bar{E}) = \frac{\hbar^2\bar{k}^2}{2\bar{m}_c} \tag{1.69}$$

It may be noted that (1.69) is the well-known two band model of Kane and is used in the literature to study the physical properties of those III–V and opto-electronic materials whose energy band structures obey the aforementioned inequalities.

The dispersion relation in HD III–V, ternary and quaternary materials whose energy spectrum in the absence of band tails obeys the two band model of Kane as defined by (1.69), can be written as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c} = \gamma_2(\bar{E},\eta_g) \tag{1.70}$$

where

$$\gamma_2(\bar{E},\eta_g) \equiv \left[\frac{2}{1+Erf(\bar{E}/\eta_g)}\right]\left[\gamma_0(\bar{E},\eta_g)+\alpha\theta_0(\bar{E},\eta_g)\right],$$

The EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{F_h},\eta_g) = \bar{m}_c\{\gamma_2(\bar{E},\eta_g)\}'|_{\bar{E}=\bar{E}_{F_h}} \tag{1.71}$$

Thus, one again observes that the EEM in this case exists in the band gap.

In the absence of band tails, $\eta_g \to 0$ and the EEM assumes the well-known form

$$\bar{m}^*(\bar{E}_F) = \bar{m}_c\{1+2\alpha\bar{E}\}|_{\bar{E}=\bar{E}_F} \tag{1.72}$$

The DOS function in this case can be written as

$$\bar{N}_{HD}(\bar{E},\eta_g) = \frac{\bar{g}_v}{2\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\sqrt{\gamma_2(\bar{E},\eta_g)}\{\gamma_2(\bar{E},\eta_g)\}' \tag{1.73}$$

Since, the original two band Kane model is an all zero and no pole function in the finite energy plane with respect to energy, therefore the HD counterpart will be totally real and the complex band vanishes.

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\left[\bar{I}_{111}(\bar{E}_{Fs},\eta_g) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_{111}(\bar{E}_{Fs},\eta_g)]\right] \tag{1.74}$$

where

$$\bar{I}_{111}(\bar{E}_{Fs}, \eta_g) = \{\gamma_2(\bar{E}_{Fs}, \eta_g)\}^{3/2}$$

In this case, $\bar{E}_{hd}$ is given by

$$\gamma_2(\bar{E}_{hd}, \eta_g) = 0 \tag{1.75}$$

One can numerically compute the entropy by using (1.74), (1.75), (1.31f) and the allied definitions in this case.

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (1.70) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{k}_s)^2}{2\bar{m}_c} = \gamma_2(\bar{E}, \eta_g) \tag{1.76}$$

The expression of the $\bar{N}_{2DT}(\bar{E})$ in this case can be written

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}} \bar{T}_{7D}{}'(\bar{E}, \eta_g, \bar{n}_z)\bar{H}(\bar{E} - \bar{E}_{n_zD7}) \tag{1.77}$$

where

$$\bar{T}_{7D}(\bar{E}, \eta_g, \bar{n}_z) = [\gamma_2(\bar{E}, \eta_g) - \hbar^2(\bar{n}_z\pi/\bar{d}_z)^2(2\bar{m}_c)^{-1}],$$

The sub-band energies $\bar{E}_{n_zD7}$ in this case given by

$$\{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2\}(2\bar{m}_c)^{-1} = \gamma_2(\bar{E}_{n_zD7}, \eta_g) \tag{1.78}$$

Thus, we observe that both the total DOS and sub-band energies of QWs of HD III–V compounds in accordance with two band model of Kane are not at all complex since the dispersion relation in accordance with the said model is an all zero function with no pole in the finite complex plane.

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) = \bar{m}_c[\gamma_2{}'(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)] \tag{1.79}$$

Therefore under the same conditions as used in obtaining (1.48) from (1.2), the 2D carrier statistics in this case can be written by using the same conditions from (1.77) as

$$\bar{n}_{2D} = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{T}_{7D}(\bar{E}_{FLHD}, \eta_g, \bar{n}_z) + \bar{T}_{8D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)] \tag{1.80}$$

where

$$\bar{T}_{8D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})\bar{T}_{7D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)$$

Therefore, combining (1.31f) and (1.80) we can get the entropyin this case.

Under the inequalities $\Delta >> \bar{E}_{g_0}$ or $\Delta << \bar{E}_{g_0}$, (1.60) assumes the form

$$\bar{E}(1+\alpha\bar{E}) = \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_c} + \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \tag{1.81a}$$

The EEM can be written from (1.81a) as

$$\bar{m}^*(\bar{E}_{Fs}) = \bar{m}_c(1+2\alpha\bar{E}_{Fs}) \tag{1.81b}$$

The total 2D DOS function assumes the form

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}(1+2\alpha\bar{E})\bar{H}(\bar{E}-\bar{E}_{n_{z_3}}) \tag{1.82}$$

where the sub-band energy $(\bar{E}_{n_{z_3}})$ can be expressed as

$$\frac{\hbar^2}{2\bar{m}_c}(\bar{n}_z\pi/\bar{d}_z)^2 = \bar{E}_{n_{z_3}}(1+\alpha\bar{E}_{n_{z_3}}) \tag{1.83}$$

The 2D electron statistics can be written as

$$\begin{aligned}\bar{n}_{2D} &= \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\int_{\bar{E}_{n_{z_3}}}^{\infty}\frac{(1+2\alpha\bar{E})d\bar{E}}{1+\exp\left(\frac{\bar{E}-\bar{E}_{Fs}}{\bar{k}_B\bar{T}}\right)} \\ &= \frac{\bar{m}_c\bar{k}_B\bar{T}\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[(1+2\alpha\bar{E}_{n_{z_3}})\bar{F}_0(\eta_{n_1}) + 2\alpha\bar{k}_B\bar{T}\bar{F}_1(\eta_{n_1})\end{aligned} \tag{1.84}$$

where $\eta_{n_1} \equiv (\bar{E}_{Fs} - \bar{E}_{n_{z_3}})/\bar{k}_B\bar{T}$ and $\bar{F}_j(\eta)$ is the one parameter Fermi–Dirac integral of order j which can be written [154] as

$$\bar{F}_j(\bar{n}) = \left(\frac{1}{\Gamma(\bar{j}+1)}\right)\int_0^{\infty}\frac{\bar{x}^j d\bar{x}}{1+\exp(\bar{x}-\eta)}, \quad \bar{j} > -1 \tag{1.85}$$

or for all j, analytically continued as a complex contour integral around the negative x-axis

$$\bar{F}_j(\eta) = \left(\frac{\Gamma(-\bar{j})}{2\pi\sqrt{-1}}\right)\int_{-\infty}^{+0}\frac{\bar{x}^j d\bar{x}}{1+\exp(-\bar{x}-\eta)} \tag{1.86}$$

where η is the dimensionless parameter and $\bar{x}$ is independent variable,

Therefore in this case the entropy can be investigated by using (1.44) and (1.84).

The forms of the DOS and the electron statistics for bulk specimens of III–V materials in the absence of band tails whose energy band structures are defined by the two-band model of Kane can, respectively, be written as

$$\bar{D}_0(\bar{E}) = 4\pi\bar{g}_v\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}, \sqrt{\bar{I}_{11e}(\bar{E})}[\bar{I}'_{11e}(\bar{E})] \tag{1.87}$$

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}[\bar{M}_2(\bar{E}_F) + \bar{N}_2(\bar{E}_F)] \tag{1.88}$$

where

$$\bar{I}_{11e}(\bar{E}) \equiv \bar{E}(1+\alpha\bar{E}), \bar{I}'_{11e}(\bar{E}) \equiv (1+2\alpha\bar{E}),$$
$$\bar{M}_2(\bar{E}_F) \equiv [\bar{I}_{11e}(\bar{E}_F)]^{3/2} \tag{1.89}$$

and

$$\bar{N}_2(\bar{E}_F) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})\bar{M}_2(\bar{E}_F) \tag{1.90}$$

(c) Under the constraints $\Delta >> \bar{E}_{g_0}$ *or* $\Delta << \bar{E}_{g_0}$ together with the inequality $\alpha\bar{E}_F << 1$, the (1.87) and (1.88) assumes the forms as

$$\bar{n}_0 = \bar{g}_v\bar{N}_c\left[\bar{F}_{1/2}(\eta) + \left(\frac{15\alpha\bar{k}_B\bar{T}}{4}\right)\bar{F}_{3/2}(\eta)\right] \tag{1.91}$$

where

$$\bar{N}_c \equiv 2\left(\frac{2\pi\bar{m}^*\bar{k}_B\bar{T}}{h^2}\right)^{3/2} \; and \; \eta \equiv \frac{\bar{E}_F}{\bar{k}_B\bar{T}}$$

and

$$\eta \equiv \frac{\bar{E}_F}{\bar{k}_B\bar{T}}$$

The entropy can be written as

$$\bar{S}_0 = \bar{g}_v\bar{N}_c\left(\frac{\pi^2\bar{k}_B}{3}\right)\left[\bar{F}_{-1/2}(\eta) + \left(\frac{15\alpha\bar{k}_B\bar{T}}{4}\right)\bar{F}_{1/2}(\eta)\right] \tag{1.92}$$

The dispersion relation in HDS whose energy spectrum in the absence of band tails obeys the parabolic energy bands (1.69) is given by

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c} = \gamma_3(\bar{E}, \eta_g) \tag{1.93}$$

where

$$\gamma_3(\bar{E}, \eta_g) \equiv \left[\frac{2}{(1 + Erf(\bar{E}/\eta_g))}\right]\gamma_0(\bar{E}, \eta_g)$$

Since the dispersion relation in accordance with the said model is an all zero function with no pole in the finite complex plane, therefore the HD counterpart will be totally real, which is also apparent form the expression (1.93).

The EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{Fh}, \eta_g) = \bar{m}_c\{\gamma_3(\bar{E}_{Fh}, \eta_g)\}' \tag{1.94}$$

In the absence of band tails, $\eta_g \to 0$ and the EEM assumes the form

$$\bar{m}^*(\bar{E}_F) = \bar{m}_c \tag{1.95}$$

It is well known that the EEM in unperturbed parabolic energy bands is a constant quantity in general excluding cross-fields configuration. However, the same mass in the corresponding HD bulk counterpart becomes a complicated function of Fermi energy and the impurity potential together with the fact that the EEM also exists in the band gap solely due to the presence of finite η_g.

The DOS function in this case can be written as

$$\bar{N}_{HD}(\bar{E}, \eta_g) = \frac{\bar{g}_v}{2\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\sqrt{\gamma_3(\bar{E}, \eta_g)}\{\gamma_3(\bar{E}, \eta_g)\}' \tag{1.96}$$

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\left[\bar{I}_{113}(\bar{E}_{F_h}, \eta_g) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_{113}(\bar{E}_{F_h}, \eta_g)]\right] \tag{1.97}$$

where

$$\bar{I}_{113}(\bar{E}_{F_h}, \eta_g) = \{\gamma_3(\bar{E}_{F_h}, \eta_g)\}^{3/2}$$

In this case, $\bar{E}_{hd}$ is given by

$$\gamma_3(\bar{E}_{hd}, \eta_g) = 0 \tag{1.98}$$

One can numerically compute the entropy by using (1.97), (1.98), (1.31f) and the allied definitions in this case.

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (1.93) as

$$\frac{\hbar^2(\bar{n}_z z/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{k}_s)^2}{2\bar{m}_c} = \gamma_3(\bar{E}, \eta_g) \tag{1.99}$$

The expression of the $\bar{N}_{2DT}(\bar{E})$ in this case can be written as

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{T}_{9D}{}'(\bar{E}, \eta_g, \bar{n}_z)\bar{H}(\bar{E} - \bar{E}_{n_z D9}) \tag{1.100}$$

where

$$\bar{T}_{9D}(\bar{E}, \eta_g, \bar{n}_z) = [\gamma_3(\bar{E}, \eta_g) - \hbar^2(\bar{n}_z\pi/\bar{d}_z)^2(2\bar{m}_c)^{-1}].$$

The sub-band energies $\bar{E}_{n_z D9}$ in this case given by

$$\{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2\}(2\bar{m}_c)^{-1} = \gamma_3(\bar{E}_{n_z D9}, \eta_g) \tag{1.101}$$

The EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) = \bar{m}_c[\gamma'_3(\bar{E}_{F1HD}, \eta_g)] \tag{1.102}$$

Therefore under the same conditions as used in obtaining (1.48) from (1.2), the 2D carrier statistics in this case can be written by using the same conditions from (1.77) as

$$\bar{n}_{2D} = \frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{T}_{9D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) + \bar{T}_{10D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)] \tag{1.103}$$

where

$$\bar{T}_{10D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{T}_{9D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)],$$

Therefore combining (1.31f) and (1.80) we can get the entropy in this case.

Under the condition $\alpha \to 0$, the expressions of total 2D DOS, for materials without forming band tails whose bulk electrons are defined by the isotropic parabolic energy bands can, be written from (1.82) as

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{H}\left(\bar{E} - \bar{E}_{n_{z_p}}\right) \tag{1.104}$$

The sub-band energy $(\bar{E}_{n_{z_p}})$ the $\bar{n}_{2D}$ and the entropy can, respectively, be expressed as

$$\bar{E}_{n_{z_p}} = \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \tag{1.105}$$

$$\bar{n}_{2D} = \frac{\bar{m}_c\bar{k}_B\bar{T}\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_0\left(\eta_{n_2}\right) \tag{1.106a}$$

$$\bar{S}_0 = \frac{\pi^2\bar{k}_B^2\bar{T}\bar{m}_c\bar{g}_v}{3\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}\left(\eta_{n_2}\right) \tag{1.106b}$$

(b) The Model of Stillman et al.

In accordance with the model of Stillman et al. [38], the electron dispersion law of III–V materials assumes the form

$$\bar{E} = \bar{t}_{11}k^2 - \bar{t}_{12}\bar{k}^4 \tag{1.107}$$

where

$$\bar{t}_{11} \equiv \frac{\hbar^2}{2\bar{m}_c};\ \bar{t}_{12} = \left(1-\frac{\bar{m}_c}{\bar{m}_0}\right)^2\left(\frac{\hbar^2}{2\bar{m}_c}\right)^2\left[\left(3\bar{E}_{g_0}+4\Delta+\frac{2\Delta^2}{\bar{E}_{g_0}}\right).\{(\bar{E}_{g_0}+\Delta)(2\Delta+3\bar{E}_{g_0})\}^{-1}\right]$$

and $\bar{m}_0$ is the free electron mass

In the presence of band tails, (1.107) gets transformed as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c} = \bar{I}_{12}(\bar{E},\eta_g) \tag{1.108}$$

where

$$\bar{I}_{12}(\bar{E},\eta_g) = \bar{a}_{11}[1-(1-\bar{a}_{12}\gamma_3(\bar{E},\eta_g))^{1/2}],\ \bar{a}_{11} \equiv \left(\frac{\hbar^2\bar{t}_{11}}{4m_c\bar{t}_{12}}\right),$$

and

$$\bar{a}_{12} = \frac{4\bar{t}_{12}}{\bar{t}_{11}^2}$$

The EEM can be written as

$$\bar{m}^*(\bar{E}_{F_h},\eta_g) = \bar{m}_c\{\bar{I}_{12}(\bar{E}_{F_h},\eta_g)\}' \tag{1.109}$$

The DOS function in this case can be written as

$$\bar{N}_{HD}(\bar{E},\eta_g) = \frac{\bar{g}_v}{2\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\sqrt{\bar{I}_{12}(\bar{E},\eta_g)}\{\bar{I}_{12}(\bar{E},\eta_g)\}' \tag{1.110}$$

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\left[\bar{I}_{121}(\bar{E}_{F_h},\eta_g) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_{121}(\bar{E}_{F_h},\eta_g)]\right] \tag{1.111}$$

where

$$\bar{I}_{121}(\bar{E}_{F_h},\eta_g) = \{\bar{I}_{12}(\bar{E}_{F_h},\eta_g)\}^{3/2}$$

In this case, $\bar{E}_{hd}$ is expressed through the equation

$$\gamma_3(\bar{E}_{hd},\eta_g) = 0 \tag{1.112}$$

One can numerically compute the entropy by using (1.111), (1.112), (1.31f) and the allied definitions in this case.

For dimensional quantization along z- direction, the dispersion relation of the 2D electrons in this case can be written following (1.108) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{k}_s)^2}{2\bar{m}_c} = \bar{I}_{12}(\bar{E},\eta_g) \tag{1.113}$$

the expression of the $\bar{N}_{2DT}(\bar{E})$ in this case can be written as

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{T}_{11D}{}'(\bar{E},\eta_g,n_z)H(\bar{E}-\bar{E}_{n_zD11}) \tag{1.114}$$

where

$$\bar{T}_{11D}((\bar{E},\eta_g,\bar{n}_z) = \left[\bar{I}_{12}(\bar{E},\eta_g) - \hbar^2(\bar{n}_z\pi/\bar{d}_z)^2(2\bar{m}_c)^{-1}\right]$$

The sub-band energies $\bar{E}_{n_zD11}$ in this case given by

$$\{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2\}(2\bar{m}_c)^{-1} = \bar{I}_{12}(\bar{E}_{n_zD11},\eta_g) \tag{1.115}$$

The EEM in this case assumes the form

$$\bar{m}^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \bar{m}_c\{\bar{I}_{12}{}'(\bar{E}_{F1HD},\eta_g,\bar{n}_z)] \tag{1.116}$$

The 2-D electron statistics in this case can be written as

$$\bar{n}_{2D} = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\left[\bar{T}_{11D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) + \bar{T}_{12D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\right] \tag{1.117}$$

where

$$\bar{T}_{12D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{T}_{11D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\right],$$

Therefore combining (1.117) and (1.31f) we can get the entropyin this case.

For unperturbed material, the 2-D EEM can be expressed as

$$\bar{m}^{*}(\bar{E}_{Fs}) = \bar{m}_c\{\bar{I}_{12}(\bar{E}_{Fs})\}' \tag{1.118}$$

where

$$\bar{I}_{12}(\bar{E}) = \bar{a}_{11}\left[1-(1-\bar{a}_{12}(\bar{E}))^{1/2}\right]$$

It appears that the EEM in this case is a function of Fermi energy alone and is independent of size quantum number.

The total 2D DOS function in the absence of band tails in this case can be written as

$$\bar{N}_{2DT}(\bar{E}) = \left(\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\left\{[\bar{I}_{12}(\bar{E})]'\bar{E}(\bar{E}-\bar{E}_{n_{z_3}})\right\} \tag{1.119}$$

where the sub-band energies $\bar{E}_{n_{z_3}}$ can be expressed as

$$\bar{I}_{12}(\bar{E}_{n_{z_3}}) = \frac{\hbar^2}{2\bar{m}_c}(\bar{n}_z\pi/\bar{d}_z)^2 \tag{1.120}$$

The 2D electron concentration assumes the form

$$\bar{N}_{2D} = \left(\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\left[\bar{T}_{55}(\bar{E}_{Fs},\bar{n}_z)+\bar{T}_{56}(\bar{E}_{Fs},\bar{n}_z)\right] \tag{1.121}$$

where

$$\bar{T}_{55}(\bar{E}_{Fs},\bar{n}_Z) \equiv \left[\bar{I}_{12}(\bar{E}_{Fs}) - \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$

and

$$\bar{T}_{56}(\bar{E}_{Fs},\bar{n}_Z) \equiv \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\bar{T}_{55}(\bar{E}_{Fs},\bar{n}_Z)$$

Thus using (1.44) and (1.121) we can study the ***Entropy*** in this case.

The expression of electron concentration for bulk specimens of III–V materials (in the absence of band tails) can be written in accordance with the model of Stillman et al. as

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\left[\bar{M}_{A_{10}}(\bar{E}_F)+\bar{N}_{A_{10}}(\bar{E}_F)\right] \tag{1.122}$$

where

$$\bar{M}_{A_{10}}(\bar{E}_F) = [\bar{I}_{12}(\bar{E}_F)]^{3/2} and\, \bar{N}_{A_{10}}(\bar{E}_F) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{M}_{A_{10}}(\bar{E}_F)]$$

Thus using (1.44) and (1.122) we can study the entropy in this case.

(c) Model of Palik et al.

The energy spectrum of the conduction electrons in III–V materials up to the fourth order in effective mass theory, taking into account the interactions of heavy hole, light hole and the split-off holes can be expressed in accordance with the model of Palik et al. [40] as

$$\bar{E} = \frac{\hbar^2 \bar{k}^2}{2\bar{m}_c} - \bar{B}_{11}\bar{k}^4 \tag{1.123}$$

where

$$\bar{B}_{11} = \left[\frac{\hbar^4}{4\bar{E}_{g_0}(\bar{m}_c)^2}\right]\left[\frac{1+\frac{\bar{x}_{11}^2}{2}}{1+\frac{\bar{x}_{11}}{2}}\right](1-\bar{y}_{11})^2, \bar{x}_{11}\left[1+\left(\frac{\Delta}{\bar{E}_{g_0}}\right)\right]^{-1} and\ \bar{y}_{11} = \frac{\bar{m}_c}{\bar{m}_0}$$

The (1.123) gets simplified as

$$\frac{\hbar^2 \bar{k}^2}{2\bar{m}_c} = \bar{I}_{13}(\bar{E}) \tag{1.124}$$

where

$$\bar{I}_{13}(\bar{E}) = \bar{b}_{12}\left[\bar{a}_{12} - ((\bar{a}_{12})^2 - 4\bar{E}\bar{B}_{11})^{1/2}\right],\ \bar{a}_{12} = \left(\frac{\hbar^2}{2\bar{m}_c}\right) \text{ and } \bar{b}_{12} = \left[\frac{\bar{a}_{12}}{2\bar{B}_{11}}\right]$$

Under the condition of heavy doping forming Gaussian band tails, (1.124) assumes the form

$$\frac{\hbar^2 \bar{k}^2}{2\bar{m}_c} = \bar{I}_{13}(\bar{E}, \eta_g) \tag{1.125}$$

where

$$\bar{I}_{13}(\bar{E}, \eta_g) = \bar{b}_{12}\left[\bar{a}_{12} - ((\bar{a}_{12})^2 - 4\bar{B}_{11}\gamma_3(\bar{E}, \eta_g))^{1/2}\right]$$

The EEM can be written as

$$\bar{m}^*(\bar{E}_{F_h}, \eta_g) = \bar{m}_c\{\bar{I}_{13}(\bar{E}_{F_h}, \eta_g)\}' \tag{1.126}$$

The DOS function in this case can be expressed as

$$\bar{N}_{HD}(\bar{E},\eta_g)=\frac{\bar{g}_v}{2\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\sqrt{\bar{I}_{13}(\bar{E},\eta_g)}\{\bar{I}_{13}(\bar{E},\eta_g)\}' \tag{1.127}$$

Since, the original band model in this case is a no pole function, in the finite complex plane therefore, the HD counterpart will be totally real and the complex band vanishes.

The electron concentration is given by

$$\bar{n}_0=\frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\left[\bar{I}_{123}(\bar{E}_{Fh},\eta_g)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_{123}(\bar{E}_{Fh},\eta_g)]\right] \tag{1.128}$$

where

$$\bar{I}_{123}(\bar{E}_{Fh},\eta_g)=\{\bar{I}_{123}(\bar{E}_{Fh},\eta_g)\}^{3/2} \tag{1.129}$$

In this case, $\bar{E}_{hd}$ is given by

$$\gamma_3(\bar{E}_{hd},\eta_g) \tag{1.130}$$

One can numerically compute the entropy by using (1.128), (1.129), (1.31f) and the allied definitions in this case.

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (1.108) as

the expression of the $\bar{N}_{2DT}(\bar{E})$ in this case can be written as

$$\bar{N}_{2DT}(\bar{E})=\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{T}'_{13D}(\bar{E},\eta_g,\bar{n}_z)\bar{H}(\bar{E}-\bar{E}_{n_zD13}) \tag{1.131}$$

where

$$\bar{T}_{13D}(\bar{E},\eta_g,\bar{n}_z)=\left[\bar{I}_{13}(\bar{E},\eta_g)-\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2(2\bar{m}_c)^{-1}\right]$$

The sub-band energies $\bar{E}_{n_zD13}$ in this case given by

$$\{\hbar(\bar{n}_z\pi/\bar{d}_z)^2\}(2\bar{m}_c)^{-1}=\bar{I}_{13}(\bar{E}_{n_zD13},\eta_g) \tag{1.132}$$

The EEM in this case can be expressed as

$$\bar{m}^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\bar{m}_c\left[\bar{I}'_{13}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\right] \tag{1.133}$$

The 2-D electron statistics in this case can be written as

$$\bar{n}_{2D}=\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{\max}}\left[\bar{T}_{13D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)+\bar{T}_{14D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\right] \tag{1.134}$$

where

$$\bar{T}_{14D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} L(r)[\bar{T}_{13D}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)]$$

Therefore combining (1.134) and (1.31f) we can get the entropy in this case.

The 2D electron dispersion relation in the absence of band tails this case assumes the form

$$\frac{\hbar^2 \bar{k}_s^2}{2\bar{m}_c} + \frac{\hbar^2}{2\bar{m}_c}(\bar{n}_z \pi / \bar{d}_z)^2 = \bar{I}_{13}(\bar{E}) \tag{1.135a}$$

The EEM in this case can be written from (1.135a) as

$$\bar{m}^*(\bar{E}_{F_S}) = \bar{m}_c[\bar{I}_{13}(\bar{E}_{F_S})]' \tag{1.135b}$$

The total 2D DOS function can be written as

$$\bar{N}_{2DT}(\bar{E}) = \left(\frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2}\right) \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \{[\bar{I}_{13}(\bar{E})]' \bar{H}(\bar{E} - \bar{E}_{n_{z_4}})\} \tag{1.136}$$

where the sub-band energies $\bar{E}_{n_{z_4}}$ can be expressed as

$$\bar{I}_{13}(\bar{E}_{n_{z_4}}) = \frac{\hbar^2}{2\bar{m}_c}(\bar{n}_z \pi / \bar{d}_z)^2 \tag{1.137}$$

The 2D electron concentration assumes the form

$$\bar{n}_{2D} = \frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{T}_{57}(\bar{E}_{Fs}, \bar{n}_z) + \bar{T}_{58}(\bar{E}_{Fs}, \bar{n}_z)] \tag{1.138}$$

where

$$\bar{T}_{57}(\bar{E}_{Fs}, \bar{n}_z) \equiv \left[\bar{I}_{13}(\bar{E}_{Fs}) - \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2\right] \text{ and } \bar{T}_{58}(\bar{E}_{Fs}, \bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) \bar{T}_{57}(\bar{E}_{Fs}, \bar{n}_z) \tag{1.139}$$

Thus by using (1.138) and (1.44) we can study the entropy in this case.

1.2.3 The entropy in quantum wells (QWs) of HD II–VI materials

The carrier energy spectra in bulk specimens of II–VI compounds in accordance with Hopfield model [57] can be written as

$$\bar{E} = \bar{a}'_0 \bar{k}_s^2 + \bar{b}'_0 \bar{k}_z^2 + \bar{\lambda}_0 \bar{k}_s \tag{1.140}$$

where $\bar{a}'_0 \equiv \hbar^2/2\bar{m}^*_{\perp}$, $\bar{b}'_0 \equiv \hbar^2/2\bar{m}^*_{||}$, and $\bar{\lambda}_0$ represents the splitting of the two-spin states by the spin orbit coupling and the crystalline field.

Therefore the dispersion relation of the carriers in HD II–VI materials in the presence of Gaussian band tails can be expressed as

$$\gamma_3(\bar{E}, \eta_g) = \bar{a}'_0 \bar{k}_s^2 + \bar{b}'_0 \bar{k}_z^2 \pm \bar{\lambda}_0 \bar{k}_s \tag{1.141}$$

Thus, the energy spectrum in this case is real since the corresponding E-k relation in the absence of band tails as given by (1.141) is a no pole function in the finite complex plane.

The transverse and the longitudinal EEMs masses are, respectively, given by

$$\bar{m}^*_{\perp}(\bar{E}_{Fn}, \eta_g) = \bar{m}^*_{\perp}\{\gamma_3(\bar{E}, \eta_g)\}' \left[1 + \left(\frac{\bar{\lambda}_0}{\sqrt{(\bar{\lambda}_0)^2 + 4\bar{a}_0{}'\gamma_3(\bar{E}, \eta_g)}}\right)\right]\Bigg|_{\bar{E}-\bar{E}_{Fn}} \tag{1.142}$$

and

$$\bar{m}^*_{||}(\bar{E}_{Fn}, \eta_g) = \bar{m}^*_{||}\{\gamma_3(\bar{E}, \eta_g)\}'|_{\bar{E}-\bar{E}_{Fn}} \tag{1.143}$$

Thus the transverse EEM in HD II–VI materials is a function of electron energy and is double valued due to the presence of $\bar{\lambda}_0$ and due to heavy doping the same mass exists in the band gap.

In the absence of band tails, $\eta_g \to 0$, we get

$$\bar{m}^*_{\perp}(\bar{E}_F) = \bar{m}^*_{\perp}\left[1 + \left(\frac{\bar{\lambda}_0}{\sqrt{(\bar{\lambda}_0)^2 + 4\bar{a}_0{}'\bar{E})}}\right)\right]\Bigg|_{\bar{E}=\bar{E}_F} \tag{1.144}$$

and

$$\bar{m}^*_{||}(\bar{E}_F) = \bar{m}^*_{||} \tag{1.145}$$

The volume in k- space as enclosed (1.141) can be expressed as

$$\bar{V}(\bar{E}, \eta_g) = \frac{4\pi}{3\bar{a}'_0\sqrt{\bar{b}'_0}}\left[\{\gamma_3(\bar{E}, \eta_g)\}^{3/2} + \frac{3}{8}\frac{(\bar{\lambda}_0)^2\sqrt{\gamma_3(\bar{E}, \eta_g)}}{\bar{a}'_0}\right.$$
$$\left. \pm \left(\frac{3}{4}\frac{\bar{\lambda}_0}{\sqrt{\bar{a}'_0}}\right)\left(\gamma_3(\bar{E}, \eta_g) + \frac{(\bar{\lambda}_0)^2}{4\bar{a}'_0}\right)\sin^{-1}\left[\frac{\sqrt{\gamma_3(\bar{E}, \eta_g)}}{\sqrt{\gamma_3(\bar{E}, \eta_g) + \frac{(\bar{\lambda}_0)^2}{4d_0}}}\right]\right] \tag{1.146}$$

Therefore, the electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2 \bar{a}'_0 \sqrt{\bar{b}'_0}} \left[\bar{I}_{124}(\bar{E}_{F_h}, \eta_g) + \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) [\bar{I}_{124}(\bar{E}_{F_h}, \eta_g)] \right] \tag{1.147}$$

where

$$\bar{I}_{124}(\bar{E}_{F_h}, \eta_g) = \left[\{\gamma_3(\bar{E}_{F_h}, \eta_g)\}^{3/2} + \frac{3}{8} \frac{(\bar{\lambda}_0)^2 \sqrt{\gamma_3(\bar{E}, \eta_g)}}{\bar{a}'_0} \right]$$

In this case, $\bar{E}_{hd}$ is given by

$$\{\gamma_3(\bar{E}_{hd}, \eta_g)\} = 0 \tag{1.148}$$

Thus, one can numerically evaluate the entropy by using (1.147), (1.31f), (1.148) and the allied definitions in this case.

The dispersion relation of the conduction electrons of QWs of HD II–VI materials for dimensional quantization along z- direction can be written following (1.141) as

$$\gamma_3(\bar{E}, \eta_g) = \bar{a}'_0 \bar{k}_s^2 + \bar{b}'_0 \left(\frac{\pi \bar{n}_z}{\bar{d}_z} \right)^2 \pm \bar{\lambda}_0 \bar{k}_s \tag{1.149}$$

The EEM can be expressed following (1.149) as

$$\bar{m}^*(\bar{E}_{F1HD}, \bar{n}_z, \eta_g) = \bar{m}^*_{\perp} \left[1 \mp \frac{(\bar{\lambda}_0)}{\left[(\bar{\lambda}_0)^2 - 4\bar{a}'_0 \bar{b}'_0 \left(\frac{\bar{n}_z \pi}{\bar{d}_z} \right)^2 + 4\bar{a}'_0 \gamma_3(\bar{E}_{F1HD}, \eta_g) \right]^{1/2}} \right] \tag{1.150}$$

Thus we observe that the doubled valued effective mass in 2-D QWs of HD II–VI materials is a function of Fermi energy, size quantum number and the screening potential, respectively, together with the fact that the same mass exists in the band gap due to the sole presence of the splitting of the two-spin states by the spin orbit coupling and the crystalline field.

The sub-band energy in this case is given by

$$\gamma_3(\bar{E}_{n_z D14}, \eta_g) = \bar{b}'_0 \left(\frac{\pi \bar{n}_z}{\bar{d}_z} \right)^2 \tag{1.151}$$

The surface electron concentration at low temperatures assumes the form

$$\bar{n}_{2D} = \frac{\bar{g}_v \bar{m}^*_{\perp}}{\pi \hbar^2} \sum_{\bar{n}_Z=1}^{\bar{n}_{z\max}} \left(\gamma_3(\bar{E}_{F1HD}, \eta_g) - \bar{E}_{n_Z D_{14}} + (\bar{\lambda})^2 \bar{m}^*_{\perp} \hbar^{-2} \right) \tag{1.152}$$

Therefore combining (1.152) and (1.31f) we can get the entropy in this case.

The dispersion relation of the conduction electrons of QWs of II–VI materials for dimensional quantization along z- direction in the absence of band tails can be written following (1.140) as

$$\bar{E} = \bar{d}_0 \bar{k}_s^2 + \bar{b}'_0 \left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2 \pm \bar{\lambda}_0 \bar{k}_s \tag{1.153}$$

Using (1.153), the EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{Fs}, \bar{n}_z) = \bar{m}^*_{\perp} \left[1 \mp \frac{(\bar{\lambda}_0)}{\left[(\bar{\lambda}_0)^2 - 4\bar{a}'_0 \bar{b}'_0 \left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2 + 4\bar{a}'_0 \bar{E}_{Fs}\right]^{1/2}}\right] \tag{1.154}$$

The sub-band energy $\bar{E}_{n_{z4}}$ assumes the form

$$\bar{E}_{n_{z5}} = \bar{b}'_0 \left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2 \tag{1.155a}$$

The area of constant energy 2D quantized surface in this case is given by

$$\bar{A}_{\pm}(\bar{E}, \bar{n}_z) = \left[\frac{\pi}{2(\bar{a}_0{}')^2}\left[(\bar{\lambda}_0)^2 + 2\bar{a}_0{}'(\bar{E} - \bar{E}_{n_{z_s}}) \pm \bar{\lambda}_0\left[(\bar{\lambda}_0)^2 + 4\bar{a}_0{}'(\bar{E} - \bar{E}_{n_{zS}})\right]^{1/2}\right]\right] \tag{1.155b}$$

The surface electron concentration can be expressed in this case as

$$\bar{n}_{2D} = \frac{-2\bar{g}_v}{2(2\pi)^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \int_{\bar{E}_{nzS}}^{\infty} \left[\bar{A}_+(\bar{E}_{Fs,} \bar{n}_z) + \bar{A}_-(\bar{E}_{Fs,} \bar{n}_z)\right] \frac{\partial}{\partial \bar{E}} \{\bar{f}_0(\bar{E})\} d\bar{E} \tag{1.156}$$

where $\bar{f}_0(\bar{E})$ is the Fermi–Dirac occupation probability factor.

From (1.156) we get

$$\bar{n}_{2D} = \frac{\bar{g}_v \bar{m}^*_{\perp} \bar{k}_B \bar{T}}{\pi \hbar^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_0(\eta_{n_{zS}}) \tag{1.157}$$

where

$$\eta_{n_{zS}} = (\bar{E}_{Fs} - \bar{E}_{n_{z_S}} + (\bar{\lambda})\bar{m}^*_{\perp} \hbar^{-2})(\bar{k}_B \bar{T})^{-1}$$

Therefore the entropy is given by

$$\bar{S}_0 = \frac{\pi^2 \bar{k}_B^2 \bar{T} \bar{m}^*_{\perp} \bar{g}_v}{3\pi\hbar^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{n_{z8}}) \tag{1.158}$$

1.2.4 The entropy in quantum wells (QWs) of HD IV–VI materials

The dispersion relation of the conduction electrons in IV–VI materials can be expressed in accordance with Dimmock [156] as

$$\left[\varepsilon - \frac{\bar{E}_{g_0}}{2} - \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_t^-} - \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_t^-}\right]\left[\varepsilon + \frac{\bar{E}_{g_0}}{2} + \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_t^-} + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_t^-}\right] = \bar{P}_\perp^2\bar{k}_s^2 + \bar{P}_{||}^2\bar{k}_z^2 \tag{1.159}$$

whereε is the energy as measured from the center of the band gap $\bar{E}_{g_0}$, $\bar{m}_t^{\pm}$ and $\bar{m}_l^{\pm}$ represent the contributions to the transverse and longitudinal effective masses of the external $\bar{L}_6^{\pm}$ *and* $\bar{L}_6^-$ bands arising from the $\vec{k}\cdot\vec{p}$ perturbations with the other bands taken to the second order.

Substituting, $\bar{P}_\perp^2 \equiv \left(\hbar^2\bar{E}_{g_0}/2\bar{m}_t^*\right), \bar{P}_{||}^2 \equiv \left(\frac{\hbar^2\bar{E}_{g_0}}{2\bar{m}_l^*}\right)$ and $\varepsilon = \left[\bar{E} + \left(\frac{\bar{E}_{g_0}}{2}\right)\right]$ (where $\bar{m}_t^*$ and $\bar{m}_l^*$ are the transverse and the longitudinal effective masses at $\bar{k} = 0$), (1.159) gets transformed as

$$\left[\bar{E} - \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_t^-} - \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_l^-}\right]\left[1 + \alpha\bar{E} + \alpha\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_t^+} + \alpha\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_l^+}\right] = \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_t^*} + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_l^*} \tag{1.160}$$

From (1.160), we can write

$$\frac{\alpha\hbar^4\bar{k}_s^4}{4\bar{m}_t^+\bar{m}_t^-} + \hbar^2\bar{k}_s^2\left[\left(\frac{1}{2\bar{m}_t^*} - \frac{1}{2\bar{m}_t^-}\right) + \alpha\bar{E}\left(\frac{1}{2\bar{m}_t^-} - \frac{1}{2\bar{m}_t^+}\right) + \frac{\alpha\hbar^2\bar{k}_z^2}{4\bar{m}_l^-\bar{m}_t^+}\right] \tag{1.161}$$

$$+\left[\left(\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_l^*} + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_l^-}\right) + \frac{\alpha\bar{E}}{2}\hbar^2\bar{k}_z^2\left(\frac{1}{\bar{m}_l^-} - \frac{1}{\bar{m}_l^+}\right) + \frac{\alpha\hbar^4\bar{k}_z^4}{4\bar{m}_l^+\bar{m}_t^-} - \bar{E}(1+\alpha\bar{E})\right] = 0$$

Using (1.161), the dispersion relation of the conduction electrons in HD IV–VI materials can be expressed as

$$\begin{aligned}\frac{\alpha\hbar^4\bar{k}_s^4}{4\bar{m}_t^+\bar{m}_l^-}\bar{Z}_0(\bar{E},\eta_g) + \hbar^2\bar{k}_s^2\left[\bar{\lambda}_{11}(\bar{E},\eta_g)\bar{k}_z^2 + \bar{\lambda}_{72}(\bar{E},\eta_g)\right] \\ + \left[\bar{\lambda}_{73}(\bar{E},\eta_g)\bar{k}_z^2 + \bar{\lambda}_{74}(\bar{E},\eta_g)\bar{k}_z^4 - \bar{\lambda}_{75}(\bar{E},\eta_g)\right] = 0\end{aligned} \tag{1.162}$$

where

$$\bar{Z}_0(\bar{E},\eta_g) \equiv \frac{1}{2}\left[1 + Erf\left(\frac{\bar{E}}{\eta_g}\right)\right],\ \bar{\lambda}_{70}(\bar{E},\eta_g) \equiv \frac{\alpha}{4\bar{m}_t^+\bar{m}_t^-}\bar{Z}_0(\bar{E},\eta_g),$$

$$\lambda_{71}(\bar{E},\eta_g) \equiv \left[\frac{\alpha\hbar^2}{4\bar{m}_t^-\bar{m}_l^+}\bar{Z}_0(\bar{E},\eta_g) + \frac{\alpha\hbar^2}{4\bar{m}_l^-\bar{m}_t^+}\bar{Z}_0(\bar{E},\eta_g)\right],$$

$$\lambda_{72}(\bar{E},\eta_g) \equiv \left[\left(\frac{1}{2\bar{m}_t^*} - \frac{1}{2\bar{E}_t^-}\right)\bar{Z}_0(\bar{E},\eta_g) + \alpha\left(\frac{1}{2\bar{m}_t^-} - \frac{1}{2\bar{m}_t^+}\right)\gamma_0(\bar{E},\eta_g)\right],$$

$$\lambda_{73}(\bar{E},\eta_g) \equiv \left[\left(\frac{\hbar^2}{2\bar{m}_l^*} + \frac{\hbar^2}{2\bar{m}_l^-}\right)\bar{Z}_0(\bar{E},\eta_g) + \frac{\alpha\hbar^2}{2}\left(\frac{1}{\bar{m}_l^-} - \frac{1}{2\bar{m}_l^+}\right)\gamma_0(\bar{E},\eta_g)\right],$$

$$\lambda_{74}(\bar{E},\eta_g) = \frac{\alpha\hbar^4\bar{Z}_0(\bar{E},\eta_g)}{4\bar{m}_l^+\bar{m}_l^-} \text{ and } \lambda_{75}(\bar{E},\eta_g) \equiv [\gamma_0(\bar{E},\eta_g) + \alpha\theta_0(\bar{E},\eta_g)]$$

Thus, the energy spectrum in this case is real since the corresponding dispersion relation in the absence of band tails as given by (1.162) is a pole-less function with respect to energy axis in the finite complex plane.

The respective transverse and the longitudinal EEMs' in this case can be written as

$$\bar{m}_\perp^*(\bar{E}_{F_h},\eta_g) = \{2Z_0(\bar{E},\eta_g)\}^{-2}\left[\bar{z}_0(\bar{E},\eta_g)\left[-\{\bar{\lambda}_{72}(\bar{E},\eta_g)\}' + \frac{\{\bar{\lambda}_{78}(\bar{E},\eta_g)\}'}{2\sqrt{\bar{\lambda}_{78}(\bar{E},\eta_g)}}\right] - \{\bar{Z}_0(\bar{E},\eta_g)\}'\left[-\bar{\lambda}_{72}(\bar{E},\eta_g) + \sqrt{\bar{\lambda}_{78}(\bar{E},\eta_g)}\right]\right]\Bigg|_{\bar{E}_{F_h}} \tag{1.163}$$

where

$$\bar{\lambda}_{78}(\bar{E},\eta_g) \equiv \left[4\bar{\lambda}_{70}(\bar{E},\eta_g)\bar{\lambda}_{75}(\bar{E},\eta_g)\right]$$

and

$$\bar{m}_\parallel^*(\bar{E}_{F_h},\eta_g) = \frac{\hbar^2}{4}\left[-\{\bar{\lambda}_{84}(\bar{E},\eta_g)\}' + \frac{\{\bar{\lambda}_{84}(\bar{E},\eta_g)\}'\{\bar{\lambda}_{84}(\bar{E},\eta_g)\}' + 2\{\{\bar{\lambda}_{85}(\bar{E},\eta_g)\}'}{\sqrt{(\bar{\lambda}_{84}(\bar{E},\eta_g))^2 + 4\bar{\lambda}_{85}(\bar{E},\eta_g)}}\right]\Bigg|_{\bar{E}-\bar{E}_{Fh}} \tag{1.164}$$

in which, $\bar{\lambda}_{84}(\bar{E},\eta_g) \equiv \frac{\bar{\lambda}_{73}(\bar{E},\eta_g)}{\bar{\lambda}_{74}(\bar{E},\eta_g)}$ *and* $\bar{\lambda}_{85}(\bar{E},\eta_g) \equiv \frac{\bar{\lambda}_{75}(\bar{E},\eta_g)}{\bar{\lambda}_{74}(\bar{E},\eta_g)}$

Thus, we can see that the both the EEMs' in this case exist in the band gap.

In the absence of band tails, $\eta_g \to 0$, we get

$$\bar{m}_\perp^*(\bar{E}_F) = \frac{\hbar^2}{2}\left[-\{\bar{a}_{11}(\bar{E})\}' + \frac{\bar{a}_{511}\{\bar{T}_{311}(\bar{E})\}'}{2\sqrt{\bar{T}_{311}(\bar{E})}}\right]\Bigg|_{\bar{E}-\bar{E}_F} \tag{1.165}$$

where

$$\alpha_{11}(\bar{E}) \equiv \frac{2\bar{m}_t^+\bar{m}_t^-}{\alpha\hbar^2}\alpha_{211}(\bar{E}), \alpha_{211}(E) \equiv \left[\frac{1}{2\bar{m}_t^*} + \frac{\alpha\bar{E}}{2\bar{m}_t^*} + \frac{1+\alpha\bar{E}}{2\bar{m}_t^-}\right],$$

$$\alpha_{511} \equiv \frac{2\bar{m}_t^+\bar{m}_t^-}{\alpha\hbar^2}\omega_{11}(\omega_{11}) \equiv \left[\frac{\alpha^2}{16}\left[\frac{1}{\bar{m}_t^+\bar{m}_t^-}\right]\right]$$

$$(\omega_{11}) \equiv \left[\frac{\alpha^2}{16}\left[\frac{1}{\bar{m}_t^-\bar{m}_t^+} + \frac{1}{\bar{m}_t^-\bar{m}_t^+}\right]^2 - \frac{\alpha^2}{4\bar{m}_t^-\bar{m}_t^+\bar{m}_t^-\bar{m}_t^+}\right]^{1/2} T_{311}(\bar{E}) \equiv \frac{\omega_{311}(\bar{E})}{(\omega_{11})^2}$$

$$\omega_{311}(\bar{E}) \equiv \left[\frac{\alpha\bar{E}(1+\alpha\bar{E})}{\bar{m}_t^+\bar{m}_t^-} + \left[\frac{1}{2\bar{m}_t^*} - \left(\frac{\alpha\bar{E}}{2\bar{m}_t^+}\right) + \frac{(1+\alpha\bar{E})}{2\bar{m}_t^-}\right]^2\right]$$

and

$$\bar{m}_{\|}^*(\bar{E}_F) = \left(\frac{\bar{m}_t^+\bar{m}_l^-}{\alpha}\right)\left[\left(\frac{\alpha}{2\bar{m}_l^+} - \frac{\alpha}{2\bar{m}_l^-}\right) + \frac{1}{2}\left\{\frac{2\left[\frac{1}{2\bar{m}_l^*} + \frac{1+\alpha\bar{E}}{2\bar{m}_l^-} - \frac{\alpha\bar{E}}{2\bar{m}_l^+}\right]\left(\frac{\alpha}{2\bar{m}_l^-} - \frac{\alpha}{2\bar{m}_l^-}\right) + \frac{\alpha(1+2\alpha\bar{E})}{\bar{m}_l^-\bar{m}_l^+}}{\left[\left[\frac{1}{2\bar{m}_l^*} + \frac{1+\alpha\bar{E}}{2\bar{m}_l^-} - \frac{\alpha\bar{E}}{2\bar{m}_l^+}\right]^2 + \frac{\alpha\bar{E}(1+\alpha\bar{E})}{\bar{m}_l^-\bar{m}_l^+}\right]}\right\}\right]_{\bar{E}-\bar{E}_F} \tag{1.166}$$

The volume in k- space as enclosed by (1.162) can be written through the integral as

$$\bar{V}(\bar{E},\eta_g) = 2\pi\int_0^{\lambda_{86}(\bar{E},\eta_g)}\left[-[\lambda_{79}(\bar{E},\eta_g)\bar{k}_z^2 + \bar{\lambda}_{80}(\bar{E},\eta_g)\right] + \sqrt{\bar{\lambda}_{81}(\bar{E},\eta_g)\bar{k}_z^4 + \bar{\lambda}_{82}(\bar{E},\eta_g)\bar{k}_z^2 + \bar{\lambda}_{83}(\bar{E},\eta_g)}]d\bar{k}_z \tag{1.167}$$

where

$$\bar{\lambda}_{86}(\bar{E},\eta_g) \equiv \left[\frac{\sqrt{[\bar{\lambda}_{84}(\bar{E},\eta_g)]^2 + 4\bar{\lambda}_{85}(\bar{E},\eta_g)} - \bar{\lambda}_{84}(\bar{E},\eta_g)}{2}\right]^{1/2}, \ \bar{\lambda}_{79}(\bar{E},\eta_g) \equiv \frac{\bar{\lambda}_{71}(\bar{E},\eta_g)}{2\hbar^2\bar{Z}_0(\bar{E},\eta_g)}$$

$$\bar{\lambda}_{81}(\bar{E},\eta_g) \equiv \frac{\bar{\lambda}_{76}(\bar{E},\eta_g)}{4\hbar^4[\bar{Z}_0(\bar{E},\eta_g)]^2}, \bar{\lambda}_{76}(\bar{E},\eta_g) \equiv [\bar{\lambda}_{71}(\bar{E},\eta_g)]^2, \bar{\lambda}_{76}(\bar{E},\eta_g) \equiv [\bar{\lambda}_{71}(\bar{E},\eta_g)]^2$$

$$\bar{\lambda}_{77} \equiv \left[2\bar{\lambda}_{71}(\bar{E},\eta_g)\bar{\lambda}_{72}(\bar{E},\eta_g) - 4\bar{\lambda}_{70}(\bar{E},\eta_g)\bar{\lambda}_{73}(\bar{E},\eta_g) - 4\bar{\lambda}_{70}(\bar{E},\eta_g)\bar{\lambda}_{74}(\bar{E},\eta_g)\right]$$

$$\bar{\lambda}_{83}(\bar{E},\eta_g) \equiv \frac{\bar{\lambda}_{78}(\bar{E},\eta_g)}{9\hbar^4[\bar{Z}_0(\bar{E},\eta_g)]^2}$$

and

$$\bar{\lambda}_{78}(\bar{E},\eta_g) \equiv [4\bar{\lambda}_{70}(\bar{E},\eta_g)\bar{\lambda}_{75}(\bar{E},\eta_g)]$$

Thus,

$$\bar{V}(\bar{E},\eta_g) = \left[\bar{\lambda}_{87}(\bar{E},\eta_g)\right]\int_0^{\lambda_{86}(\bar{E},\eta_g)}\left[\sqrt{\bar{k}_z^4 + \bar{\lambda}_{88}(\bar{E},\eta_g)\bar{k}_z^2 + \bar{\lambda}_{89}(\bar{E},\eta_g)} - \bar{\lambda}_{90}(\bar{E},\eta_g)\right]d\bar{k}_z \tag{1.168}$$

Where

$$\bar{\lambda}_{87}(\bar{E},\eta_g) \equiv 2\pi\sqrt{\lambda_{81}(\bar{E},\eta_g)}, \bar{\lambda}_{88}(\bar{E},\eta_g) \equiv \frac{\bar{\lambda}_{82}(\bar{E},\eta_g)}{\bar{\lambda}_{81}(\bar{E},\eta_g)}, \bar{\lambda}_{89}(\bar{E},\eta_g) \equiv \frac{\bar{\lambda}_{83}(\bar{E},\eta_g)}{\bar{\lambda}_{81}(\bar{E},\eta_g)}$$

and

$$\bar{\lambda}_{90}(\bar{E},\eta_g) \equiv 2\pi\left[\frac{\bar{\lambda}_{79}(\bar{E},\eta_g)\{\bar{\lambda}_{86}(\bar{E},\eta_g)\}^3}{3} + \bar{\lambda}_{80}(\bar{E},\eta_g)\bar{\lambda}_{89}(\bar{E},\eta_g)\right]$$

The (1.168) can be written as

$$\bar{V}(\bar{E},\eta_g) = \left[\bar{\lambda}_{87}(\bar{E},\eta_g)\bar{\lambda}_{95}(\bar{E},\eta_g) - \bar{\lambda}_{90}(\bar{E},\eta_g)\right] \tag{1.169}$$

in which,

$$\bar{\lambda}_{95}(\bar{E},\eta_g) \equiv \left[\frac{\bar{\lambda}_{91}(\bar{E},\eta_g)}{3}[-\bar{E}_t[\bar{\lambda}_{93}(\bar{E},\eta_g),\bar{\lambda}_{94}(\bar{E},\eta_g)]\right.$$

$$\left.[\{\bar{\lambda}_{91}(\bar{E},\eta_g)\}^2 + \{\bar{\lambda}_{92}(\bar{E},\eta_g)\}^2 + 2\{\bar{\lambda}_{92}(\bar{E},\eta_g)\}^2\bar{F}_t[\bar{\lambda}_{93}(\bar{E},\eta_g),\bar{\lambda}_{94}(\bar{E},\eta_g)]]\right.$$

$$\left. + \left(\frac{\{\bar{\lambda}_{86}(\bar{E},\eta_g)\}}{3}\right)[\{\bar{\lambda}_{86}(\bar{E},\eta_g)\}^2 + \{\bar{\lambda}_{91}(\bar{E},\eta_g)\}^2 + 2\{\bar{\lambda}_{92}(\bar{E},\eta_g)\}^2]\right.$$

$$\left.[[\{\bar{\lambda}_{91}(\bar{E},\eta_g)\}^2 + \{\bar{\lambda}_{86}(\bar{E},\eta_g)\}^2]^{1/2}[\{\bar{\lambda}_{92}(\bar{E},\eta_g)\}^2 + \{\bar{\lambda}_{86}(\bar{E},\eta_g)\}^2]^{-1/2}],\right.$$

$$\{\bar{\lambda}_{91}(\bar{E},\eta_g)\}^2 \equiv \frac{1}{2}\left[\sqrt{\{\bar{\lambda}_{88}(\bar{E},\eta_g)\}^2 - 4\lambda_{89}(\bar{E},\eta_g)} + \bar{\lambda}_{88}(\bar{E},\eta_g)], \bar{E}_i[\bar{\lambda}_{93}(\bar{E},\eta_g),\bar{\lambda}_{94}(\bar{E},\eta_g)\right],$$

is the incomplete elliptic integral of the 2nd kind and is given by [133, 134],

$$\bar{E}_i[\bar{\lambda}_{93}(\bar{E},\eta_g),\bar{\lambda}_{94}(\bar{E},\eta_g)] \equiv \int_0^{\bar{\lambda}_{93}(\bar{E},\eta_g)} \left[\{1-\{\bar{\lambda}_{94}(\bar{E},\eta_g)\}^2\sin^2\xi\}^{1/2}\right] d\xi,$$

ξ is the variable of integration in this case,

$$\bar{\lambda}_{93}(\bar{E},\eta_g) \equiv \tan^{-1}\left[\frac{\bar{\lambda}_{86}(\bar{E},\eta_g)}{\bar{\lambda}_{92}(\bar{E},\eta_g)}\right]\{\bar{\lambda}_{92}(\bar{E},\eta_g)\}^2 \equiv \frac{1}{2}\left[\bar{\lambda}_{88}(\bar{E},\eta_g) - \sqrt{\{\bar{\lambda}_{88}(\bar{E},\eta_g)\}^2 - 4\bar{\lambda}_{89}(\bar{E},\eta_g)}\right],$$

$$\bar{\lambda}_{94}(\bar{E},\eta_g) \equiv \frac{\sqrt{\{\bar{\lambda}_{91}(\bar{E},\eta_g)\}^2 - \{\bar{\lambda}_{92}(\bar{E},\eta_g)\}^2}}{\bar{\lambda}_{91}(\bar{E},\eta_g)}, \bar{F}_i[\bar{\lambda}_{93}(\bar{E},\eta_g),\bar{\lambda}_{94}(\bar{E},\eta_g)]$$

is the incomplete elliptic integral of the 1st kind and is given by [133, 134],

$$\bar{F}_i[\bar{\lambda}_{93}(\bar{E},\eta_g),\bar{\lambda}_{94}(\bar{E},\eta_g)] \equiv \int_0^{\bar{\lambda}_{93}(\bar{E},\eta_g)} \left[\{1-\{\bar{\lambda}_{94}(\bar{E},\eta_g)\}^2\sin^2\xi\}^{-1/2}\right] d\xi.$$

The DOS function in this case is given by

$$\bar{N}_{HD}(\bar{E},\eta_g) = \frac{\bar{g}_v}{4\pi^3}\left[\{\bar{\lambda}_{87}(\bar{E},\eta_g)\}'\bar{\lambda}_{95}(\bar{E},\eta_g) + \{\bar{\lambda}_{95}(\bar{E},\eta_g)\}'\bar{\lambda}_{87}(\bar{E},\eta_g) - \{\bar{\lambda}_{90}(\bar{E},\eta_g)\}'\right] \tag{1.170}$$

Therefore the electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v}{4\pi^3}\left[\bar{I}_{125}(\bar{E}_{F_h},\eta_g) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{I}_{125}(\bar{E}_{F_h},\eta_g)\right]\right] \tag{1.171}$$

where

$$\bar{I}_{125}(\bar{E}_{F_h},\eta_g) = \left[\{\bar{\lambda}_{87}(\bar{E}_{F_h},\eta_g)\}\bar{\lambda}_{95}(\bar{E}_{F_h},\eta_g) - \{\bar{\lambda}_{90}(\bar{E}_{F_h},\eta_g)\}\right]$$

In this case, $\bar{E}_{hd}$ is given by

$$\bar{\lambda}_{95}(\bar{E}_{hd},\eta_g) = 0 \tag{1.172}$$

Thus, one can numerically evaluate the entropy by using (1.31f), (1.171) and (1.172) and the allied definitions in this case.

The 2D dispersion relation of the conduction electrons in QWs of IV–VI materials in the absence of band tails for the dimensional quantization along z direction can be expressed as

$$\bar{E}(1+\alpha\bar{E})+\alpha\bar{E}\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_4}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_5}\right)+\alpha\bar{E}\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)-(1+\alpha\bar{E})\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_2}\right)$$
$$-\alpha\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_2}\right)\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_4}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_5}\right)-\alpha\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_2}\right)\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2$$
$$-(1+\alpha\bar{E})\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2.-\alpha\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_4}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_5}\right)$$
$$-\alpha\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2=\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{m}_2}+\frac{\hbar^2}{2\bar{m}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right) \tag{1.173}$$

where

$$\bar{x}_4=\bar{m}_t^+,\bar{x}_5=\frac{\bar{m}_t^+ +2\bar{m}_l^+}{3},x_6=\frac{3\bar{m}_t^+\bar{m}_l^+}{2\bar{m}_l^+ +\bar{m}_t^+},\bar{x}_1=\bar{m}_t^-,\bar{x}_2=\frac{\bar{m}_t^- +2\bar{m}_l^-}{3},x_3=\frac{3\bar{m}_t^-\bar{m}_l^-}{2\bar{m}_l^- +\bar{m}_t^-}$$

$$\bar{m}_1=\bar{m}_t^*,\bar{m}_2=\frac{\bar{m}_t^*+2\bar{m}_l^*}{3}$$

and

$$\bar{m}_3=\frac{3\bar{m}_l^*\bar{m}_t^*}{\bar{m}_t^*+2\bar{m}_l^*}.$$

Therefore, the HD 2-D dispersion relation In this case assumes the form

$$\gamma_2(\bar{E},\eta_g)+\alpha\gamma_3(\bar{E},\eta_g)\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_4}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_5}\right)+\alpha\gamma_3(\bar{E},\eta_g)\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2$$
$$-(1+\alpha\gamma_3(\bar{E},\eta_g))\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_2}\right)-\alpha\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_2}\right)\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_4}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_5}\right)$$
$$-\alpha\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_2}\right)\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-(1+\alpha\gamma_3(\bar{E},\eta_g))\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2$$
$$-\alpha\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\left(\frac{\hbar^2\bar{k}_x^2}{2\bar{x}_4}+\frac{\hbar^2\bar{k}_y^2}{2\bar{x}_5}\right)$$
$$-\alpha\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2=\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{m}_2}+\frac{\hbar^2}{2\bar{m}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \tag{1.174}$$

Substituting, $\bar{k}_x=\bar{r}Cos\theta$ *and* $\bar{k}_y=\bar{r}Sin\theta$ (where $\bar{r}$ *and* θ are 2D polar coordinates in 2D wave vector space) in (1.174), we can write

$$\bar{r}^4\left[\alpha\frac{1}{4}\left(\frac{\hbar^2\cos^2\theta}{\bar{x}_1}+\frac{\hbar^2\sin^2\theta}{\bar{x}_2}\right)\left(\frac{\hbar^2\cos^2\theta}{\bar{x}_4}+\frac{\hbar^2\sin^2\theta}{\bar{x}_5}\right)\right]+\bar{r}^2\frac{1}{2}\left[\left(\frac{\hbar^2\cos^2\theta}{\bar{m}_1}+\frac{\hbar^2\sin^2\theta}{\bar{m}_2}\right)\right.$$
$$+\alpha\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{d_z}\right)^2\left(\frac{\hbar^2\cos^2\theta}{\bar{x}_4}+\frac{\hbar^2\sin^2\theta}{\bar{x}_5}\right)+\alpha\left(\frac{\hbar^2\cos^2\theta}{\bar{x}_1}+\frac{\hbar^2\sin^2\theta}{\bar{x}_2}\right)\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{d_z}\right)^2$$
$$\left.+\hbar^2(1+\alpha\gamma_3(\bar{E},\eta_g))\left(\frac{\cos^2\theta}{\bar{x}_1}+\frac{\sin^2\theta}{x_2}\right)-\hbar^2\alpha\gamma_3(\bar{E},\eta_g)\left(\frac{\cos^2\theta}{\bar{x}_4}+\frac{\sin^2\theta}{\bar{x}_5}\right)\right]$$
$$-\left[\gamma_2(\bar{E},\eta_g)+\alpha\gamma_3(\bar{E},\eta_g)\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{d_z}\right)^2-(1+\alpha\gamma_3(\bar{E},\eta_g))\frac{\hbar^2}{2\bar{x}_3}\left(\frac{n_z\pi}{d_z}\right)^2\right.$$
$$\left.-\alpha\left(\frac{\hbar^4}{4\bar{x}_3\bar{x}_6}\left(\frac{\bar{n}_z\pi}{d_z}\right)^4\right)\right]=0 \tag{1.175}$$

The area $\bar{A}(\bar{E},\bar{n}_z)$ of the 2D wave vector space can be expressed as

$$\bar{A}(\bar{E},\bar{n}_z)=\bar{J}_1-\bar{J}_2 \tag{1.176}$$

where

$$\bar{J}_1\equiv 2\int_0^{\pi/2}\frac{\bar{c}_1}{\bar{b}_1}d\theta \tag{1.177}$$

and

$$\bar{J}_2\equiv 2\int_0^{\pi/2}\frac{\bar{a}\,\bar{c}_1^2}{\bar{b}_1^3}d\theta \tag{1.178}$$

in which

$$\bar{a}\equiv\left[\alpha\left(\frac{\hbar^4}{4}\right)\left(\frac{\cos^2\theta}{\bar{x}_1}+\frac{\sin^2\theta}{\bar{x}_2}\right)\left(\frac{\cos^2\theta}{\bar{x}_4}+\frac{\sin^2\theta}{\bar{x}_5}\right)\right],$$
$$\bar{b}_1\equiv\left(\frac{\hbar^2}{2}\right)\left[\left(\frac{\cos^2\theta}{\bar{m}_1}+\frac{\sin^2\theta}{\bar{m}_2}\right)+\alpha\left(\frac{\hbar^2}{2\bar{x}_3}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\left[\left(\frac{\cos^2\theta}{\bar{x}_4}+\frac{\sin^2\theta}{\bar{x}_5}\right)\right.\right.$$
$$+\alpha\left(\frac{\hbar^2}{2\bar{x}_6}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\left[\left(\frac{\cos^2\theta}{\bar{m}_1}+\frac{\sin^2\theta}{\bar{m}_2}\right)\right.$$
$$\left.\left.\left.+(1+\alpha\gamma_3(\bar{E},\eta_g))\left(\frac{\cos^2\theta}{\bar{x}_1}+\frac{\sin^2\theta}{\bar{x}_2}\right)-\alpha\gamma_3(E,\eta_g)\left(\frac{\cos^2\theta}{\bar{x}_4}+\frac{\sin^2\theta}{\bar{x}_5}\right)\right]\right]\right]$$

and

$$\bar{c}_1 \equiv \left[\gamma_2(\bar{E},\eta_g) + \alpha\gamma_3(\bar{E},\eta_g)\left(\frac{\hbar^2}{2\bar{x}_6}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 - (1+\alpha\gamma_3(\bar{E},\eta_g))\left(\frac{\hbar^2}{2\bar{x}_3}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 - \alpha\left(\frac{\hbar^4}{4\bar{x}_3\bar{x}_6}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^4\right]$$

The (1.177) can be expressed as

$$\bar{J}_1 = 2\int_0^{\pi/2} \frac{\bar{t}_{31}(\bar{E},\bar{n}_z)d\theta}{\bar{A}_{11}(\bar{E},\bar{n}_z)\cos^2\theta + \bar{B}_{11}(\bar{E},\bar{n}_z)\sin^2\theta}$$

where

$$\bar{t}_{31}(\bar{E},\bar{n}_z) \equiv \bar{c}_1, \bar{A}_{11}(\bar{E},\bar{n}_z) \equiv \frac{\hbar^2}{2m_1}\bar{t}_{11}(\bar{E},\bar{n}_z),$$

$$\bar{t}_{11}(\bar{E},\bar{n}_z) \equiv \left[1 + \bar{m}_1\left[\frac{1}{\bar{x}_4}\frac{\alpha\hbar^2}{2\bar{x}_3}\left(\frac{n_z\pi}{d_z}\right)^2 + \frac{\alpha\hbar^2}{2\bar{x}_1\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \frac{1+\alpha\gamma_2(\bar{E},\bar{n}_z)}{\bar{x}_1} - \frac{\alpha\gamma_3(\bar{E},\bar{n}_z)}{\bar{x}_4}\right]\right]$$

$$\bar{B}_{11}(\bar{E},\bar{n}_z) \equiv \frac{\hbar^2}{2m_2}t_{21}(\bar{E},\bar{n}_z)$$

and

$$\bar{t}_{21}(\bar{E},\bar{n}_z) \equiv \left[1 + m_2\left[\frac{\alpha\hbar^2}{2\bar{x}_3\bar{x}_5}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \frac{\alpha\hbar^2}{2\bar{x}_2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \frac{1+\alpha\gamma_3(\bar{E},\bar{n}_z)}{\bar{x}_2} - \frac{\alpha\gamma_3(\bar{E},\bar{n}_z)}{\bar{x}_5}\right]\right]$$

Performing the integration, we get

$$\bar{J}_1 = \pi\bar{t}_{31}(\bar{E},\bar{n}_z)[\bar{A}_{11}(\bar{E},\bar{n}_z)\bar{B}_{11}(\bar{E},\bar{n}_z)]^{-1/2} \tag{1.179}$$

From (1.178) we can write

$$\bar{J}_2 = \frac{\alpha\bar{t}_{31}^2(\bar{E},\bar{n}_z)\hbar^4}{2\bar{B}_{11}^3(\bar{E},\bar{n}_z)}\bar{I} \tag{1.180}$$

where

$$\bar{I} \equiv \int_0^\infty \frac{(\bar{a}_1 + \bar{a}_2\bar{z}^2)(\bar{a}_3 + \bar{a}_4\bar{z}^2)dz}{[(\bar{a})^2 + \bar{z}^2]^3}, (\bar{a})^2 = \left(\frac{\bar{A}_{11}(\bar{E},\bar{n}_z)}{\bar{B}_{11}(\bar{E},\bar{n}_z)}\right), \tag{1.181}$$

in which $\bar{a}_1 \equiv \frac{1}{\bar{x}_1}$, $\bar{a}_2 \equiv \frac{1}{\bar{x}_2}$, $\bar{z} = \tan\theta$, θ is a new variable, $\bar{a}_3 \equiv \frac{1}{\bar{x}_4}$, $\bar{a}_4 \equiv \frac{1}{\bar{x}_5}$ and $(\bar{a})^2 \equiv \left(\frac{\bar{A}_1(\bar{E},\bar{n}_z)}{\bar{B}_1(\bar{E},\bar{n}_z)}\right)$.

The use of the Residue theorem leads to the evaluation of the integral in (1.181) as

$$\bar{I} = \frac{\pi}{4\bar{a}}[\bar{a}_1\bar{a}_4 + 3\bar{a}_2\bar{a}_4] \tag{1.182}$$

Therefore, the 2D area of the 2D wave vector space can be written as

$$\bar{A}_{HD}(\bar{E}, \bar{n}_z) = \frac{\pi\bar{t}_{31}(\bar{E}, \bar{n}_z)}{\sqrt{\bar{A}_{11}(\bar{E}, \bar{n}_z)\bar{B}_{11}(\bar{E}, \bar{n}_z)}}\left[1 - \frac{1}{\bar{x}_5}\left(\frac{1}{\bar{x}_1} + \frac{3}{\bar{x}_2}\right)\frac{\alpha\bar{t}_{31}(\bar{E}, \bar{n}_z)\hbar^4}{8\bar{B}_{11}^2(\bar{E}, \bar{n}_z)}\right] \tag{1.183}$$

The EEM for the HD QWs of IV–VI materials can thus be written as

$$\bar{m}^*(\bar{E}, n_z) = \frac{\hbar^2}{2}[\theta_{5HD}(\bar{E}, n_z)]\Big|_{\bar{E}=\bar{E}_{F1HD}} \tag{1.184}$$

Thus, the EEM is a function of Fermi energy and the quantum number due to the band nonparabolicity.

The total DOS function can be written as

$$\bar{N}_{2DT}(\bar{E}) = \left(\frac{\bar{g}_v}{2\pi}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\theta_{5HD}(\bar{E}, n_z)\bar{H}(\bar{E} - \bar{E}_{n_{z_{7HD}}}) \tag{1.185}$$

where the sub-band energy $(\bar{E}_{n_{z_{7HD}}})$ in this case can be written as

$$\gamma_2(\bar{E}_{n_{z_{7HD}}}, \bar{\eta}_g) + \bar{\alpha}\gamma_3(\bar{E}_{n_{z_{7HD}}}, \bar{\eta}_g)\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 - (1 + \bar{\alpha}\gamma_3(\bar{E}_{n_{z_{7HD}}}, \bar{\eta}_g))\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2$$
$$-\alpha\frac{\hbar^{2=0}}{2x_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\frac{\hbar^2}{2x_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 - \left[\frac{\hbar^2}{2m_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right] \tag{1.186}$$

The use (1.185) leads to the expression of 2D electron statistics as

$$\bar{n}_{2D} = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{\max}}[\bar{T}_{55HD}(\bar{E}_{F1HD}, n_z) + \bar{T}_{56HD}(\bar{E}_{F1HD}, n_z)] \tag{1.187}$$

where

$$\bar{T}_{55HD}(\bar{E}_{F1HD}, n_z) \equiv \frac{\bar{A}_{HD}(\bar{E}_{F1HD}, n_z)}{\pi} \text{ and } \bar{T}_{56HD}(\bar{E}_{F1HD}, n_z) \equiv \sum_{r=1}^{s}\bar{L}(\bar{r})T_{55HD}(\bar{E}_{F1HD}, n_z)$$

Using (1.187) and (1.31f) we can numerically study the entropy in this case.

In the absence of heavy doping the EEM in QWs of IV–VI materials can be written as

$$\bar{m}^*(\bar{E}, n_z) = \frac{\hbar^2}{2}[\theta_5(\bar{E}, n_z)]\Big|_{\bar{E}=\bar{E}_{Fs}} \tag{1.188}$$

where

$$\theta_5(\bar{E},n_z)\equiv\left[1-\frac{1}{\bar{x}_5}\left(\frac{1}{\bar{x}_1}+\frac{3}{\bar{x}_2}\right)\frac{\bar{\alpha}\bar{t}_{30}(\bar{E},n_z)\hbar^4}{8[\bar{B}_{10}(\bar{E},n_z)]^2}\right][\bar{A}_{10}(\bar{E},n_z)\bar{B}_{10}(\bar{E},n_z)]^{-1}$$

$$\left[\sqrt{\bar{A}_{10}(\bar{E},n_z)\bar{B}_{10}(\bar{E},n_z)}\{\bar{t}_{30}(\bar{E},n_z)\}'-\{\bar{t}_{30}(\bar{E},n_z)\}'\left\{\frac{1}{2}\{\bar{A}_{10}(\bar{E},n_z)\}'\left[\frac{\bar{B}_{10}(\bar{E},n_z)}{\bar{A}_{10}(\bar{E},n_z)}\right]^{1/2}\right.\right.$$
$$\left.\left.+\frac{1}{2}\{\bar{B}_{10}(\bar{E},n_z)\}'\left[\frac{\bar{A}_{10}(\bar{E},n_z)}{\bar{B}_{10}(\bar{E},n_z)}\right]\right\}\right]$$
$$-\frac{1}{8}\frac{\bar{t}_{30}(\bar{E},n_z)\alpha\hbar^4}{\sqrt{\bar{A}_{10}(\bar{E},n_z)\bar{B}_{10}(\bar{E},n_z)}}\frac{1}{\bar{x}_5}\left(\frac{1}{\bar{x}_1}+\frac{3}{\bar{x}_2}\right)[\bar{B}_{10}(\bar{E},n_z)]^{-4}[\{\bar{B}_{10}(\bar{E},n_z)\}^2\{\bar{t}_{30}(\bar{E},n_z)\}'$$
$$-2\bar{B}_{10}(\bar{E},n_z)\{\bar{B}_{10}(\bar{E},n_z)\}'\bar{t}_{30}(\bar{E},n_z)],\ \bar{t}_{30}(\bar{E},n_z)=\bar{c}_0,$$

$$\bar{c}_0\equiv\left[\bar{E}(1+\bar{\alpha}\bar{E})+\bar{\alpha}\bar{E}\left(\frac{\hbar^2}{2\bar{x}_6}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-(1+\bar{\alpha}\bar{E})\left(\frac{\hbar^2}{2\bar{x}_3}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-\bar{\alpha}\left(\frac{\hbar^2}{4\bar{x}_3\bar{x}_6}\right)\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^4\right],$$

$$\bar{A}_{10}(\bar{E},n_z)\equiv\frac{\hbar^2}{2\bar{m}_1}\bar{t}_{10}(\bar{E},n_z),\bar{t}_{10}(\bar{E},n_z)$$
$$\equiv\left[1+\bar{m}_1\left[\frac{1}{\bar{x}_4}\frac{\bar{\alpha}\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\frac{\bar{\alpha}\hbar^2}{2\bar{x}_1\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\frac{1+\alpha\bar{E}}{\bar{x}_1}-\frac{\alpha\bar{E}}{\bar{x}_4}\right]\right]$$

$$\bar{B}_{10}(\bar{E},n_z)\equiv\frac{\hbar^2}{2\bar{m}_2}\bar{t}_{20}(\bar{E},n_z)$$

and

$$\bar{t}_{20}(\bar{E},n_z)\equiv\left[1+\bar{m}_2\left[\frac{\bar{\alpha}\hbar^2}{2\bar{x}_3\bar{x}_5}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\frac{\bar{\alpha}\hbar^2}{2\bar{x}_2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\frac{1+\bar{\alpha}\bar{E}}{\bar{x}_2}-\frac{\bar{\alpha}\bar{E}}{\bar{x}_5}\right]\right]$$

Thus, the EEM is a function of Fermi energy and the quantum number due to the band nonparabolicity.

The total DOS function can be written as

$$\bar{N}_{2DT}(\bar{E})=\left(\frac{\bar{g}_v}{2\pi}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\theta_5(\bar{E},n_z)\bar{H}(\bar{E}-\bar{E}_{n_{z_7}}) \tag{1.189}$$

where the sub-band energy $(\bar{E}_{n_{z_7}})$ in this case can be written as

$$\bar{E}_{n_{z_7}}(1+\bar{\alpha}\bar{E}_{n_{z_7}})+\bar{\alpha}\bar{E}_{n_{z_7}}\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-(1+\bar{\alpha}\bar{E}_{n_{z_7}})\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 - \alpha\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\frac{\hbar^2}{2\bar{x}_6}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-\left[\frac{\hbar^2}{2\bar{m}_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]=0 \tag{1.190}$$

In the absence of heavy doping, the expression of 2D electron statistics can be written as

$$\bar{n}_{2D}=\frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{\max}}[\bar{T}_{550}(\bar{E}_{Fs},n_z)+\bar{T}_{560}(\bar{E}_{Fs},n_z)] \tag{1.191}$$

where

$$\bar{T}_{550}(\bar{E}_{Fs},n_z)\equiv\frac{\bar{A}_0(\bar{E}_{Fs},n_z)}{\pi},\bar{A}_0(\bar{E},n_z) = \frac{\pi\bar{t}_{30}(\bar{E},n_z)}{\sqrt{\bar{A}_{10}(\bar{E},n_z)\bar{B}_{10}(\bar{E},n_z)}}\left[1-\frac{1}{\bar{x}_5}\left(\frac{1}{\bar{x}_1}+\frac{3}{\bar{x}_2}\right)\frac{\alpha\bar{t}_{30}(\bar{E},n_z)\hbar^4}{8\bar{B}^2_{10}(\bar{E},n_z)}\right],$$

and

$$\bar{T}_{560}(\bar{E}_{Fs},n_z)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\bar{T}_{550}(\bar{E}_{Fs},n_z) \tag{1.192}$$

Thus using (1.44) and (1.192) we can study the entropy in this case.

For bulk specimens of IV–VI materials, the expressions of electron concentration and the ENTROPY assume the forms

$$\bar{n}_0=\left(\frac{\bar{g}_v}{2\pi^2}\right)[\bar{M}_{A4}(\bar{E}_{F_b})+\bar{N}_{A_4}(\bar{E}_{F_b})] \tag{1.193}$$

$$\bar{S}_0=\bar{g}_v\left[\frac{\bar{k}_B{}^2\bar{T}}{6}\right][\bar{M}'_{A_4}(\bar{E}_{F_b})+\bar{N}'_{A_4}(\bar{E}_{F_b})] \tag{1.194}$$

where

$$\bar{M}_{A_4}(\bar{E}_{F_b})=\left[\alpha\bar{J}_{A_1}(\bar{E}_{F_b})-\alpha_3(\bar{E}_{F_b})\bar{\tau}_{A_1}(\bar{E}_{F_b})-\frac{\alpha_4}{3}[\bar{\tau}_{A_1}(\bar{E}_{F_b})]^3\right],\alpha_5=\left[\frac{2\bar{m}_t^+\bar{m}_t^-}{\alpha\hbar^2}\omega_{A_1}\right],$$

$$\bar{J}_{A_1}(\bar{E}_{F_b})=\frac{\bar{A}_4(\bar{E}_{F_b})}{3}-[-(\bar{A}^2_A(\bar{E}_{F_b})+\bar{B}^2_A(\bar{E}_{F_b}))\bar{E}(\lambda,q)+2\bar{B}^2_A(\bar{E}_{F_b})\bar{F}(\lambda,\bar{q})]+\frac{\bar{\tau}_{A_1}(\bar{E}_{F_b})}{3}$$

$$[(\bar{\tau}_{A_1}(\bar{E}_{F_b}))^2+\bar{A}^2_A(\bar{E}_{F_b})+2\bar{B}^2_A(\bar{E}_{F_b})][\bar{A}^2_A(\bar{E}_{F_b})+\bar{\tau}^2_{A_1}(\bar{E}_{F_b})]^{1/2}[\bar{B}^2_A(\bar{E}_{F_b})+\bar{\tau}^2_{A_1}(\bar{E}_{F_b})]^{-1/2}$$

$$\lambda=\tan^{-1}\frac{\bar{\tau}_A(\bar{E}_{F_b})}{\bar{B}_A(\bar{E}_{F_b})},\ \bar{q}=\left[\frac{\sqrt{\bar{A}^2_A(\bar{E}_{F_b})-\bar{B}^2_A(\bar{E}_{F_b})}}{\bar{A}_A(\bar{E}_{F_b})}\right],$$

$$\bar{A}_A(\bar{E}_{F_b}) = \left[\tau_{A_2}(\bar{E}_{F_b}) + \sqrt{\tau_{A_2}^2(\bar{E}_{F_b}) - 4\tau_{A_3}(\bar{E}_{F_b})}\right]^{1/2} \Big/ \sqrt{2},$$

$$\bar{B}_A(\bar{E}_{F_b}) = \left[\tau_{A_2}(\bar{E}_{F_b}) - \sqrt{\tau_{A_2}^2(\bar{E}_{F_b}) - 4\tau_{A_3}(\bar{E}_{F_b})}\right]^{1/2} \Big/ \sqrt{2},$$

$$\tau_{A_2}(\bar{E}_{F_b}) = \frac{\omega_{A_2}(\bar{E}_{F_b})}{\omega_{A_1}^2},\ \tau_{A_3}(\bar{E}_{F_b}) = \frac{\omega_{A_3}(\bar{E}_{F_b})}{\omega_{A_1}^2},$$

$$\omega_{A_2}(\bar{E}_{F_b}) = \left[\frac{\alpha}{2}\left[\frac{1}{2\bar{m}_t^*} - \frac{\alpha.\bar{E}_{F_b}}{2\bar{m}_t^+} + \frac{1+\alpha\bar{E}_{F_b}}{2\bar{m}_t^-}\right]\cdot\left[\frac{1}{\bar{m}_t^- m_l^+} + \frac{1}{\bar{m}_l^- \bar{m}_t^+}\right]\right.$$
$$\left. - \frac{\alpha}{\bar{m}_t^+ \bar{m}_t^-}\left[\frac{1}{\bar{m}_l^*} + \frac{\alpha\bar{E}_{F_b}}{2\bar{m}_l^+} + \frac{1+\alpha\bar{E}_{F_b}}{2\bar{m}_l^-}\right]\right]$$

$$\omega_{A_3}(\bar{E}_{F_b}) = \left[\frac{\alpha\bar{E}_{F_b}1+\alpha\bar{E}_{F_b}}{\bar{m}_t^+\bar{m}_t^-} + \left[\frac{1}{2\bar{m}_t^*} - \frac{\alpha\bar{E}_{F_b}}{2\bar{m}_t^+} + \frac{1+\alpha\bar{E}_{F_b}}{2\bar{m}_t^-}\right]\frac{\alpha\bar{E}_{F_b}1+\alpha\bar{E}_{F_b}}{\bar{m}_t^+\bar{m}_t^-}\right.$$
$$\left. + \left[\frac{1}{2\bar{m}_t^*} - \frac{\alpha\bar{E}_{F_b}}{2\bar{m}_t^+} + \frac{1+\alpha\bar{E}_{F_b}}{2\bar{m}_t^-}\right]\right], \alpha_2(\bar{E}_{F_b}) = \left[\frac{1}{2\bar{m}_t^*} - \frac{\alpha\bar{E}_{F_b}}{2\bar{m}_t^+} + \frac{1+\alpha\bar{E}_{F_b}}{2\bar{m}_t^-}\right],$$

$$\alpha_3 = \frac{\alpha\hbar^2}{4}\left[\frac{1}{\bar{m}_t^-\bar{m}_l^+} + \frac{1}{\bar{m}_l^-\bar{m}_t^+}\right],$$

$$\tau_{A_1}(\bar{E}_{F_b}) = \left[\frac{2\bar{m}_l^+\bar{m}_l^-}{\alpha\hbar^2}\right]^{1/2}\left[-\left[\frac{1}{2\bar{m}_l^*} + \frac{1+\alpha\bar{E}_{F_b}}{\bar{m}_l^-} - \frac{\alpha\bar{E}_{F_b}}{2\bar{m}_l^+}\right]\right.$$
$$\left. + \left[\left[\frac{1}{2\bar{m}_l^*} + \frac{1+\alpha\bar{E}_{F_b}}{\bar{m}_l^-} - \frac{\alpha\bar{E}_{F_b}}{2\bar{m}_l^+}\right]^2 + \frac{\alpha\bar{E}_{F_b}(1+\alpha\bar{E}_{F_b})}{\bar{m}_l^-\bar{m}_l^+}\right]^{1/2}\right]^{1/2},$$

is the in complete Elliptic integral of second kind, $F(\lambda, q)$ is the incomplete Elliptic integral of first kind $\bar{N}_{A_4}(\bar{E}_{Fb}) = \sum_{\bar{r}=1}^{\bar{S}} \bar{L}(\bar{r})[\bar{M}_{A_4}(\bar{E}_{Fb})]$

1.2.5 The entropy in quantum wells (QWs) of HD stressed Kane type materials

The electron energy spectrum in stressed Kane type materials can be written [152–157] as

$$\left(\frac{\bar{k}_x}{\bar{a}_0(\bar{E})}\right)^2 + \left(\frac{\bar{k}_y}{\bar{b}_0(\bar{E})}\right)^2 + \left(\frac{\bar{k}_z}{\bar{c}_0(\bar{E})}\right)^2 = 1 \tag{1.195}$$

where

$$[\bar{a}_0(\bar{E})]^2 \equiv \frac{\bar{K}_0(\bar{E})}{\bar{A}_0(\bar{E}) + \frac{1}{2}\bar{D}_0(\bar{E})},\ \bar{K}_0(\bar{E}) \equiv \left[\bar{E} - \bar{C}_1\bar{\varepsilon} - \frac{2\bar{C}_2^2\bar{\varepsilon}_{xy}^2}{3\bar{E}'_g}\right]\left(\frac{3\bar{E}'_g}{2\bar{B}_2^2}\right)$$

$\bar{C}_1$ is the conduction band deformation potential, ε is the trace of the strain tensor $\hat{\varepsilon}$ which can be written as

$$\hat{\varepsilon} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{xy} & \varepsilon_{yy} & 0 \\ 0 & 0 & \bar{\varepsilon}_{zz} \end{bmatrix},$$

$\bar{C}_2$ is a constant which describes the strain interaction between the conduction and valance bands, $\bar{E}'_{g_0} \equiv \bar{E}_{g_0} + \bar{E} - \bar{C}_1\bar{\varepsilon},\ \bar{B}_2$, is the momentum matrix element,

$$\bar{A}_0(\bar{E}) \equiv \left[1 - \frac{(\bar{a}_0 + \bar{C}_1)}{\bar{E}'_{g_0}} + \frac{3\bar{b}_0\bar{\varepsilon}_{xx}}{2\bar{E}'_{g_0}} - \frac{\bar{b}_0\bar{\varepsilon}}{2\bar{E}'_{g_0}}\right],$$

$$\bar{a}_0 \equiv -\frac{1}{3}(\bar{b}_0 + 2\bar{m}),\ \bar{b}_0 \equiv \frac{1}{3}(\bar{l} - \bar{m}),\ \bar{d}_0 \equiv \frac{2\bar{n}}{\sqrt{3}},$$

$\bar{l}, \bar{m}, \bar{n}$ are the matrix elements of the strain perturbation operator, $\bar{D}_0(\bar{E}) \equiv (\bar{d}_0\sqrt{3})\dfrac{\bar{\varepsilon}_{xy}}{\bar{E}'_{g_0}}$

$$[\bar{b}_0(\bar{E})]^2 \equiv \frac{\bar{K}_0(\bar{E})}{\bar{A}_0(\bar{E}) - \frac{1}{2}\bar{D}_0(\bar{E})},\ [\bar{c}_0(\bar{E})]^2 \equiv \frac{\bar{K}_0\bar{c}_0(\bar{E})}{\bar{L}_0\bar{c}_0(\bar{E})}$$

and

$$\bar{L}_0(\bar{E}) = \left[1 - \frac{(\bar{a}_0 + \bar{C}_1)}{\bar{E}'_{g_0}} + \frac{3\bar{b}_0\bar{\varepsilon}_{zz}}{\bar{E}'_{g_0}} - \frac{\bar{b}_0\bar{\varepsilon}}{2\bar{E}'_{g_0}}\right]$$

The use of (1.195) can be written as

$$(\bar{E} - \bar{\alpha}_1)\bar{k}_x^2 + (\bar{E} - \bar{\alpha}_2)\bar{k}_Y^2 + (\bar{E} - \bar{\alpha}_3)\bar{k}_z^2 = \bar{t}_1\bar{E}^3 - \bar{t}_2\bar{E}^2 + \bar{t}_3\bar{E} + t_4 \tag{1.196a}$$

where

$$\bar{\alpha}_1 \equiv \left[\bar{E}_{g_0} - \bar{C}_1\bar{\varepsilon} - (\bar{a}_0 + \bar{C}_1)\bar{\varepsilon} + \frac{3}{2}\bar{b}_0\bar{\varepsilon}_{xx} - \frac{\bar{b}_0}{2}\bar{\varepsilon} + \left(\frac{\sqrt{3}}{2}\right)\bar{\varepsilon}_{xy}\bar{d}_0\right],$$

$$\bar{\alpha}_2 \equiv \left[\bar{E}_{g_0} - \bar{C}_1\bar{\varepsilon} - (\bar{a}_0 + \bar{C}_1)\bar{\varepsilon} + \frac{3}{2}\bar{b}_0\bar{\varepsilon}_{xx} - \frac{\bar{b}_0}{2}\varepsilon - \left(\frac{\sqrt{3}}{2}\right)\bar{\varepsilon}_{xy}\bar{d}_0\right]$$

$$\bar{\alpha}_3 \equiv \left[\bar{E}_{g_0} - \bar{C}_1\bar{\varepsilon} - (\bar{a}_0 + \bar{C}_1)\bar{\varepsilon} + \frac{3}{2}\bar{b}_0\bar{\varepsilon}_{zz} - \frac{\bar{b}_0}{2}\bar{\varepsilon}\right],$$

$$\bar{t}_1 \equiv \left(\frac{3}{2\bar{B}_2^2}\right), \bar{t}_2 \equiv \left(\frac{1}{2\bar{B}_2^2}\right)\left[6(\bar{E}_{g_0} - \bar{C}_1\bar{\varepsilon}) + 3\bar{C}_1\bar{\varepsilon}\right],$$

$$\bar{t}_3 \equiv \left(\frac{1}{2\bar{B}_2^2}\right)\left[3(\bar{E}_{g_0} - \bar{C}_1\bar{\varepsilon})^2 + 6\bar{C}_1\bar{\varepsilon}(\bar{E}_{g_0} - \bar{C}_1\bar{\varepsilon}) - 2\bar{C}_2^2\bar{\varepsilon}_{xy}^2\right]$$

and

$$\bar{t}_4 \equiv \left(\frac{1}{2\bar{B}_2^2}\right)\left[3 - \bar{C}_1\bar{\varepsilon}((\bar{E}_{g_0} - \bar{C}_1\bar{\varepsilon})^2 + 2\bar{C}_2^2\bar{\varepsilon}_{xy}^2\right].$$

The (1.196a) can be written as

$$\bar{E}\bar{k}^2 - \bar{T}_{17}\bar{k}_x^2 - \bar{T}_{27}\bar{k}_y^2 - \bar{T}_{37}\bar{k}_z^2 = \left[\bar{q}_{67}\bar{E}^3 - \bar{R}_{67}\bar{E}^2 + \bar{V}_{67}\bar{E} + \bar{\rho}_{67}\right] \tag{1.196b}$$

where

$$\bar{T}_{17} = \bar{\alpha}_1,\ \bar{T}_{27} = \bar{\alpha}_2,\ \bar{T}_{37} = \bar{\alpha}_3,\ \bar{t}_1 = \bar{q}_{67},\ \bar{t}_2 = \bar{R}_{67},\ \bar{t}_3 = \bar{V}_{67}$$

and

$$\bar{t}_4 = \bar{\rho}_{67}$$

Under the condition of heavy doping, (1.196b) can be written as

$$\bar{I}(4)\bar{k}^2 - \bar{T}_{17}\bar{I}(1)\bar{k}_x^2 - \bar{T}_{27}\bar{I}(1)\bar{k}_y^2 - \bar{T}_{37}\bar{k}_z^2\bar{I}(1) = \left[\bar{q}_{67}\bar{I}(6) - \bar{R}_{67}\bar{I}(5) + \bar{V}_{67}\bar{I}(4) + \bar{\rho}_{67}\bar{I}(1)\right] \tag{1.196c}$$

where

$$\bar{I}(6) = \int_{-\infty}^{\bar{E}} (\bar{E} - \bar{V})^3\bar{F}(\bar{V})d\bar{V} \tag{1.197}$$

The (1.197) can be written as

$$\bar{I}(6) = \bar{E}^3\bar{I}(1) - 3\bar{E}^2\bar{I}(7) + 3\bar{E}\bar{I}(8) - \bar{I}(9) \tag{1.198}$$

In which,

$$\bar{I}(7) = \int_{-\infty}^{\bar{E}} \bar{V}\bar{F}(\bar{V})d\bar{V} \tag{1.199}$$

$$\bar{I}(8) = \int_{-\infty}^{\bar{E}} \bar{V}^2 \bar{F}(\bar{V}) \bar{d}\bar{V} \tag{1.200}$$

$$\bar{I}(9) = \int_{-\infty}^{\bar{E}} \bar{V}^3 \bar{F}(\bar{V}) \bar{d}\bar{V} \tag{1.201}$$

Using (1.4), together with simple algebraic manipulations, one obtains

$$\bar{I}(7) = \frac{-\bar{\eta}_g}{2\sqrt{\pi}} \exp\left(\frac{-\bar{E}^2}{\bar{\eta}_g^2}\right) \tag{1.202}$$

$$\bar{I}(8) = \frac{\bar{\eta}_g^2}{4}\left[1 + Erf\left(\frac{\bar{E}}{\bar{\eta}_g}\right)\right] \tag{1.203}$$

and

$$\bar{I}(9) = \frac{-\bar{\eta}_g^3}{2\sqrt{\pi}} \exp\left(\frac{-\bar{E}^2}{\bar{\eta}_g^2}\right)\left[1 + \frac{\bar{E}^2}{\bar{\eta}_g^2}\right] \tag{1.204}$$

Thus (1.197) can be written as

$$\bar{I}(6) = \left[\frac{\bar{E}}{2}\left[1 + Erf\left(\frac{\bar{E}}{\eta_g}\right)\right]\left[\bar{E}^2 + \frac{3}{2}\eta_g^2\right] + \frac{\eta_g}{2\sqrt{\pi}} \exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)\left[4\bar{E}^2 + \eta_g^2\right]\right] \tag{1.205}$$

Thus, combining the appropriate equations, the dispersion relations of the conduction electrons in HD stressed materials can be expressed as

$$\bar{P}_{11}(\bar{E}, \eta_g)\bar{k}_x^2 + \bar{Q}_{11}(\bar{E}, \eta_g)\bar{k}_y^2 + \bar{S}_{11}(\bar{E}, \eta_g)\bar{k}_z^2 = 1 \tag{1.206}$$

where

$$\bar{P}_{11}(\bar{E}, \eta_g) \equiv \left[\frac{\gamma_0(\bar{E}, \eta_g) - (\bar{T}_{17}/2)[1 + Erf(\bar{E}, \eta_g)]}{\bar{\Delta}_{14}(\bar{E}, \eta_g)}\right],$$

$$\Delta_{14}(\bar{E}, \eta_g) \equiv \left[\bar{q}_{67}\left\{\frac{\bar{E}}{2}\left[1 + Erf\left(\frac{\bar{E}}{\eta_g}\right)\right]\left[\bar{E}^2 + \frac{3}{2}\eta_g^2\right] + \frac{\eta_g}{2\sqrt{\pi}} \exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)[4\bar{E}^2 + \eta_g^2]\right\}\right.$$

$$\left. - \bar{R}_{67}\theta_0(\bar{E}, \eta_g) + \bar{V}_{67}\gamma_0(\bar{E}, \eta_g) + \frac{\bar{\rho}_{67}}{2}[1 + Erf(\bar{E}/\eta_g)]\right],$$

$$\bar{Q}_{11}(\bar{E}, \eta_g) \equiv \left[\frac{\gamma_0(\bar{E}, \eta_g) - (\bar{T}_{27}/2)[1 + Erf(\bar{E}/\eta_g)]}{\Delta_{14}(\bar{E}, \eta_g)}\right]$$

and

$$\bar{S}_{11}(\bar{E},\eta_g) \equiv\equiv \left[\frac{\gamma_0(\bar{E},\eta_g)-(\bar{T}_{27}/2)[1+Erf(\bar{E}/\eta_g)]}{\Delta_{14}(\bar{E},\eta_g)}\right]$$

Thus, the energy spectrum in this case is real since the dispersion relation of the corresponding materials in the absence of band tails as given by (1.195) is a pole-less function in the finite complex plane.

The EEMs along $\bar{x}$, $\bar{y}$ *and* $\bar{z}$ directions in this case can be written as

$$\begin{aligned}\bar{m}^*_{xx}(\bar{E}_{F_h},\eta_g) = \frac{\hbar^2}{2}\Bigg[&[\gamma_0(\bar{E}_{F_h},\eta_g)\\ &-(\bar{T}_{17}/2)[1+Erf(\bar{E}_{F_h},\eta_g)]]^{-2}[\Delta_{14}(\bar{E}_{F_h},\eta_g)\}'[\gamma_0(\bar{E}_{F_h},\eta_g)\\ &-(\bar{T}_{27}/2)[1+Erf(\bar{E}_{F_h},\eta_g)]]]\\ &-\Delta_{14}(\bar{E}_{F_h},\eta_g)\left[\frac{1}{2}\left[1+Erf\left(\frac{\bar{E}_{F_h}}{\eta_g}\right)\right]-\left\{\frac{\bar{T}_{17}}{\eta_g\sqrt{\bar{x}}}\exp\left(\frac{\bar{E}^2{}_{F_h}}{\eta_g^2}\right)\right\}\right]\Bigg]\end{aligned} \tag{1.207}$$

$$\begin{aligned}\bar{m}^*_{yy}(\bar{E}_{F_h},\eta_g) = \frac{\hbar^2}{2}\Bigg[&[\gamma_0(\bar{E}_{F_h},\eta_g)\\ &-(\bar{T}_{27}/2)[1+Erf(\bar{E}_{F_h},\eta_g)]]^{-2}[\Delta_{14}(\bar{E}_{F_h},\eta_g)\}'[\gamma_0(\bar{E}_{F_h},\eta_g)\\ &-(\bar{T}_{27}/2)[1+Erf(\bar{E}_{F_h},\eta_g)]]]\\ &-\Delta_{14}(\bar{E}_{F_h},\eta_g)\left[\frac{1}{2}\left[1+Erf\left(\frac{\bar{E}_{F_h}}{\eta_g}\right)\right]-\left\{\frac{\bar{T}_{27}}{\eta_g\sqrt{\bar{x}}}\exp\left(\frac{\bar{c}}{\eta_g^2}\right)\right\}\right]\Bigg]\end{aligned} \tag{1.208}$$

and

$$\begin{aligned}\bar{m}^*_{zz}(\bar{E}_{F_h},\eta_g) = \frac{\hbar^2}{2}\Bigg[&[\gamma_0(\bar{E}_{F_h},\eta_g)\\ &-(\bar{T}_{37}/2)[1+Erf(\bar{E}_{F_h},\eta_g)]]^{-2}[\Delta_{14}(\bar{E}_{F_h},\eta_g)\}'[\gamma_0(\bar{E}_{F_h},\eta_g)\\ &-(\bar{T}_{37}/2)[1+Erf(\bar{E}_{F_h},\eta_g)]]]\\ &-\Delta_{14}(\bar{E}_{F_h},\eta_g)\left[\frac{1}{2}\left[1+Erf\left(\frac{\bar{E}_{F_h}}{\eta_g}\right)\right]-\left\{\frac{\bar{T}_{37}}{\eta_g\sqrt{x}}\exp\left(\frac{\bar{E}^2{}_{F_h}}{\eta_g^2}\right)\right\}\right]\Bigg]\end{aligned} \tag{1.209}$$

Thus, we can see that the EEMs in this case exist within the band gap.

In the absence of band tails, $\eta_g \to 0$ we get

$$\bar{m}^{*}_{xx}(\bar{E}_F) = \hbar^2 \bar{a}_0(\bar{E}_F)\{\bar{a}_0(\bar{E}_F)\}' \tag{1.210}$$

$$\bar{m}^{*}_{xx}(\bar{E}_F) = \hbar^2 \bar{b}_0(\bar{E}_F)\{\bar{b}_0(\bar{E}_F)\}' \tag{1.211}$$

and

$$\bar{m}^{*}_{xx}(\bar{E}_F) = \hbar^2 \bar{c}_0(\bar{E}_F)\{\bar{c}_0(\bar{E}_F)\}' \tag{1.212}$$

The DOS function in this case can be written as

$$\bar{N}_{HD}(\bar{E},\eta_g) = \frac{\bar{g}_v}{3\pi^2}\{\Delta_{15}(\bar{E}/\eta_g)\}^{-2}\left[\frac{3}{2}\{\Delta_{15}(\bar{E},\eta_g)\}\sqrt{\Delta_{14}(\bar{E},\eta_g)}\{\Delta_{14}(\bar{E},\eta_g)\}' - \{\Delta_{14}(\bar{E},\eta_g)\}^{3/2}\{\Delta_{15}(\bar{E},\eta_g)\}'\right] \tag{1.213}$$

where

$$\Delta_{15}(\bar{E},\eta_g) \equiv [[\gamma_0(\bar{E},\eta_g) - (\bar{T}_{17}/2)[1+Erf(\bar{E},\eta_g)]][\gamma_0(\bar{E},\eta_g) - (\bar{T}_{27}/2)[1+Erf(\bar{E},\eta_g)]]$$
$$[\gamma_0(\bar{E},\eta_g) - (\bar{T}_{37}/2)[1+Erf(\bar{E},\eta_g)]]]^{1/2}$$

Using (1.213), the electron concentration at can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left[\bar{I}_{126}(\bar{E}_{F_h},\eta_g) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_{126}(\bar{E}_{F_h},\eta_g)]\right] \tag{1.214}$$

where

$$\bar{I}_{126}(\bar{E}_{F_h},\eta_g) = \left[\frac{\{\Delta_{14}(\bar{E}_{F_h},\eta_g)\}^{3/2}}{\Delta_{15}(\bar{E}_{F_h},\eta_g)}\right]$$

In this case, $\bar{E}_{hd}$ is given by

$$\{\Delta_{14}(\bar{E}_{hd},\eta_g)\} = 0 \tag{1.215}$$

Thus, one can numerically evaluate the entropy by using (1.214), (1.215), (1.31f) and the allied definitions in this case.

The dispersion relation of the conduction electrons in HD QWs of Kane type materials can be written as

$$\bar{P}_{11}(\bar{E},\eta_g)\bar{k}_x^2 + \bar{Q}_{11}(\bar{E},\eta_g)\bar{k}_y^2 + \bar{S}_{11}(\bar{E},\eta_g)\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 \equiv 1 \tag{1.216}$$

The EEM can be expressed as

$$\bar{m}^{*}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\frac{\hbar^2}{2}\bar{A}'_{56}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) \tag{1.217}$$

where

$$\bar{A}_{56}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\frac{\pi\left[1-\bar{S}_{11}(\bar{E},\eta_g)\left(\frac{\bar{\eta}_z\pi}{\bar{d}_z}\right)^2\right]}{\sqrt{\bar{P}_{11}(\bar{E},\eta_g)\bar{Q}_{11}(\bar{E},\eta_g)}}$$

From (1.217), it appears that the EEM is a function of Fermi energy, and size quantum number and the same mass exists in the band gap.

Thus, the total 2D DOS function can be expressed

$$\bar{N}_{2DT}(\bar{E})=\frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{A}'_{56}(\bar{E}_{F1HD},\eta_g,n_z) \tag{1.218}$$

The sub-band energies ($\bar{E}_{n_{z_{8HD}}}$) are given by

$$\bar{S}_{11}(\bar{E}_{n_{z_{8HD}}},\eta_g)(\pi\bar{n}_z/\bar{d}_z)^2=1 \tag{1.219}$$

The 2D surface electron concentration per unit area for QWs of stressed HD Kane type compounds can be written as

$$\bar{n}_{2D}=\frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{\max}}[\bar{T}_{57HD}(\bar{E}_{F1HD},\eta_g,\bar{\eta}_z)+\bar{T}_{58HD}(\bar{E}_{F1HD},\eta_g,\bar{\eta}_z)] \tag{1.220}$$

where

$$\bar{T}_{57HD}(\bar{E}_{F1HD},\eta_g,\bar{\eta}_z)\equiv\bar{A}_{56HD}(\bar{E}_{F1HD},\eta_g,\bar{\eta}_z)$$

and

$$\bar{T}_{58HD}(\bar{E}_{F1HD},\eta_g,\bar{\eta}_z)\equiv\sum_{r=l}^{s}\bar{L}(\bar{r})\bar{T}_{57HD}(\bar{E}_{F1HD},\eta_g,\bar{\eta}_z)$$

Using (1.31f) and (1.220) we can study the entropy in this case.

In the absence of band tails, the 2D electron energy spectrum in QWs of stressed materials assumes the form

$$\frac{\bar{k}_x^2}{[\bar{a}_0(\bar{E})]^2}+\frac{\bar{k}_y^2}{[\bar{b}_0(\bar{E})]^2}+\frac{1}{[\bar{c}_0(\bar{E})]^2}(\bar{n}_z\pi/\bar{d}_z)^2=1 \tag{1.221}$$

The area of 2D wave vector space enclosed by (1.221) can be written as

$$\bar{A}(\bar{E},\bar{n}_z)=\pi\bar{P}^2(\bar{E},\bar{n}_z)\bar{a}_0(\bar{E})\bar{b}_0(\bar{E})$$

where

$$\bar{P}^2(\bar{E},\bar{n}_z) = [1 - [\bar{n}_z\pi/\bar{d}_z\bar{c}_0(\bar{E})]^2]$$

From (1.221), the EEM can be written as

$$\bar{m}^*(\bar{E}_{Fs},\bar{n}_z) = \frac{\hbar^2}{2}[\bar{P}^2(\bar{E}_{Fs},\bar{n}_z)\bar{a}_0(\bar{E}_{Fs})\bar{b}_0(\bar{E}_{Fs})]' \tag{1.222}$$

Thus, the total 2D DOS function can be expressed as

$$\bar{N}_{2DT}(\bar{E}) = \left(\frac{\bar{g}_v}{2\pi}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\theta_6(\bar{E},\bar{n}_z)\bar{H}(\bar{E}-\bar{E}_{n_{z_{11}}}) \tag{1.223}$$

in which,

$$\bar{\theta}_6(\bar{E},\bar{n}_z) = [2\bar{P}(\bar{E},\bar{n}_z)\{\bar{P}(\bar{E},\bar{n}_z)\}'\bar{a}_0(\bar{E})\bar{b}_0(\bar{E}) + \{\bar{P}(\bar{E},\bar{n}_z)\}^2\{\bar{a}_0(\bar{E})\}'\bar{b}_0(\bar{E}) + \{\bar{P}(\bar{E},\bar{n}_z)\}^2\{\bar{b}_0(\bar{E})\}'\bar{a}_0(\bar{E})]$$

The sub-band energies $(\bar{E}_{n_{z_{11}}})$ are given by

$$\bar{c}_0(\bar{E}_{n_{z_{11}}}) = \bar{n}_z\pi/\bar{d}_z \tag{1.224}$$

The 2D surface electron concentration per unit area for QWs of stressed Kane type compounds can be written as

$$\bar{n}_{2D} = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{T}_{61}(\bar{E}_{Fs},\bar{n}_z) + \bar{T}_{62}(\bar{E}_{Fs},\bar{n}_z)] \tag{1.225}$$

where

$$\bar{T}_{61}(\bar{E}_{Fs},\bar{n}_z) \equiv [\bar{p}^2(\bar{E}_{Fs},\bar{n}_z)\bar{a}_0(\bar{E}_{Fs})\bar{b}_0(\bar{E}_{Fs})]$$

and

$$\bar{T}_{62}(\bar{E}_{Fs},\bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\bar{T}_{61}(\bar{E}_{Fs},\bar{n}_z)$$

The entropy in this case assumes the form

$$\bar{S}_0 = \left[\frac{\bar{g}_v\pi\bar{k}_B{}^2\bar{T}}{6}\right]\left[\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\left[\overline{T'}_{61}(\bar{E}_{Fs},\bar{n}_z) + \overline{T'}_{62}(\bar{E}_{Fs},\bar{n}_z)\right]\right] \tag{1.226}$$

The DOS function for bulk specimens of stressed Kane type materials in the absence of band tail can be written as

$$\bar{D}_0(\bar{E}) = \bar{g}_v(3\pi^2)^{-1}\left[\bar{a}_0(\bar{E})\bar{b}_0(\bar{E})[\bar{c}_0(\bar{E})]' + \bar{a}_0(\bar{E})[\bar{b}_0(\bar{E})]'\bar{c}_0(\bar{E}) + [\bar{a}_0(\bar{E})]'\bar{b}_0(\bar{E})\bar{c}_0(\bar{E})\right] \tag{1.227}$$

Combining (1.227) with the Fermi–Dirac occupation probability factor and using the generalized Summerfield lemma the electron concentration in this case can be expressed as

$$\bar{n}_0 = \bar{g}_v(3\pi^2)^{-1}[\bar{M}_4(\bar{E}_F) + \bar{N}_4(\bar{E}_F)] \tag{1.228}$$

where

$$\bar{M}_4(\bar{E}_F) \equiv [\bar{a}_0(\bar{E}_F)\bar{b}_0(\bar{E}_F)\bar{c}_0(\bar{E}_F)]$$

and

$$\bar{N}_4(\bar{E}_F) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})M_4(\bar{E}_F)$$

The entropy in this case is given by

$$\bar{S}_0 = \left[\frac{\bar{k}_B{}^2\bar{T}\,\bar{g}_v}{9}\right]\left[\bar{M}'_4(\bar{E}_F) + \bar{N}'_4(\bar{E}_F)\right] \tag{1.229}$$

1.2.6 The entropy in quantum wells (QWs) of HD Te

The dispersion relation of the conduction electrons in Te can be expressed as [158]

$$\bar{E} = \psi_1\bar{k}_z^2 + \psi_2\bar{k}_s^2 \pm \left[\psi_3^2\bar{k}_z^2 + \psi_4^2\bar{k}_s^2\right]^{1/2} \tag{1.230}$$

where the values of the system constants are given in table as given annexure (15).

The carrier energy spectrum in HD Te can be written as

$$\gamma_3(\bar{E},\eta_g) = \psi_1\bar{k}_z^2 + \psi_2\bar{k}_s^2 \pm \left[\psi_3^2\bar{k}_z^2 + \psi_4^2\bar{k}_s^2\right]^{1/2} \tag{1.231}$$

The EEMs along $\bar{k}_z$ and $\bar{k}_s$ directions assume the forms

$$\bar{m}_z^*(\bar{E}_{F_h},\eta_g) = \frac{\hbar^2}{2\psi_1}\left[1 - \frac{\psi_3}{\sqrt{\psi_3^2 + 4\psi_1\gamma_3(\bar{E}_{F_h},\eta_g)}}\right]\gamma_3(\bar{E}_{F_h},\eta_g) \tag{1.232}$$

and

$$\bar{m}_s^*(\bar{E}_{F_h},\eta_g) = \frac{\hbar^2}{2\psi_1}\left[1 - \frac{\psi_3}{\sqrt{\psi_4^2 + 4\psi_1\gamma_3(\bar{E}_{F_h},\eta_g)}}\right]\gamma_3(\bar{E}_{F_h},\eta_g) \tag{1.233}$$

The investigations of EEMs require the expression of electron concentration, which can be written from (1.231) as

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left[\bar{t}_{1HD}(\bar{E}_{F_h}, \eta_g) + \bar{t}_{2HD}(\bar{E}_{F_h}, \eta_g)\right]$$

where

$$\bar{t}_{1HD}(\bar{E}_{F_h}, \eta_g) = [3\psi_{5HD}(\bar{E}_{F_h}, \eta_g)\Gamma_{3HD}(\bar{E}_{F_h}, \eta_g) - \psi_6\Gamma^3_{3HD}(\bar{E}_{F_h}, \eta_g)]$$

$$\psi_{5HD}(\bar{E}_{F_h}, \eta_g) = \left[\frac{\gamma_3(\bar{E}_{F_h}, \eta_g)}{\psi_2} + \frac{\psi_4^2}{2\psi_2^2}\right],\ \Gamma_{3HD}(\bar{E}_{F_h}, \eta_g) = \frac{\sqrt{\psi_3^2 + 4\psi_1\gamma_3(\bar{E}_{F_h}, \eta_g)}}{2\psi_1}$$

$$\psi_6 = \frac{\psi_1}{\psi_2}$$

and

$$\bar{t}_{2HD}(\bar{E}_{F_h}, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})\bar{t}_{1HD}(\bar{E}_{F_h}, \eta_g) \tag{1.234a}$$

In this case $\bar{E}_{Fhd}$ is given by

$$\{\gamma_3(\bar{E}_{F_{hd}}, \eta_g)\} = 0 \tag{1.234b}$$

Therefore by using (1.31f), (1.234a) and (1.234b) we can study the entropy in this case

The 2D electron energy spectrum in HD QW of Te can be written using (1.230) as

$$\bar{k}_s^2 = \psi_5(\bar{E}, \eta_g) - \psi_6\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 \pm \psi_7\left[\psi_{8HD}^2(\bar{E}, \eta_g) - \left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]^{1/2} \tag{1.235}$$

where

$$\psi_7 = \frac{\psi_4\sqrt{\psi_1}}{\psi_2^{3/2}}$$

and

$$\psi_{8HD}(\bar{E}, \eta_g) = \left[\frac{\psi_4^4 + 4\gamma_3(\bar{E}, \eta_g)\psi_2\psi_4^2 + 4\psi_2^2\psi_2^2}{4\psi_1\psi_2\psi_4^2}\right]$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F_s}, \bar{n}_z) = \frac{\hbar^2}{2}\bar{t}'_{40}(\bar{E}_{F_s}, \bar{n}_z)$$

$$\bar{m}^{*}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\frac{\hbar^2}{2}\left[\psi_{5HD}(\bar{E}_{F1HD},\eta_g)+\frac{\psi_{8HD}(\bar{E}_{F1HD},\eta_g)\psi'_{8HD}(\bar{E}_{F1HD},\eta_g)}{\sqrt{\psi_{8HD}(\bar{E}_{F1HD},\eta_g)-(\pi\bar{n}_z/\bar{d}_z)^2}}\right] \tag{1.236}$$

The total DOS function in this case can be expressed as

$$\bar{N}_{2DT}(\bar{E})=\frac{\bar{g}_v}{\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\psi'_{5HD}(\bar{E},\eta_g)\bar{H}(\bar{E}-\bar{E}_{n_{z59HD}}) \tag{1.237}$$

where $\bar{E}_{n_{z59HD}}$ is the lowest positive root of the equation

$$\psi'_{5HD}(\bar{E}_{n_{z59HD}},\eta_g)-\psi_6\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)\pm\psi_7\left[\psi^2_{8HD}(\bar{E}_{n_{z59HD}},\eta_g)-\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]^{1/2}=0 \tag{1.238}$$

The surface electron concentration is given by

$$\bar{n}_{2D}=\frac{\bar{g}_v}{\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{\max}}[\bar{t}_{1HDTe}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)+\bar{t}_{2HDTe}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)] \tag{1.239}$$

where

$$\bar{t}_{1HDTe}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\bar{t}_{1HDTe}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\left[\psi_{5HD}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)-\psi_6\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]$$

and

$$\bar{t}_{2HDTe}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{t}_{1HDTe}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)]$$

Thus using (1.239) and (1.31f) we can study the entropy in this case.

The 2D electron energy spectrum in QWs of Te in the absence of band tails assumes the form

$$\bar{k}_s^2=\psi_5(\bar{E})-\psi_6\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)\pm\psi_7\left[\psi_8^2(\bar{E})-\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]^{1/2} \tag{1.240}$$

where

$$\psi_5(\bar{E})\left[\frac{\bar{E}}{\psi_2}+\frac{\psi_4^2}{2\psi_2^2}\right]$$

and

$$\psi_8^2(\bar{E}) = \frac{\psi_4^4 + 4\bar{E}\psi_2\psi_4^2 + 4\psi_2^2\psi_3^2}{4\psi_1\psi_2\psi_4^2}$$

Thus, the total 2D DOS function can be expressed as

$$\bar{n}_{2DT}(\bar{E}) = \left(\frac{g_v}{\pi}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{\max}} \bar{t}'_{40}(\bar{E}, \bar{n}_z)\bar{H}(\bar{E} - \bar{E}_{n_{z12}}) \tag{1.241}$$

where

$$\bar{t}_{40}(\bar{E}, \bar{n}_z) = \left[\psi_5(\bar{E}) - \psi_6\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right) \pm \psi_7\left[\psi_8^2(\bar{E}) - \left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]^{1/2}\right]^{1/2}$$

The sub-band energies ($\bar{E}_{n_{z12}}$) are given by

$$\bar{E}_{n_{z12}} = \psi_1\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 \pm \psi_3\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right) \tag{1.242a}$$

Using (1.240) the EEM can be expressed as

$$\bar{m}^*(\bar{E}_{Fs}, \bar{n}_z) = \frac{\hbar^2}{2}\bar{t}'_{40}(\bar{E}_{Fs}, \bar{n}_z) \tag{1.242b}$$

The 2D surface electron concentration per unit area for QWs of Te can be written as

$$\bar{n}_{2D} = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{t}'_{40}(\bar{E}_{Fs}, \bar{n}_z)\bar{H}(\bar{E}_{Fs}, \bar{n}_z) \tag{1.243}$$

where

$$\bar{t}_{41}(\bar{E}_{Fs}, \bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})t_{40}(\bar{E}_{Fs}, \bar{n}_z)$$

The entropyin this case is given by

$$\bar{S}_0 = \left[\frac{\bar{g}_v\pi\bar{k}_B{}^2\bar{T}}{3}\right]\left[\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{t}'_{40}(\bar{E}_{Fs}, \bar{n}_z) + \bar{t}'_{41}(\bar{E}_{Fs}, \bar{n}_z)]\right] \tag{1.244}$$

The electron concentration and the entropy for bulk specimens of Te in the absence of band tails can, respectively, be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}[\bar{M}_9(\bar{E}_F) + \bar{N}_9(\bar{E}_F)] \tag{1.245}$$

and

$$\bar{S}_0 = \left[\frac{\bar{g}_v \bar{k}_B{}^2 \bar{T}}{9}\right][\bar{M}'_9(\bar{E}_F) + \bar{N}'_9(\bar{E}_F)]] \tag{1.246}$$

where

$$\bar{M}_9(\bar{E}_F) = [3\psi_5(\bar{E}_F)\Gamma_3(\bar{E}_F) - \psi_6\Gamma_3^3(\bar{E}_F)], \psi_5(\bar{E}_F) = \left[\frac{\bar{E}_F}{\psi_5} + \frac{\psi_4^2}{2\psi_2^2}\right]$$

$$\Gamma_3(\bar{E}_F) = [2\psi_1]^{-1}\left[\sqrt{\psi_3^2 + 4\psi_1\bar{E}_F} - \psi_3\right] \text{ and } \bar{N}_9(\bar{E}_F) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})\bar{M}_9(\bar{E}_F)$$

1.2.7 The entropy in quantum wells (QWs) of HD gallium phosphide

The energy spectrum of the conduction electrons in n-GaP can be written as [159]

$$\bar{E} = \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^*} + \frac{\hbar^2}{2\bar{m}_{||}^*}[\bar{A}'\bar{k}_s^2 + \bar{k}_z^2] - \left[\frac{\hbar^4\bar{k}_0^2}{2\bar{m}_{||}^{*2}}(\bar{k}_s^2 + \bar{k}_z^2) + |\bar{V}_G|^2\right]^{1/2} + |\bar{V}_G| \tag{1.247}$$

where $\bar{k}_0$ and $|V_G|$ are constants of the energy spectrum and $\bar{A}'$=1.

The dispersion relation of the conduction electrons in HD n- GaP can be expressed as

$$\gamma_3(\bar{E}, \eta_g) = \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^*} + \frac{\hbar^2}{2\bar{m}_{||}^*}[\bar{A}'\bar{k}_s^2 + \bar{k}_z^2] - \left[\frac{\hbar^4\bar{k}_0^2}{\bar{m}_{||}^{*2}}(\bar{k}_s^2 + \bar{k}_z^2) + |V_G|^2\right]^{1/2} - |V_G| \tag{1.248}$$

The EEMs assume the forms as

$$\bar{m}_z^*(\bar{E}_{F_h}, \eta_g) = \frac{\hbar^2\gamma'_3(\bar{E}_{F_h}, \eta_g)}{b}\left[1 \pm (\bar{C} + \bar{b}\bar{D})[\bar{C}^2 + 4\bar{b}\bar{D}^2 + 4\bar{b}\bar{C}\gamma_3(\bar{E}_{F_h}, \eta_g) - 4\bar{b}\bar{C}\bar{D} + 4\bar{b}^2\gamma_3(\bar{E}_{F_h}, \eta_g)\bar{D}]^{-1/2}\right] \tag{1.249}$$

And

$$\bar{m}_s^*(\bar{E}_{F_h}, \eta_g) = \frac{\hbar^2}{2}[\bar{t}_{11}\gamma'_3(\bar{E}_{F_h}, \eta_g) - \bar{t}_{41}\bar{t}'_5(\bar{E}_{F_h}, \eta_g)] \tag{1.250}$$

where

$$\bar{b} = \frac{\hbar^2}{2\bar{m}_{||}^*},\ \bar{C} = \frac{1}{2}\left(\frac{\hbar^2\bar{k}_0}{\bar{m}_{||}^*}\right)^2,\ \bar{D} = |V_G|, \bar{t}_{11} = \frac{1}{\bar{a}},\ \bar{a} = \frac{\hbar^2}{2\bar{m}_\perp^*} + \bar{A}'\bar{b},\ \bar{t}_{41} = \frac{\sqrt{\bar{g}_3}}{2\bar{a}^2}$$

$$\bar{g}_3 = (4\bar{a}\bar{b}c + 4\bar{a}^2\bar{c}), \bar{t}_5^2(\bar{E}_{F_h}, \eta_g) = [\bar{g}_2 - 4\bar{a}\bar{C}\gamma_3(\bar{E}_{F_h}, \eta_g)](\bar{g}_3)^{-1}, \bar{g}_2 = (4\bar{a}^2\bar{b}^2 + \bar{C}^2 + 4\bar{a}\bar{C}\bar{D})$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v}{4\pi^2}[\bar{I}_{127}(\bar{E}_{F_h}, \eta_g) + \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{I}_{127}(\bar{E}_{F_h}, \eta_g)]] \tag{1.251}$$

where

$$\bar{I}_{127}(\bar{E}_{F_h}, \eta_g) = [\bar{M}_{1HD}(\bar{E}_{F_h}, \eta_g)]$$

$$\bar{M}_{1HD}(\bar{E}_{F_h}, \eta_g) = \left[2(\bar{t}_{11}\gamma_3(\bar{E}_{F_h}, \eta_g) + \bar{t}_{21})\sqrt{t_{81} + t_{91}\gamma_3(\bar{E}_{F_h}, \eta_g)} + \left(\frac{\bar{t}_{31}}{3}\right)\theta_{,-}^3(\bar{E}_{F_h}, \eta_g)\right.$$
$$+ \left(\frac{\bar{t}_{41}}{2}\right)\left[\theta_{,-}(\bar{E}_{F_h}, \eta_g)\sqrt{\theta_-^2(\bar{E}_{F_h}, \eta_g) + t_5(\bar{E}_{F_h}, \eta_g)} - \sqrt{t_5(\bar{E}_{F_h}, \eta_g)}\right]$$
$$\left. + (\bar{t}_{41}\bar{t}_5(\bar{E}_{F_h}, \eta_g)/2)\ln\left|\frac{\theta_{,-}(\bar{E}_{F_h}, \eta_g) + \sqrt{\theta_-^2(\bar{E}_{F_h}, \eta_g) + \bar{t}_5(\bar{E}_{F_h}, \eta_g)}}{\sqrt{\bar{t}_5(\bar{E}_{F_h}, \eta_g)}}\right|\right]$$

$$\bar{t}_{21} = \frac{\bar{g}_1}{2\bar{a}^2}, \bar{g}_1 = -(\bar{C} + 2\bar{a}\bar{D}), \bar{t}_{81} = [\bar{t}_{41}^4 + 4\bar{t}_{41}^2\bar{t}_{21}\bar{t}_{31} + (4\bar{t}_{31}^2\bar{t}_{41}^2\bar{g}_2)(\bar{g}_3)^{-1}], \bar{t}_{31} = \frac{\bar{b}}{\bar{a}},$$

$$\bar{t}_{91} = [4\bar{t}_{11}\bar{t}_{31}\bar{t}_{41}^2 + 8\bar{t}_{11}\bar{t}_{21}\bar{t}_{31}^2 - (16\bar{t}_{31}^2\bar{t}_{41}^2\bar{a}\bar{C})(\bar{g}_3)^{-1}],$$

$$\theta_-(\bar{E}_{F_h}, \eta_g) = (\bar{t}_{31}\sqrt{2})^{-1}\left[\bar{t}_{61} + \bar{t}_{71}\gamma_3(\bar{E}_{F_h}, \eta_g) - \sqrt{\bar{t}_{81} + \bar{t}_{91}\gamma_3(\bar{E}_{F_h}, \eta_g)}\right], \bar{t}_{61} = (\bar{t}_{41}^2 + 2\bar{t}_{21}\bar{t}_{31})$$

and $\bar{t}_{71} = (2\bar{t}_{11}\bar{t}_{31})$

The $\bar{E}_{hd}$ in this case is given by the equation

$$\gamma_3(\bar{E}_{hd}, \eta_g) = 0 \tag{1.252}$$

Therefore using (1.251), (1.252), and (1.31f) we can study the entropyin this case.

The 2D dispersion relation in QW of HD GaP can be expressed following (1.248) as

$$\bar{k}_s^2 = \bar{t}_{11}\gamma_3(\bar{E}, \eta_g) + \bar{t}_{21} - \bar{t}_{31}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 - \bar{t}_{41}\left[\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + \bar{t}_5^2(\bar{E}, \eta_g)\right]^{1/2} \tag{1.253}$$

The EEM in this case can be written following (1.253) as

$$\bar{m}^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\frac{\hbar^2}{2}\left[\bar{t}_{11}\gamma'_3(\bar{E}_{F1HD},\eta_g)-\bar{t}_{41}\bar{t}_5(\bar{E}_{F1HD},\eta_g)t'_5(\bar{E}_{F1HD},\eta_g)\right.$$
$$\left.\left[\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2+\bar{t}_5^2(\bar{E}_{F1HD},\eta_g)\right]^{-1/2}\right] \tag{1.254}$$

The total DOS function assumes the form

$$\bar{N}_{2DT}(\bar{E},\eta_g)=\frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\left[\bar{t}_{11}\gamma'_3(\bar{E}_{F1HD},\eta_g)-\bar{t}_{41}\bar{t}_5(\bar{E}_{F1HD},\eta_g)\bar{t}'_5(\bar{E}_{F1HD},\eta_g)\right.$$
$$\left.\left[\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2+\bar{t}_5^2(\bar{E}_{F1HD},\eta_g)\right]^{-1/2}\right]\bar{H}(\bar{E}-\bar{E}_{n_{z8tHD}}) \tag{1.255}$$

where $\bar{E}_{n_{z8THD}}$ is given by the equation

$$\bar{t}_{11}y_3(\bar{E}_{n_{z8THD}})+\bar{t}_{21}-\bar{t}_{31}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)-\bar{t}_{41}\left[\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2+\bar{t}_5^2(\bar{E}_{n_{z8THD}},\eta_g)\right]^{1/2}=0 \tag{1.256}$$

The surface electron concentration in QW of HD n-GaP can be written as

$$\bar{n}_s=\frac{\bar{g}_v}{\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{\max}}\left[\bar{t}_{3HDGaP}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)+\bar{t}_{4HDGaP}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\right] \tag{1.257}$$

where

$$\bar{t}_{1HDGap}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\bar{t}_{11}\gamma_3(\bar{E}_{F1HD},\eta_g,\bar{n}_z)+\bar{t}_{21}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2-t_{41}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2$$
$$+\bar{t}_5^2(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\Big]^{1/2}$$
$$\bar{t}_{4HDGap}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{t}_{3HDGap}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\right]$$

Thus using (1.257) and (1.31f) we can study the entropy in this case.

The 2D electron dispersion relation in size-quantized n-GaP in the absence of band tails assumes the form

$$\bar{E}=\bar{a}\bar{k}_s^2+\bar{b}\left(\frac{\bar{n}_z}{\bar{d}_z}\right)^2-\left[\bar{c}\left(\frac{\bar{n}_z}{\bar{d}_z}\right)^2+\bar{c}\bar{k}_s^2+|V_G|^2\right]^{1/2}+|V_G| \tag{1.258}$$

The sub-band energy $(\bar{E}_{n_{z13}})$ are given by

$$\bar{E}_{n_{z13}} = \bar{c}(\pi\bar{n}_z/\bar{d}_z)^2 + |V_G| - \left[|V_G|^2 + \bar{D}(\pi\bar{n}_z/\bar{d}_z)^2\right]^{1/2} \tag{1.259}$$

The (1.258) can be expressed as

$$\bar{k}_s^2 = \bar{t}_{42}(\bar{E}, n_z) \tag{1.260}$$

in which,

$$\bar{t}_{42}(\bar{E}, n_z) \equiv [\{2\bar{a}(\bar{E} - \bar{t}_1) + \bar{D}\} - \{[2\bar{a}(\bar{E} - \bar{t}_1) + \bar{D}]^2 - 4\bar{a}^2[(\bar{E} - \bar{t}_1)^2 - \bar{t}_2]\}^{1/2}]$$

$$\bar{t}_1 \equiv |V_G| + \bar{C}(\pi\bar{n}_z/\bar{d}_z)^2$$

and

$$\bar{t}_2 \equiv |V_G|^2 + \bar{C}(\pi\bar{n}_z/\bar{d}_z)^2,$$

The total DOS function is given by

$$N_{2DT}(E) = \frac{\bar{g}_v}{4\pi\bar{a}^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{t}_{42}{}'(\bar{E}, \bar{n}_z)]\bar{H}(\bar{E} - \bar{E}_{n_{z13}}) \tag{1.261a}$$

Using (1.260) the EEM can be expressed as

$$\bar{m}^*(\bar{E}_{F_s}, \bar{n}_z) = \frac{\hbar^2}{2}\bar{t}'_{42}(\bar{E}_{F_s}, \bar{n}_z) \tag{1.261b}$$

The electron statistics in QWs in n-GaP assumes the form

$$\bar{n}_{2D} = \left[\left(\frac{\bar{g}_v}{4\pi\bar{a}^2}\right) \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{t}_{42}(\bar{E}_{F_s}, \bar{n}_z) + \bar{t}_{43}(\bar{E}_{F_s}, \bar{n}_z)\ ]\right]$$

$$\bar{t}_{43}(\bar{E}_{F_s}, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} [\bar{t}_{42}(\bar{E}_{F_s}, \bar{n}_z)\ ] \tag{1.262}$$

where

$$\bar{t}_{43}(\bar{E}_{F_s}, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} [\bar{t}_{42}(\bar{E}_{F_s}, \bar{n}_z).]$$

The entropy in this case is given by

$$\bar{S}_0 = \left[\frac{\bar{g}_v \pi \bar{k}_B{}^2 \bar{T}}{12\bar{a}^2}\right] \left[\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{t}'_{42}(\bar{E}_{Fs}, \bar{n}_z) + \bar{t}'_{43}(\bar{E}_{Fs}, \bar{n}_z)]\right] \tag{1.263}$$

The EEMs in bulk specimens of n-GaP in the absence of band tails can be written as

$$\bar{m}_s^*(\bar{E}_F) = \frac{\hbar^2}{2}[\bar{t}'_{11} - \bar{t}_{41}(\bar{E}_F)\bar{t}'_5(\bar{E}_F)] \tag{1.264}$$

$$m_z^*(\bar{E}_F) = \frac{\hbar^2}{b}[1 - \bar{C}[4\bar{b}\bar{C}\bar{E}_F + 4\bar{b}^2\bar{D}^2 + \bar{C}^2 - 4\bar{b}\bar{V}\bar{C}\bar{D}]^{-1/2}] \tag{1.265}$$

where

$$\bar{t}_5(\bar{E}_F) = \left[\frac{\bar{g}_2 - 4\bar{a}\bar{C}\bar{E}}{\bar{g}_3}\right]^{1/2}$$

The electron concentration and the entropy in this case assume the forms

$$\bar{n}_0 = \frac{\bar{g}_v}{4\pi^2}[\bar{M}_1(\bar{E}_F) + \bar{N}_1(\bar{E}_F)] \tag{1.266}$$

$$\bar{S}_0 = \left[\frac{\bar{g}_v \bar{k}_B{}^2 \bar{T}}{12}\right][\bar{M}'_1(\bar{E}_F) + \bar{N}'_1(\bar{E}_F)] \tag{1.267}$$

where

$$\bar{M}_1(\bar{E}_F) = \left[2(\bar{t}_{11}\bar{E}_F + \bar{t}_{21})\sqrt{\bar{t}_{91}\bar{E}_F + \bar{t}_{81}} + \frac{\bar{t}_{31}}{3}\phi^3(\bar{E}_F) + \frac{\bar{t}_{41}}{2}\left[\phi(\bar{E}_F)\sqrt{\phi^2(\bar{E}_F) + \bar{t}_5(\bar{E}_F)}\right.\right.$$

$$\left.\left. + \frac{\bar{t}_{41}\bar{t}_5(\bar{E}_F)}{2}\left[\ln\left|\frac{\phi(\bar{E}_F) + \sqrt{\phi^2(\bar{E}_F) + \bar{t}_5(\bar{E}_F)}}{\sqrt{\bar{t}_5(\bar{E}_F)}}\right|\right]\right],$$

$$\phi(\bar{E}_F) = (\bar{t}_{31}\sqrt{2})^{-1}\left[\bar{t}_{61} + \bar{E}_F\bar{t}_{71} - [\bar{t}_{81} + \bar{t}_{91}\bar{E}_F]\right]^{1/2}$$

$$\bar{N}_1(\bar{E}_F) = \sum_{\bar{r}=1}^{\bar{s}}[\bar{L}(\bar{r})\bar{M}_1(\bar{E}_F)]$$

1.2.8 The entropy in quantum wells (QWs) of HD platinum antimonide

The dispersion relation for the n-type $PtSb_2$ can be written as [160]

$$\left[\bar{E} + \lambda_0\frac{\bar{a}^2}{4}\bar{k}^2 - \overline{lk}_s^2\frac{\bar{a}^2}{4}\right]\left[\bar{E} + \delta_0 - \bar{v}\frac{\bar{a}^2}{4}\bar{k}^2 - \bar{n}'\bar{k}_s^2\frac{\bar{a}^2}{4}\right] = \bar{I}\left(\frac{\bar{a}^4}{16}\right)\bar{k}^4 \tag{1.268}$$

The (1.268) assumes the form

$$[\bar{E}+\omega_1\bar{k}_s^2+\omega_2\bar{k}_z^2][\bar{E}+\delta_0+\omega_3\bar{k}_s^2-\omega_4\bar{k}_z^2]=\bar{I}_1(\bar{k}_s^2+\bar{k}_z^2)^2 \tag{1.269}$$

where

$$\omega_1=\left[\lambda_0\frac{\bar{a}^2}{4}+\bar{l}\frac{\bar{a}^2}{4}\right],\omega_2=\lambda_0\frac{\bar{a}^2}{4},\omega_3=\left[\bar{n}'\frac{\bar{a}^2}{4}-\bar{\nu}\frac{\bar{a}^2}{4}\right],\omega_4=\bar{\nu}\frac{\bar{a}^2}{4},\bar{I}_1=\bar{I}\left(\frac{\bar{a}^2}{4}\right)^2,$$

$\lambda_0,\bar{l},\delta_0,\bar{\nu},\bar{n}'$ and $\bar{a}$ are the band constants.

The carrier dispersion law in HD $PtSb_2$ can be written as

$$\bar{T}_{11}\bar{k}_s^4-\bar{k}_s^2[\bar{T}_{21}(\bar{E},\eta_g)-\bar{T}_{31}\bar{k}_z^2]+[\bar{T}_{41}k_z^4-\bar{T}_{51}(\bar{E},\eta_g)\bar{k}_z^2-\bar{T}_{61}(\bar{E},\eta_g)]=0 \tag{1.270}$$

Where

$$\bar{T}_{11}=(\bar{I}_1-\omega_2\omega_3),\bar{T}_{21}(\bar{E},\eta_g)=[\omega_1\delta_0+\omega_1\gamma_3(\bar{E},\eta_g)+\omega_3\gamma_3(\bar{E},\eta_g)],$$

$$\bar{T}_{31}=[2\bar{I}_1+\omega_2\omega_4-\omega_2\omega_3],\bar{T}_{41}=[2\bar{I}_1+\omega_2\omega_4],\bar{T}_{51}(\bar{E},\eta_g)=[\omega_2\gamma_0-\omega_4\gamma_3(\bar{E},\eta_g)$$
$$+\omega_2\gamma_3(\bar{E},\eta_g)],\bar{T}_{61}(\bar{E},\eta_g)=[\gamma_8(\bar{E},\eta_g)+\gamma_0\gamma_3(\bar{E},\eta_g)]$$
$$\text{and }\gamma_8(\bar{E},\eta_g)=2\theta_0(\bar{E},\eta_g)[1+Erf(\bar{E},\eta_g)]^{-1}$$

The EEMs are given by

$$\bar{m}_s^*(\bar{E}_{F_h},\eta_g)=\frac{\hbar^2}{2\bar{T}_{11}}\left[\bar{T}_{21}{}'(\bar{E}_{F_h},\eta_g)+\frac{(\bar{T}_{21}(\bar{E}_{F_h},\eta_g)\bar{T}_{21}{}'(\bar{E}_{F_h},\eta_g)+2\bar{T}_{11}\bar{T}_{61}{}'(\bar{E}_{F_h},\eta_g)}{\sqrt{\bar{T}_{21}^2(\bar{E}_{F_h},\eta_g)+4\bar{T}_{11}\bar{T}_{61}{}'(\bar{E}_{F_h},\eta_g)}}\right] \tag{1.271}$$

$$\bar{m}_z^*(\bar{E}_{F_h},\eta_g)=\left(\frac{\hbar^2}{2\bar{T}_{11}}\right)\left[\bar{T}_{51}{}'(\bar{E}_{F_h},\eta_g)+[\bar{T}_{51}{}'(\bar{E}_{F_h},\eta_g)\bar{T}_{51}{}'(\bar{E}_{F_h},\eta_g)+2\bar{T}_{51}{}'(\bar{E}_{F_h},\eta_g)]\right.$$
$$\left.[\bar{T}_{51}^2(\bar{E}_{F_h},\eta_g)+4\bar{T}_{41}\bar{T}_{51}{}'(\bar{E}_{F_h},\eta_g)]^{-1/2}\right] \tag{1.272}$$

The electron concentration assumes the form

$$\bar{n}_0=\frac{\bar{g}_\nu}{3\pi^2}\left[\bar{I}_{128}(\bar{E}_{F_h},\eta_g)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_{128}(\bar{E}_{F_h},\eta_g)]\right] \tag{1.273}$$

where

$$\bar{I}_{128}(\bar{E}_{F_h},\eta_g)=[\bar{M}_{6HD}(\bar{E}_{F_h},\eta_g)]$$

$$\bar{M}_{6HD}(\bar{E}_{F_h},\eta_g)=\left[\bar{T}_{91HD}(\bar{E}_{F_h},\eta_g)\rho_{2HD}(\bar{E}_{F_h},\eta_g)-\bar{T}_{101}\frac{\rho'_{2HD}(\bar{E}_{F_h},\eta_g)}{3}-\bar{T}_{11}\bar{J}_3(\bar{E}_{F_h},\eta_g)\right]$$

$$\bar{T}_{91HD}(\bar{E}_{F_h},\eta_g)=\frac{\bar{T}_{21}(\bar{E}_{F_h},\eta_g)}{2\bar{T}_{11}}$$

$$\rho_{2HD}(\bar{E}_{F_h},\eta_g)=\left[(2\bar{T}_{41})^{-1}\left[\bar{T}_{51}(\bar{E}_{F_h},\eta_g)+\sqrt{\bar{T}^2_{51}(\bar{E}_{F_h},\eta_g)+4\bar{T}_{41}\bar{T}_{61}(\bar{E}_{F_h},\eta_g)}\right]\right]^{1/2},$$

$$\bar{T}_{101}=[\bar{T}_{31}/2\bar{T}_{11}]$$

$$\begin{aligned}\bar{J}_3(\bar{E}_{F_h},\eta_g)=&\frac{\rho_{2HD}(\bar{E}_{F_h},\eta_g)}{3}[[\bar{A}^2_{3HD}(\bar{E}_{F_h},\eta_g)+\bar{B}^2_{3HD}(\bar{E}_{F_h},\eta_g)]\bar{E}_0(\bar{\eta}(\bar{E}_{F_h},\eta_g),\bar{t}(\bar{E}_{F_h},\eta_g))\\&-[\bar{A}^2_{3HD}(\bar{E}_{F_h},\eta_g)-\bar{B}^2_{3HD}(\bar{E}_{F_h},\eta_g)]\bar{F}_0(\eta(\bar{E}_{F_h},\eta_g),\bar{t}(\bar{E}_{F_h},\eta_g))]\\&+\frac{\rho_{2HD}(\bar{E}_{F_h},\eta_g)}{3}[(\bar{A}^2_{3HD}(\bar{E}_{F_h},\eta_g)-\rho^2_{2HD}(\bar{E}_{F_h},\eta_g))(\bar{B}^2_{3HD}(\bar{E}_{F_h},\eta_g)\\&-\rho^2_{2HD}(\bar{E}_{F_h},\eta_g))]^{1/2},\end{aligned}$$

$$\bar{E}_0(\eta(\bar{E}_{F_h},\eta_g)),\bar{t}(\bar{E}_{F_h},\eta_g)$$

and

$$\bar{F}_0\,\bar{E}_0(\eta(\bar{E}_{F_h},\eta_g)),\bar{t}(\bar{E}_{F_h},\eta_g)$$

are the incomplete elliptic integrals of second and first, respectively.

$$\bar{A}^2_{3HD}(\bar{E}_{F_h},\eta_g)=\frac{1}{2}\left[\left[\bar{T}_{12}(\bar{E}_{F_h},\eta_g)+\sqrt{\bar{T}^2_{12}(\bar{E}_{F_h},\eta_g)-4\bar{T}_{13}(\bar{E}_{F_h},\eta_g)}\right]\right],$$

$$\bar{T}_{12}(\bar{E}_{F_h},\eta_g)=[\bar{T}_7(\bar{E}_{F_h},\eta_g)/\bar{T}_{61}]$$

$$\bar{T}_{61}=[\bar{T}^2_{31}-4\bar{T}_{11}\bar{T}_{41}],\ \bar{T}_7(\bar{E}_{F_h},\eta_g)=[2\bar{T}_{31}\bar{T}_{21}(\bar{E}_{F_h},\eta_g)-4\bar{T}_{11}\bar{T}_{51}(\bar{E}_{F_h},\eta_g)]$$

$$\bar{T}_{13}(\bar{E}_{F_h},\eta_g)=(\bar{T}_8(\bar{E}_{F_h},\eta_g)/\bar{T}_8),\ \bar{T}_8(\bar{E}_{F_h},\eta_g)=[\bar{T}^2_{21}(\bar{E}_{F_h},\eta_g)+4\bar{T}_{11}\bar{T}_{61}(\bar{E}_{F_h},\eta_g)],$$

$$\bar{B}^2_{3HD}(\bar{E}_{F_h},\eta_g)=\frac{1}{2}\left[\left[\bar{T}_{12}(\bar{E}_{F_h},\eta_g)-\sqrt{\bar{T}^2_{12}(\bar{E}_{F_h},\eta_g)-4\bar{T}_{13}(\bar{E}_{F_h},\eta_g)}\right]\right],\ \bar{T}_{11}=[\sqrt{\bar{T}_{61}}/2\bar{T}_{11}]$$

$$\bar{t}(\bar{E}_{F_h},\eta_g)=[\bar{B}_3(\bar{E}_{F_h},\eta_g)/\bar{A}_3(\bar{E}_{F_h},\eta_g)],\eta(\bar{E}_{F_h},\eta_g)=\sin^{-1}\left[\frac{\rho_2(\bar{E}_{F_h},\eta_g)}{\bar{B}_3(\bar{E}_{F_h},\eta_g)}\right]$$

The $\bar{E}_{hd}$ in this case is given by the equation

$$\bar{T}_{61}(\bar{E}_{hd},\eta_g)=0 \tag{1.273b}$$

Using (1.273a), (1.273b), and (1.31f), we can study the entropy in this case.

From (1.270) the dispersion relation in QWs of HD PtSb2can be expressed as

$$\bar{T}_{11}\bar{k}_s^4 - \bar{P}_{1HD}(\bar{E},\eta_g,\bar{n}_z)\bar{k}_s^2 + \bar{P}_{2HD}(\bar{E},\eta_g,\bar{n}_z) = 0 \tag{1.274}$$

where

$$\bar{P}_{1HD}(\bar{E},\eta_g,\bar{n}_z) = [\bar{T}_{21}(\bar{E},\eta_g,\bar{n}_z) - \bar{T}_{31}(\pi\bar{n}_z/\bar{d}_z)]$$

$$\bar{P}_{2HD}(\bar{E},\eta_g,\bar{n}_z) = [\bar{T}_{41}(\pi\bar{n}_z/\bar{d}_z)^4 - \bar{T}_{51}(\bar{E}_{F_h},\eta_g)(\pi\bar{n}_z/\bar{d}_z)^2 - \bar{T}_{61}(\bar{E}_{F_h},\eta_g)]$$

(1.274) can be written as

$$\bar{k}_s^2 = \bar{A}_{60}\ (\bar{E}_{F_h},\eta_g,\bar{n}_z) \tag{1.275}$$

where

$$\bar{A}_{60}(\bar{E}_{F_h},\eta_g,\bar{n}_z) = \left[\bar{P}_{1HD}(\bar{E}_{F_h},\eta_g,\bar{n}_z) - \sqrt{\bar{P}_{1HD}^2(\bar{E}_{F_h},\eta_g,\bar{n}_z) - 4\bar{T}_{11}\bar{P}_{2HD}(\bar{E}_{F_h},\eta_g,\bar{n}_z)}\right]$$

The EEM assumes the form

$$\bar{m}^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \frac{\hbar^2}{2}\bar{A}'_{60}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) \tag{1.276}$$

The surface electron concentration is given by

$$\bar{n}_{2D} = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) + \bar{B}_{60}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)] \tag{1.277}$$

where

$$\bar{B}_{60}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{A}_{60}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)]$$

Thus by using (1.277) and (1.31f) we can study the entropy in this case.

From (1.269), we can write the expression of the 2D dispersion law in QWs of n-$PtSb_2$ in the absence of band tails as

$$\bar{k}_s^2 = \bar{t}_{44}(\bar{E},\bar{n}_z) \tag{1.278}$$

where

$$\bar{t}_{44}(\bar{E},\bar{n}_z) = [2\bar{A}_9]^{-1}[-\bar{A}_{10}(\bar{E},\bar{n}_z) + \sqrt{\bar{A}_{10}^2(\bar{E},\bar{n}_z) + 4\bar{A}_9\bar{A}_{11}(\bar{E},\bar{n}_z)}],$$

$$\bar{A}_9 \equiv [\bar{I}_1 + \omega_1\omega_3], \bar{A}_{10}(\bar{E}, \bar{n}_z) \equiv \left[\omega_3\bar{E} + \omega_1\left\{\bar{E} + \delta_0 - \omega_4\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right\} + \omega_2\omega_3\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + 2\bar{I}_1\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right],$$

and

$$\bar{A}_{11}(\bar{E}, \bar{n}_z) \equiv \left[\bar{E}\left[\bar{E} + \delta_0 - \omega_4\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right] + \omega_2\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\left[\bar{E} + \delta_0 - \omega\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right] - \bar{I}_1\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^4\right]$$

The area of k_s space can be expressed as

$$\bar{A}(\bar{E}, \bar{n}_z) = \pi\bar{t}_{44}(\bar{E}, \bar{n}_z) \tag{1.279}$$

The total DOS function assumes the form

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{t}'_{44}(\bar{E}, \bar{n}_z)]H(\bar{E} - \bar{E}_{n_{z_{14}}}) \tag{1.280}$$

where the quantized levels $(\bar{E}_{n_{z_{14}}})$ can be expressed through the equation

$$\bar{E}_{n_{z_{14}}} = (2)^{-1}\left[-\left[\bar{\omega}_2\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + \delta_0 - \omega_4\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right] + \left\{\left[\omega_2\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + \delta_0 - \omega_4\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]^2 + 4\left[\bar{I}_1\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^4 + \omega_2\omega_4\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^4 - \omega_2\delta_0\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]\right\}^{1/2}\right] \tag{1.281a}$$

Using (1.278), the EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{F_S}, \bar{n}_z) = \frac{\hbar^2}{2}\overline{t}'_{44}(\bar{E}_{F_S}, \bar{n}_z) \tag{1.281b}$$

The electron statistics can be written as

$$\bar{n}_{2D} = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{t}_{44}(\bar{E}_{Fs}, \bar{n}_z) + \bar{t}_{45}(\bar{E}_{Fs}, \bar{n}_z)] \tag{1.282}$$

where

$$\bar{t}_{45}(\bar{E}_{Fs}, \bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{S}}\bar{L}(\bar{r})[\bar{t}_{44}(\bar{E}_{Fs}, \bar{n}_z) + \bar{t}_{45}(\bar{E}_{Fs}, \bar{n}_z)]$$

The entropyin this case is given by

$$\bar{S}_0 = \left[\frac{\bar{g}_v \pi \bar{k}_B{}^2 \bar{T}}{6}\right]\left[\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{t}'_{44}(\bar{E}_{Fs}, \bar{n}_z) + \bar{t}'_{45}(\bar{E}_{Fs}, \bar{n}_z)]\right] \tag{1.283}$$

1.2.9 The entropy in quantum wells (QWs) of HD bismuth telluride

The dispersion relation of the conduction electrons in Bi_2Te_3 can be written as [161]

$$\bar{E}(1+\alpha\bar{E}) = \omega_1\bar{k}_x^2 + \omega_2\bar{k}_y^2 + \omega_3\bar{k}_z^2 + 2\omega_4\bar{k}_z\bar{k}_y \tag{1.284}$$

where

$$\omega_1 = \frac{\hbar^2}{2\bar{m}_0}\alpha_{11}, \omega_2 = \frac{\hbar^2}{2\bar{m}_0}\alpha_{22}, \omega_3 = \frac{\hbar^2}{2\bar{m}_0}\alpha_{33}, \omega_4 = \frac{\hbar^2}{2\bar{m}_0}\alpha_{23},$$

in which $\bar{\alpha}_{11}, \bar{\alpha}_{22}, \bar{\alpha}_{33}$ and $\bar{\alpha}_{23}$ are system constants.

The dispersion relation in HD Bi_2Te_3 assumes the form

$$\gamma_2(\bar{E}, \eta_g) = \omega_1\bar{k}_x^2 + \omega_2\bar{k}_y^2 + \omega_3\bar{k}_z^2 + 2\omega_4\bar{k}_z\bar{k}_y \tag{1.285}$$

The EEMs can, respectively, be expressed as

$$\bar{m}_x^*(\bar{E}_{F_h}, \eta_g) = \frac{\hbar^2}{2\bar{w}_1}\gamma_2(\bar{E}_{F_h}, \eta_g) \tag{1.286}$$

$$\bar{m}_y^*(\bar{E}_{F_h}, \eta_g) = \frac{\hbar^2}{2\bar{w}_2}\gamma_2(\bar{E}_{F_h}, \eta_g) \tag{1.287}$$

$$\bar{m}_z^*(\bar{E}_{F_h}, \eta_g) = \frac{\hbar^2}{2\bar{w}_3}\gamma(\bar{E}_{F_h}, \eta_g) \tag{1.288}$$

The DOS function in this case is given by

$$\bar{N}(\bar{E}) = 4\pi\bar{g}_v\left(\frac{2\bar{m}_0}{h^2}\right)^{3/2}\frac{\sqrt{\gamma_2(\bar{E}, \eta_g)}\gamma'_2(\bar{E}, \eta_g)}{\sqrt{\alpha_{11}\alpha_{22}\alpha_{33} - 4\alpha_{11}\alpha_{23}^2}} \tag{1.289}$$

Thus combining (1.289) with the Fermi–Dirac occupation probability factor, the electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_0}{\hbar^2}\right)^{3/2}(\alpha_{11}\alpha_{22}\alpha_{33} - 4\alpha_{11}\alpha_{23}^2)^{-1/2}[\bar{U}_{1HD}(\bar{E}_{F_h}, \eta_g) + \bar{U}_{2HD}(\bar{E}_{F_h}, \eta_g)] \tag{1.290a}$$

where

$$\bar{U}_{1HD}(\bar{E}_{F_h}, \eta_g) = [\gamma_2(\bar{E}_{F_h}, \eta_g)]^{3/2}, \bar{U}_{2HD}(\bar{E}_{F_h}, \eta_g) = \sum_{r=1}^{s} \bar{L}(\bar{r})[\bar{U}_{1HD}(\bar{E}_{F_h}, \eta_g)]$$

The $\bar{E}_{hd}$ in this case is given by the equation

$$\gamma_2(\bar{E}_{hd}, \eta_g) = 0 \tag{1.290b}$$

Using (1.290a), (1.290b), and (1.31f), we can study the entropy in this case.

The dispersion relation in QWs of HD Bi_2Te_3 can be expressed as

$$\gamma_2(\bar{E}, \eta_g) = \omega_1\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \omega_2\bar{k}_y^2 + \omega_3\bar{k}_z^2 + 2\omega_4\bar{k}_z\bar{k}_y \tag{1.291}$$

The EEM can be expressed as

$$\bar{m}^*(\bar{E}_{F1HD}, \eta_g) = \frac{\bar{m}_0}{\sqrt{\alpha_1\alpha_{33} - 4\alpha_{23}^2}}\gamma'_2(\bar{E}_{F1HD}, \eta_g) \tag{1.292}$$

The surface electron concentration can be written as

$$\bar{n}_{2D} = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{R}_{60}(\bar{E}_{F1HD}, \eta_g, \bar{n}_x) + \bar{R}_{61}(\bar{E}_{F1HD}, \eta_g, \bar{n}_x)] \tag{1.293}$$

$$\bar{R}_{60}(\bar{E}_{F1HD}, \eta_g, \bar{n}_x) = \frac{1}{\sqrt{\bar{a}_{11}\bar{a}_{33} - 4\bar{a}_{23}^2}}\left[\frac{2\bar{m}_0\gamma'_2(\bar{E}_{F1HD}, \eta_g)}{\hbar^2} - \frac{2\bar{m}_0}{\hbar^2}\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2\bar{\alpha}_{11}\right]$$

and

$$\bar{R}_{61}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{R}_{60}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)]$$

Using (1.293) and (1.31f) we can study the entropy in this case.

The 2D electron dispersion law in QWs of Bi_2Te_3 in the absence of band tails assumes the form

$$\bar{E}(1 + \alpha\bar{E}) = \omega_1\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \omega_2\bar{k}_y^2 + \omega_3\bar{k}_z^2 + 2\omega_4\bar{k}_z\bar{k}_y \tag{1.294}$$

The area of the ellipse is given by

$$\bar{A}_n(\bar{E}, \bar{n}_x) = \frac{\pi}{\sqrt{\bar{\alpha}_{22}\bar{\alpha}_{23} - 4\bar{\alpha}_{23}}}\left[\frac{2\bar{m}_0\bar{E}(1 + \bar{\alpha}\bar{E})}{\hbar^2} - \bar{\omega}_1\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2\right] \tag{1.295}$$

The total DOS function assumes the form

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{g}_v \bar{m}_0}{\pi\hbar^2\sqrt{\bar{\alpha}_{22}\bar{\alpha}_{33} - 4\bar{\alpha}_{23}^2}} \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} (1 + 2\alpha\bar{E})\bar{H}(\bar{E} - \bar{E}_{n_{z_{15}}}) \tag{1.296}$$

where $(\bar{E}_{n_{z_{15}}})$ can be expressed through the equation

$$\bar{E}_{n_{z_{15}}}(1 + \alpha\bar{E}_{n_{z_{15}}}) = \omega_1\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 \tag{1.297a}$$

The EEM in this case assumes the form as

$$\bar{m}^*(\bar{E}_{F_s}) = \frac{\bar{m}_0(1 + 2\alpha(\bar{E}_{F_s}))}{\sqrt{\alpha_{22}\alpha_{33} - 4\alpha^2{}_{23}}} \tag{1.297b}$$

The electron concentration can be written as

$$\bar{n}_{2D} = \left(\frac{\bar{m}_0\bar{g}_v}{\sqrt{\alpha_{22}\alpha_{33} - 4\alpha_{23}^2}}\right) \sum_{n_z=1}^{n_{z\max}} [(1 + 2\alpha\bar{E}_{n_{z_{15}}})\bar{F}_o(\eta_{n_{15}}) + 2\alpha\bar{k}_B\bar{T}F_1(\eta_{n_{15}})] \tag{1.298}$$

where

$$\eta_{n_{15}} = \frac{\bar{E}_{Fs} - \bar{E}_{n_{z15}}}{\bar{k}_B\bar{T}}$$

Using (1.298) the entropy in this case is given by

$$\bar{S}_0 = \left(\frac{\bar{m}_0}{\sqrt{\alpha_{22}\alpha_{33} - 4\alpha_{23}^2}}\right)\left[\frac{\bar{g}_v\pi^2\bar{k}^2{}_B\bar{T}}{3}\right]\left[\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [(1 + 2\alpha\bar{E}_{n_{z15}})\vec{F}_{-1}(\eta_{n_{z15}}) + 2\alpha\bar{k}_B\bar{T}F_0(\eta_{n_{z15}})\,]\right] \tag{1.299}$$

1.2.10 The entropy in quantum wells (QWs) of HD germanium

It is well known that the conduction electrons of n-Ge obey two different types of dispersion laws since band nonparabolicity has been included in two different ways as given in the literature [162, 163].

(a) The energy spectrum of the conduction electrons in bulk specimens of n-Ge can be expressed in accordance with Cardona et al. [162] as

$$\bar{E} = \frac{\bar{E}_{g_0}}{2} + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{||}^*} + \left[\left(\frac{\bar{E}_{g_0}^2}{2}\right) + \bar{E}_{g_0}\bar{k}_z^2\left(\frac{\hbar^2}{2\bar{m}_{\perp}^*}\right)\right]^{1/2} \tag{1.300}$$

where in this case $m_{\|}^{*}$ and $m_{\perp}^{*}$ are the longitudinal and transverse effective masses along <111> direction at the edge of the conduction band, respectively

The (1.300) can be written as

$$\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\|}^{*}} = \bar{E}(1+\alpha\bar{E}) + \alpha\left(\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{\|}^{*}}\right) - (1+2\alpha\bar{E})\left(\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{\|}^{*}}\right) \tag{1.301}$$

The dispersion relation under the condition of heavy doping can be expressed from (1.301) as

$$\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^{*}} = \gamma_2(\bar{E},\eta_g) + \alpha\left(\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{\|}^{*}}\right) - (1+2\alpha\bar{E}\gamma_3(\bar{E},\eta_g))\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{\|}^{*}} \tag{1.302}$$

The EEMs can be written as

$$\bar{m}^{*}(\bar{E}_{Fh},\eta_g) = \bar{m}_{\perp}^{*}\gamma'_2(\bar{E}_{Fh},\eta_g) \tag{1.303}$$

and

$$\bar{m}^{*}(\bar{E}_F,\eta_g) = \bar{m}_{\|}^{*}\gamma'_3(\bar{E}_F,\eta_g) - \frac{\gamma'_3(\bar{E}_F,\eta_g)\ [1+2\alpha\gamma_3(\bar{E}_F,\eta_g)] - \gamma'_2(\bar{E}_F,\eta_g)}{\sqrt{[1+2\alpha\gamma_3(\bar{E}_F,\eta_g)]^2 - 4\alpha\gamma_2(\bar{E}_F,\eta_g)}} \tag{1.304}$$

The electron concentration can be written as

$$\bar{N}_0 = \frac{8\pi\bar{g}_v\bar{m}_{\perp}^{*}\sqrt{2\bar{m}_{\|}^{*}}}{\bar{h}^3}\left[\bar{I}_{129}(\bar{E}_{F_h},\eta_g) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_{129}(\bar{E}_{F_h},\eta_g)]\right] \tag{1.305a}$$

where

$$\bar{I}_{129}(\bar{E}_{F_h},\eta_g) = [\bar{M}_{8HD}(\bar{E}_{F_h},\eta_g)],$$

$$\bar{M}_{8HD}(\bar{E}_{F_h},\eta_g) = \left[\gamma_3(\bar{E}_{F_h},\eta_g)^{1/2}\left[\gamma_2(\bar{E}_{F_h},\eta_g) + \frac{\alpha}{5}\gamma_3^2(\bar{E}_{F_h},\eta_g)\right] - \frac{\gamma_3(\bar{E}_{F_h},\eta_g)}{3}[1+2\alpha\gamma_3(\bar{E}_{F_h},\eta_g)]\right]$$

The $\bar{E}_{hd}$ in this case is given by the equation

$$\gamma_2(\bar{E}_{hd},\eta_g) = 0 \tag{1.305b}$$

Thus by using (1.305a), (1.305b) and (1.31f), we can study the entropy in this case.

In the presence of size quantization, the dispersion law in QW of HD Ge can be written following (1.302) as

$$\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^{*}} = \gamma_2(\bar{E},\eta_g) + \alpha\left(\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_{\|}^{*}}\right)^2 - (1+2\alpha\gamma_3(\bar{E},\eta_g))\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_{\|}^{*}} \tag{1.306a}$$

The EEM assumes the form

$$\bar{m}^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\bar{m}^*_{\perp}\left[\gamma'_2(\bar{E}_{F1HD},\eta_g)-\frac{\alpha\hbar^2}{\bar{m}^*_{||}}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\gamma_3(\bar{E}_{F_h},\eta_g)\right] \tag{1.306b}$$

The surface electron concentration per unit area is given by

$$\bar{N}_{2D}=\frac{\bar{g}_v\bar{m}^*_{\perp}}{\pi\hbar^2}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}[\bar{R}_1(\bar{E}_{F1HD},\eta_g,\bar{n}_z)+\bar{S}_1(\bar{E}_{F1HD},\eta_g,\bar{n}_z)] \tag{1.307}$$

where

$$\bar{R}_1(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\left[\gamma_2(\bar{E}_{F1HD},\eta_g)+\bar{\alpha}\left(\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{||}}\right)^2-(1+2\bar{\alpha}\gamma_3(\bar{E}_{F1HD},\eta_g))\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{||}}\right]$$

and

$$\bar{S}_1(\bar{E}_{F1HD},\eta_g,\bar{n}_z)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{R}_1(\bar{E}_{F1HD},\eta_g,\bar{n}_z)]$$

Thus using (1.307) and (1.31f) we can study the entropyin this case.

In the presence of size quantization along k_z direction, the 2D dispersion relation of the conduction relations in QWs of n-Ge in the absence of band tails can be written by extending the method as given in [158] as

$$\frac{\hbar^2\bar{k}_x^2}{2\bar{m}^*_1}+\frac{\hbar^2\bar{k}_y^2}{2\bar{m}^*_2}=\gamma(\bar{E},\bar{n}_z) \tag{1.308}$$

where,

$$m^*_1=m^*_{\perp}$$

$$\bar{m}^*_2=\frac{\bar{m}^*_{\perp}}{3},\ \gamma(\bar{E},\bar{n}_z)\equiv\left[\bar{E}(1+\alpha\bar{E})-(1+2\alpha\bar{E})\frac{\hbar^2}{2\bar{m}^*_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\alpha\left[\frac{\hbar^2}{2\bar{m}^*_3}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]^2\right]$$

and

$$\bar{m}^*_3=\frac{3\bar{m}^*_{||}\bar{m}^*_{\perp}}{2\bar{m}^*_{||}+\bar{m}^*_{\perp}}$$

The area of ellipse of the 2D surface as given by (1.308) can be written as

$$\bar{A}(\bar{E},\bar{n}_z)=\frac{2\pi\sqrt{\bar{m}_1^*\bar{m}_2^*}}{\hbar^2}\gamma(\bar{E},\bar{n}_z) \tag{1.309a}$$

The EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{Fs},\bar{n}_z)=\left(\sqrt{\bar{m}_1^*\bar{m}_2^*}\right)[\gamma(\bar{E}_{Fs},\bar{n}_z)]' \tag{1.309b}$$

The DOS function per sub-band can be expressed as

$$\bar{n}_{2D}=\frac{4\sqrt{\bar{m}_1^*\bar{m}_2^*}}{\pi\hbar^2}\left[1+2\alpha\bar{E}-2\alpha\left(\frac{\hbar^2}{2\bar{m}_3^*}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right)\right] \tag{1.310}$$

The total DOS function is given by

$$\bar{N}_{2D}(\bar{E})=\frac{4}{\pi\hbar^2}\sqrt{\bar{m}_1^*\bar{m}_2^*}\left[1+2\alpha\bar{E}-2\alpha\left(\frac{\hbar^2}{2\bar{m}_3^*}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right)\right]\bar{H}(\bar{E}-\bar{E}_{n_{z16}}) \tag{1.311}$$

where $\bar{E}_{n_{z16}}$ is the positive root of the following equation

$$\bar{E}_{n_{z16}}(1+\bar{E}_{n_{z16}})-(1+2\alpha\bar{E}_{n_{z16}})\left(\frac{\hbar^2}{2\bar{m}_3^*}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right)+\alpha\left(\frac{\hbar^2}{2\bar{m}_3^*}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right)^2=0 \tag{1.312}$$

Thus combining (1.311) with the Fermi–Dirac occupation probability factor, the 2D electron statistics in this case can be written as

$$\bar{n}_{2D}=\frac{4\sqrt{\bar{m}_1^*\bar{m}_2^*}k_B\bar{T}}{\pi\hbar^2}\times\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[(\bar{A}_1(\bar{n}_z)+1+2\alpha\eta_{n_{z16}})\bar{F}_0(\eta_{n_{16}})2\alpha\bar{k}_B\bar{T}\bar{F}_1(\eta_{n_{z16}})] \tag{1.313}$$

where

$$\bar{A}_1(\bar{n}_z)\equiv\left[1+2\bar{\alpha}\left(\frac{\hbar^2}{2\bar{m}_3^*}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right)\right]$$

and

$$\eta_{n_{z16}}=\frac{1}{\bar{k}_B\bar{T}}[\bar{E}_{F2D}-\bar{E}_{n_{z16}}]$$

The entropy in this case is given by

$$\bar{S}_0=\left[\frac{4\pi\sqrt{\bar{m}_1^*\bar{m}_2^*}\bar{k}^2{}_B\bar{T}}{3\hbar^2}\right]\left[\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[(\bar{A}_1(\bar{n}_z)+2\alpha\bar{E}_{n_{z16}})\bar{F}_{-1}(\eta_{n_{z16}})+2\alpha\bar{k}_B\bar{T}\bar{F}_0(\eta_{n_{z16}})]\right] \tag{1.314}$$

The expressions of EEMs' in bulk specimens of Ge in the absence of band tails can be written following (1.301)

$$\bar{m}^*(\bar{E}_F) = \bar{m}^*_{||} \tag{1.315}$$

$$\bar{m}^*(\bar{E}_F) = \bar{m}^*_{\perp}(1 + 2\alpha\bar{E}_F) \tag{1.316}$$

The DOS function for bulk specimens of Ge in the absence of band tails can be written following (1.301) as

$$\bar{N}(\bar{E}) = 4\pi\bar{g}_v\left(\frac{2\bar{m}^*_D}{\hbar^2}\right)^{3/2}\left[\bar{E}^{\frac{1}{2}} - \frac{5}{6}\alpha\bar{E}^{3/2} + \frac{18\bar{\alpha}}{5}\left(\frac{\bar{m}^*_{11}}{\hbar^2}\right)^2\bar{E}^{\frac{1}{2}}\right];\ \bar{m}_D = (\bar{m}^{*2}_{\perp}\bar{m}^*_{||})^{1/3} \tag{1.317}$$

Using (1.317), the electron concentration in bulk specimens of Ge can be written as

$$\bar{n}_0 = \bar{N}_{c1}\left[\bar{F}_{\frac{1}{2}}(\eta) - \frac{5}{4}\alpha\bar{k}_B\bar{T}\bar{F}_{\frac{3}{2}}(\eta) + \frac{189}{4}\alpha\bar{k}_B\bar{T}\left(\frac{\bar{m}^*_{11}\bar{k}_B\bar{T}}{\hbar^2}\right)^2\bar{F}_{\frac{7}{2}}(\eta)\right];\ \bar{N}_{c1} = 2\bar{g}_v\left(\frac{2\pi\bar{m}^*_D\bar{k}_B\bar{T}}{\bar{h}^2}\right)^{3/2} \tag{1.318}$$

The use of (1.318) leads to the expression of entropy in this case as

$$\bar{S}_0 = \left[\frac{\bar{N}_{c1}\pi^2\bar{k}_B}{3}\right]\left[\bar{F}_{\frac{1}{2}}(\eta) - \frac{5}{4}\alpha\bar{k}_B\bar{T}\bar{F}_{\frac{3}{2}}(\eta) + \frac{189}{4}\alpha\bar{k}_B\bar{T}\left(\frac{\bar{m}^*_{||}\bar{k}_B\bar{T}}{\hbar^2}\right)^2\bar{F}_{\frac{7}{2}}(\eta)\right] \tag{1.319}$$

(b) The dispersion relation of the conduction electron in bulk specimens of n-Ge can be expressed in accordance with the model of Wang and Ressler [163] can be written as

$$\bar{E} = \frac{\hbar^2\bar{k}^2_z}{2\bar{m}^*_{||}} + \frac{\hbar^2\bar{k}^2_s}{2\bar{m}^*_{\perp}} - \alpha_4\left(\frac{\hbar^2\bar{k}^2_s}{2\bar{m}^*_{\perp}}\right) - \alpha_5\left(\frac{\hbar^2\bar{k}^2_s}{2\bar{m}^*_{\perp}}\right)\left(\frac{\hbar^2\bar{k}^2_z}{2\bar{m}^*_{||}}\right) - \alpha_6\left(\frac{\hbar^2\bar{k}^2_z}{2\bar{m}^*_{||}}\right) \tag{1.320}$$

where

$$\alpha_4 = \bar{\beta}_4\left(\frac{2\bar{m}^*_{\perp}}{\hbar^2}\right), \bar{\beta}_4 = 1.4\bar{\beta}_5,$$

$$\bar{\beta}_5 = \frac{\alpha\hbar^4}{4}[(\bar{m}^*_{\perp})^{-1} - (\bar{m}_0)^{-1}]^2, \alpha_5 = \bar{\alpha}_7\left(\frac{4\bar{m}^*_{\perp}\bar{m}^*||}{\hbar^4}\right), \alpha_7 = 0.8\bar{\beta}_5$$

and

$$\alpha = (0.005\bar{\beta}_5)\left(\frac{2\bar{m}^*_{||}}{\hbar^2}\right)^2$$

The energy spectrum under the condition of heavy doping can be written as

$$\gamma_3(\bar{E},\eta_g)=\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{\|}^*}+\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^*}-\alpha_4\left(\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^*}\right)-\bar{\alpha}_5\left(\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^*}\right)\left(\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{\|}^*}\right)-\alpha_6\left(\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{\|}^*}\right)^2 \tag{1.321a}$$

The (1.321) can be expressed as

$$\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_{\perp}^*}=\alpha_8-\alpha_9\bar{k}_z^2-\alpha_{10}[\bar{k}_z^4+\alpha_{11}\bar{k}_z^2+\alpha_{12}(\bar{E},\eta_g) \tag{1.321b}$$

where

$$\alpha_8=\frac{1}{2\bar{\alpha}_4},\alpha_9=\frac{\alpha_5}{2\alpha_4}\left(\frac{\hbar^2}{2\bar{m}_{\|}^*}\right),\alpha_{10}=\frac{1}{2\alpha_4}\left(\frac{\hbar^2}{2\bar{m}_{\|}^*}\right)\sqrt{\alpha_5^2-4\alpha_4\alpha_6},\alpha_{11}=\frac{2\bar{m}_{\|}^*}{\hbar^2}\left[\frac{4\bar{\alpha}_4-2\bar{\alpha}_5}{\alpha_5^2-4\alpha_4\alpha_6}\right]$$

and

$$\alpha_{12}(\bar{E},\eta_g)=\left(\frac{2\bar{m}_{\|}^*}{\hbar^2}\right)\left[\frac{(1-4\alpha_4\gamma_3(\bar{E},\eta_g)}{\alpha_5^2-4\alpha_4\alpha_6}\right]$$

The EEMs' can be written as

$$m_z^2(\bar{E}_{Fh},\eta_g)=\left(\frac{2\bar{m}_{\|}^*}{\hbar^2}\right)\left[\frac{\bar{m}_{\|}^*\gamma_3(\bar{E}_{Fh},\eta_g)}{1-4\alpha_4\gamma_3(\bar{E}_{Fh},\eta_g)}\right] \tag{1.322}$$

$$m_{\perp}^2(\bar{E}_{Fh},\eta_g)=\left(\frac{2\bar{m}_{\|}^*}{\hbar^2}\right)\left[\frac{m_{\perp}^2\gamma_3(\bar{E}_{Fh},\eta_g)}{1-4\alpha_4\gamma_3(\bar{E}_{Fh},\eta_g)}\right] \tag{1.323}$$

The electron concentration in HD Ge in accordance with the model of Wang and Ressler can be expressed as

$$\bar{n}_0=\frac{\bar{m}_{\perp}^2\bar{g}_v}{\pi^2\hbar^2}\left[\bar{I}_3(\bar{E}_{Fh},\eta_s)+\bar{I}_4(\bar{E}_{Fh},\eta_s)\right] \tag{1.324}$$

where

$$\bar{I}_3(\bar{E}_{Fh},\eta_s)[\alpha_8\rho_{10}(\bar{E}_{Fh},\eta_s)-\frac{\alpha_9}{3}\rho_{10}^3(\bar{E}_{Fh},\eta_s)\alpha_{10}\bar{J}_{10}(\bar{E}_{Fh},\eta_s)]$$

$$\rho_{10}(\bar{E}_{Fh},\eta_s)=\frac{1}{\hbar}\left[\frac{\bar{m}_{\|}^2}{\alpha_6}\right]^{\frac{1}{2}}\left[1-\sqrt{1-4\alpha_6\gamma_3(\bar{E}_{Fh},\eta_s)}\right]^{\frac{1}{2}}$$

$$\bar{J}_{10}(\bar{E}_{Fh},\eta_g)=\frac{\bar{A}_1^2(\bar{E}_{Fh},\eta_g)}{3}[-\bar{E}_0(\lambda(\bar{E}_{Fh},\eta_g),\bar{q}(\bar{E}_{Fh},\eta_g))$$
$$[\bar{A}_1^2(\bar{E}_{Fh},\eta_g)+\bar{B}_1^2(\bar{E}_{Fh},\eta_g)]+2\bar{B}_1^2(\bar{E}_{Fh},\eta_g)\bar{F}_0(\lambda(\bar{E}_{Fh},\eta_g),\bar{q}(\bar{E}_{Fh},\eta_g))]$$
$$+\frac{\bar{A}_1^2(\bar{E}_{Fh},\eta_g)}{3}[\rho_{10}(\bar{E}_{Fh},\eta_s)+\bar{A}_1^2(\bar{E}_{Fh},\eta_g)+2\bar{B}_1^2(\bar{E}_{Fh},\eta_g)]\left[\frac{\bar{A}_1^2(\bar{E}_{Fh},\eta_g)+\rho_{10}^2(\bar{E}_{Fh},\eta_s)}{\bar{B}_1^2(\bar{E}_{Fh},\eta_g)+\rho_{10}^2(\bar{E}_{Fh},\eta_s)}\right]$$

$$\bar{A}_1^2(\bar{E}_{Fh},\eta_g)=\frac{1}{2}\left[\alpha_{11}+\sqrt{\alpha_{11}^2-4\alpha_{12}^2(\bar{E}_{Fh},\eta_g)}\right],\bar{B}_1^2(\bar{E}_{Fh},\eta_g)=\frac{1}{2}\left[\alpha_{11}+\sqrt{\alpha_{11}^2-4\alpha_{12}^2(\bar{E}_{Fh},\eta_g)}\right]$$

$$\lambda(\bar{E}_{Fh},\eta_g)=\tan^{-1}\left[\frac{\rho_{10}(\bar{E}_{Fh},\eta_g)}{\bar{B}_1(\bar{E}_{Fh},\eta_g)}\right],\bar{q}(\bar{E}_{Fh},\eta_g)=\left[\left[\frac{\bar{A}_1^2(\bar{E}_{Fh},\eta_g)-\bar{B}_1^2(\bar{E}_{Fh},\eta_g)}{\bar{A}_1^2(\bar{E}_{Fh},\eta_g)}\right]\right.$$

and

$$\bar{I}_4(\bar{E}_{Fh},\eta_g)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{I}_3(\bar{E}_{Fh},\eta_g)]$$

The $\bar{E}_{hd}$ in this case is given by the equation

$$\gamma_2(\bar{E}_{hd},\eta_g) \tag{1.324b}$$

Thus using (1.324a), (1.324b), and (1.31f) we can study the entropy in this case.

The dispersion relation in QW of HD Ge can be written as

$$\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^*}=\alpha_8-\alpha_9\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-\alpha_{10}\left[\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^4+\alpha_{11}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\alpha_{12}(\bar{E},\eta_g)\right]^{1/2} \tag{1.325}$$

The (1.325) can be expressed as

$$\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^*}=\bar{A}_{15}(\bar{E},\eta_g,\bar{n}_z) \tag{1.326}$$

where

$$\bar{A}_{15}(\bar{E},\eta_g,\bar{n}_z)=\left[\alpha_8-\alpha_9\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2-\alpha_{10}\left[\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^4+\alpha_{11}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2+\alpha_{12}(\bar{E},\eta_g)\right]^{1/2}\right]$$

The EEM is given by

$$\bar{m}_s^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\bar{m}_\perp^*=\bar{A}'_{75}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) \tag{1.327}$$

The electron concentration per unit area assumes the form

$$\bar{n}_{2D} = \frac{\bar{m}_{\perp}^{*} g_v}{\pi\hbar^2} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{A}_{75}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) + \bar{A}_{76}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)] \tag{1.328}$$

where

$$\bar{A}_{76}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{A}_{75}(\bar{E}_{F1HD}, \eta_g, \bar{n}_z)]$$

Using (1.328) and (1.31f) we can study the entropy in this case

The 2D dispersion law in the absence of band tails can be expressed as

$$\bar{E} = \bar{A}_5(\bar{n}_z) + \bar{A}_6(\bar{n}_z)\beta - \alpha_4\beta^2 \tag{1.329}$$

where

$$\bar{A}_5(\bar{n}_z) = \frac{\hbar^2}{2\bar{m}_3^{*}}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\left[1-\alpha_6\left(\frac{\hbar^2}{2\bar{m}_3^{*}}\right)\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right], \bar{A}_6(\bar{n}_z) = \left[1-\alpha_5\left(\frac{\hbar^2}{2\bar{m}_3^{*}}\right)\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]$$

and

$$\beta = \frac{\hbar^2\bar{k}_x^2}{2\bar{m}_1^{*}} + \frac{\hbar^2\bar{k}_y^2}{2\bar{m}_2^{*}}$$

The (1.329) can be written as

$$\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_1^{*}} + \frac{\hbar^2\bar{k}_y^2}{2\bar{m}_2^{*}} = \bar{I}_1(\bar{E}, \bar{n}_z) \tag{1.330}$$

where

$$\bar{I}_1(\bar{E}, \bar{n}_z) = (2\alpha_4)^{-1}\left[\bar{A}_6(\bar{n}_z) - \bar{A}_6^2(\bar{n}_z) - 4\alpha_4\bar{E} + 4\alpha_4\bar{A}_5(\bar{n}_z)\right]^{1/2}\Big]$$

From (1.330), the area of the 2D k_s -space is given by

$$\bar{A}_6(\bar{E}, \bar{n}_z) = \frac{2\pi\sqrt{\bar{m}_1^{*}\bar{m}_2^{*}}}{\hbar^2}\bar{I}_1(\bar{E}, \bar{n}_z) \tag{1.331a}$$

Using (1.331a) in this case can be expressed as

$$\bar{m}^{*}(\bar{E}_{F_s}, \bar{n}_z) = \left(\sqrt{\bar{m}_1^{*}\bar{m}_2^{*}}\right)\left[\bar{I}_1(\bar{E}_{F_s}, \bar{n}_z)\right]' \tag{1.331b}$$

The DOS function per sub-band can be written as

$$\bar{N}_{2D}(\bar{E}) = \frac{4}{\pi}\frac{\sqrt{\bar{m}_1^{*}\bar{m}_2^{*}}}{\hbar^2}\{\bar{I}_1(\bar{E}, \bar{n}_z)\}' \tag{1.332}$$

where, $\{\bar{I}_1(\bar{E},\bar{n}_z)\}' = \dfrac{\partial}{\partial \bar{E}}[\bar{I}_1(\bar{E},\bar{n}_z)]$

The total DOS function assumes the form

$$\bar{N}_{2DT}(\bar{E}) = \frac{4\sqrt{\bar{m}_1^*\bar{m}_2^*}}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\{\bar{I}_1(\bar{E},\bar{n}_z)\}' H(E - E_{n_{z17}}) \tag{1.333}$$

where the sub-band energy $(E_{n_{z17}})$ are given by

$$\bar{E}_{n_{z17}} = \left(\frac{\hbar^2}{2\bar{m}_3^*}\right)\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\left[1-\alpha_6\left(\frac{\hbar^2}{2\bar{m}_3^*}\right)\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right] \tag{1.334}$$

The electron statistics can be written as

$$\bar{n}_{2D} = \frac{4\sqrt{\bar{m}_1^*\bar{m}_2^*}}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{t}_{46}(\bar{E}_{Fs},\bar{n}_z)+\bar{t}_{47}(\bar{E}_{Fs},\bar{n}_z)] \tag{1.335}$$

where

$$\bar{t}_{46}(\bar{E}_{Fs},\bar{n}_z) = \bar{I}_1(\bar{E}_{Fs},\bar{n}_z), \bar{t}_{47}(\bar{E}_{Fs},\bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})([\bar{t}_{46}(\bar{E}_{Fs},\bar{n}_z))$$

Using (1.335), the entropy in this case is given by

$$\bar{S}_0 = 4\sqrt{\bar{m}_1^*\bar{m}_2^*}\left[\frac{\pi^2\bar{k}_B^2\bar{T}}{3\pi\hbar^2}\right]\left[\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{t}'_{47}(\bar{E}_{Fs},\bar{n}_z)+\bar{t}'_{48}(\bar{E}_{Fs},\bar{n}_z)]\right] \tag{1.336}$$

1.2.11 The entropy in quantum wells (QWs) of HD gallium antimonide

The dispersion relation of the conduction electrons in n-GaSb can be written as [164]

$$\bar{E} = \frac{\hbar^2\bar{k}^2}{2\bar{m}_0} - \frac{\bar{E}'_{g_0}}{2}\frac{\bar{E}'_{g_0}}{2}\left[1+\frac{2\hbar^2\bar{k}^2}{\bar{E}'_{g_0}}\left(\frac{1}{\bar{m}_c}-\frac{1}{\bar{m}_0}\right)\right]^{1/2} \tag{1.337}$$

where

$$\bar{E}'_{g_0} = \left[\bar{E}_{g_0}+\frac{5.10^{-5}\bar{T}^2}{2(112+\bar{T})}\right]\bar{e}V$$

The (1.337) can be expressed as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c} = \bar{I}_{36}(\bar{E}) \tag{1.338}$$

where

$$\bar{I}_{36}(\bar{E}) = [\bar{E} + \bar{E}_{g_0}^{'} - (\bar{m}_c/\bar{m}_0)(\bar{E}_{g_0}^{'}/2) - [(\bar{E}_{g_0}^{'}/2)^2[((\bar{E}_{g_0}^{'})^2/2)(1-(\bar{m}_c/\bar{m}_0))] + [(\bar{E}_{g_0}^{'}/2)(1-(\bar{m}_c/\bar{m}_0))]2 + \bar{E}\bar{E}_{g_0}^{'}(1-(\bar{m}_c/\bar{m}_0))]^{1/2}]$$

Under the condition of heavy doping (1.338) assumes the form

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c} = \bar{I}_{36}(\bar{E},\eta_g) \tag{1.339}$$

where

$$\bar{I}_{36}(\bar{E},\eta_g) = [\gamma_3(\bar{E},\eta_g) + \bar{E}_{g_0}^{'} - (\bar{m}_c/\bar{m}_0)(\bar{E}_{g_0}^{'}/2) - [(\bar{E}_{g_0}^{'}/2)^2[((\bar{E}_{g_0}^{'})^2/2)(1-(\bar{m}_c/\bar{m}_0))] + [(\bar{E}_{g_0}^{'}/2)(1-(\bar{m}_c/\bar{m}_0))]^2 + \bar{E}_{g_0}^{'}(1-(\bar{m}_c/\bar{m}_0))]^{1/2}]$$

where

$$\bar{I}_{36}(\bar{E},\eta_g) = \left[\left[\gamma_3(\bar{E},\eta_g) + \bar{E}_g^{'} - \frac{\bar{m}_c}{\bar{m}_0}.\frac{\bar{E}_g^{'}}{2} - \left[\left(\frac{\bar{E}_g^{'}}{2}\right)^2 + \left[\frac{\bar{E}_g^{'}}{2}\left(1-\frac{\bar{m}_c}{\bar{m}_0}\right)\right]\right]\right]^2 + \left(\frac{\bar{E}_{g_0}^{'}}{2}\right)^2\left(1-\frac{\bar{m}_c}{\bar{m}_0}\right) + \gamma_3(\bar{E},\eta_g)\bar{E}_{g_0}^{'}\left(1-\frac{\bar{m}_c}{\bar{m}_0}\right)\right]^{1/2}\right]$$

The EEM can be written as

$$\bar{m}^*(\bar{E}_{F_h},\eta_g) = \bar{m}_c\{\bar{I}_{36}(\bar{E}_{F_h},\eta_g)\}' \tag{1.340}$$

The DOS function in this case can be written as

$$\bar{N}_{HD}(\bar{E}_{F_h},\eta_g) = \frac{\bar{g}_v}{2\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\sqrt{\bar{I}_{36}(\bar{E}_{F_h},\eta_g)}\{\bar{I}_{36}(\bar{E}_{F_h},\eta_g)\}' \tag{1.341}$$

Since, the original band model in this case is a no pole function, therefore, the HD counterpart will be totally real, and the complex band vanishes.

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}[\{\bar{I}_{36}(\bar{E}_{F_h},\eta_g)\}^{3/2}] \tag{1.342}$$

In this case, $\bar{E}_{hd}$ is given by

$$\bar{I}_{36}(\bar{E}_{F_h},\eta_g) = 0 \tag{1.343}$$

One can numerically compute the entropy by using (1.342), (1.343), (1.31f) and the allied definitions in this case.

For dimensional quantization along z- direction, the dispersion relation of the 2D electrons in QWs of *HD GaSb* can be written following (1.339) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{k}_s)^2}{2\bar{m}_c} = \bar{I}_{36}(\bar{E},\eta_g) \tag{1.344}$$

The expression of the $\bar{N}_{2DT}(\bar{E})$ in this case can be written as

$$\bar{N}_{2DT}(\bar{E}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\overline{T'}_{119D}(\bar{E}_{F_h},\eta_g,\bar{n}_z)\bar{H}(\bar{E}-\bar{E}_{n_{zD119}}) \tag{1.345}$$

where

$$\bar{T}_{119D}(\bar{E}_{F_h},\eta_g,\bar{n}_z) = [\bar{I}_{36}(\bar{E}_{F_h},\eta_g) - \hbar^2(\bar{n}_z\pi/\bar{d}_z)^2(2\bar{m}_c)^{-1}],$$

The sub-band energies $\bar{E}_{n_{zD119}}$ in this case given by

$$\left\{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2\right\}(2\bar{m}_c)^{-1} = \bar{I}_{36}(\bar{E}_{n_{zD119}},\eta_g) \tag{1.346}$$

The EEM in this case assumes the form

$$\bar{m}^*(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \bar{m}_c[\overline{I'}_{36}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)] \tag{1.347}$$

The 2-D electron statistics in this case can be written as

$$\bar{N}_{2DT}(E) = \left(\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{T}_{119D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) + \bar{T}_{129D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)] \tag{1.348}$$

where

$$\bar{T}_{129D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\sum_{n_z=}^{n_{z\max}}[\bar{T}_{119D}(\bar{E}_{F1HD},\eta_g,\bar{n}_z)\right]$$

Therefore combining (1.348) and (1.31f) we can get the entropyin this case.

The total 2D DOS function in the absence of band tails in this case can be written as

$$\bar{N}_{2DT}(\bar{E}) = \left(\frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2}\right) \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \{[\bar{I}_{36}(\bar{E})]' \bar{H}(\bar{E} - \bar{E}_{n_{z44}})\} \tag{1.349}$$

where the sub-band energies $\bar{E}_{n_{z3}}$ can be expressed as

$$\bar{I}_{36}(\bar{E}_{n_{z44}}) = \frac{\hbar^2}{2\bar{m}_c}(\pi\bar{n}_z/\bar{d}_z)^2 \tag{1.350a}$$

The EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{Fs}) = (\bar{m}_c)[\bar{I}_{36}(\bar{E}_{Fs})]' \tag{1.350b}$$

The 2D carrier concentration assumes the form

$$\bar{N}_{2DT} = \left(\frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2}\right) \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{T}_{55}(\bar{E}_{Fs}, \bar{n}_z) + \bar{T}_{56}(\bar{E}_{Fs}, \bar{n}_z)] \tag{1.351}$$

where

$$\bar{T}_{55}(\bar{E}_{Fs}, \bar{n}_z) = [\bar{I}_{36}(\bar{E}_{Fs}) - \frac{\hbar^2}{2\bar{m}_c}(\pi\bar{n}_z/\bar{d}_z)^2]$$

and

$$\bar{T}_{56}(\bar{E}_{Fs}, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{T}_{55}(\bar{E}_{Fs}, \bar{n}_z)]$$

Using (1.351), the entropy in this case is given by

$$\bar{S}_0 = \bar{m}_c \bar{g}_v \left[\frac{\pi \bar{k}_B{}^2 \bar{T}}{3\hbar^2}\right] \left[\sum_{\bar{n}_z=1}^{\bar{n}_{\max}} [(\bar{T}_{55}(\bar{E}_{Fs}, \bar{n}_z))' + (\bar{T}_{56}(\bar{E}_{Fs}, \bar{n}_z))']\right] \tag{1.352}$$

The expression of electron concentration for bulk specimens of GaSb (in the absence of band tails) can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2} [\bar{M}_{A_{10}}(\bar{E}_F) + \bar{N}_{A_{10}}(\bar{E}_F)] \tag{1.353}$$

where

$$\bar{M}_{A_{10}}(\bar{E}_F)[I_{36}(\bar{E}_F)]^{3/2}$$

and

$$\bar{N}_{A_{10}}(\bar{E}_F) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{M}_{A_{10}}(\bar{E}_F)]$$

The entropy in this case can be expressed as

$$\bar{S}_0 = \left(\frac{2\bar{m}_c}{\hbar^2}\right)^{3/2}\left[\frac{\bar{g}_v\bar{k}_B^2\bar{T}}{9}\right]\left[(\overline{M}_{A_{10}}(\bar{E}_F))' + (\overline{N}_{A_{10}}(\bar{E}_F))'\right] \tag{1.354}$$

1.2.12 The entropy in quantum wells (QWs) of HD II–V materials

The dispersion relation (DR) of the holes in II–V compounds in accordance with Yamada [165] can be expressed as

$$\bar{E} = \bar{A}_{10}\bar{k}_x^2 + \bar{A}_{11}\bar{k}_y^2 + \bar{A}_{12}\bar{k}_z^2 + \bar{A}_{13}\bar{k}_x \pm [(\bar{A}_{14}\bar{k}_x^2 + \bar{A}_{15}\bar{k}_y^2 + \bar{A}_{16}\bar{k}_z^2 + \bar{A}_{17}\bar{k}_x)^2 + \bar{A}_{18}\bar{k}_y^2 + \bar{A}_{19}^2] \tag{1.355}$$

where $\bar{A}_{10}$, $\bar{A}_{11}$, $\bar{A}_{12}$, $\bar{A}_{13}$, $\bar{A}_{14}$, $\bar{A}_{15}$, $\bar{A}_{16}$, $\bar{A}_{17}$, $\bar{A}_{18}$ and $\bar{A}_{19}$ are energy band constants. The DR under the condition of formation of band tails can be written in this case as

$$\begin{aligned}\gamma_3(\bar{E},\eta_g) = {} & \bar{A}_{10}\bar{k}_x^2 + \bar{A}_{11}\bar{k}_y^2 + \bar{A}_{12}\bar{k}_z^2 + \bar{A}_{13}\bar{k}_x \\ & \pm [(\bar{A}_{14}\bar{k}_x^2 + \bar{A}_{15}\bar{k}_y^2 + \bar{A}_{16}\bar{k}_z^2 + \bar{A}_{17}\bar{k}_x)^2 + \bar{A}_{18}\bar{k}_y^2 + \bar{A}_{19}^2]^{1/2}\end{aligned} \tag{1.356}$$

The whole energy spectrum in this case assumes the form

$$\begin{aligned}\gamma_3(\bar{E},\eta_g) = {} & \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{11}\bar{k}_y^2 + \bar{A}_{12}\bar{k}_z^2 + \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right) \\ & \pm \left[(\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{15}\bar{k}_y^2 + \bar{A}_{16}\bar{k}_z^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2\right) + \bar{A}_{18}\bar{k}_y^2 + \bar{A}_{19}^2]^{1/2}\end{aligned} \tag{1.357}$$

The subband energy $(\bar{E}_{n_zHD401})$ is the lowest positive root of the following equation

$$\gamma_3(\bar{E}_{n_zHD401},\eta_g) = \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right) \pm \left[\left(\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right)^2 + \bar{A}_{19}^2\right]^{1/2} \tag{1.358}$$

The EEM and the DOS function for both the cases should be calculated numerically.

Using (1.31f) and (1.358) we can study the entropy numerically.

1.2.13 The entropy in quantum wells (QWs) of HD lead germanium telluride

The dispersion law of n-type $Pb_{1-x}Ge_xTe$ with x = 0.01 can be expressed following Vassilev [125] as

$$\left[\bar{E} - 0.606\bar{k}_s^2 - 0.722\bar{k}_z^2\right]\left[\bar{E} + \bar{E}_{g_0} + 0.411\bar{k}_s^2 + 0.377\bar{k}_z^2\right] = 0.23\bar{k}_s^2 + 0.02\bar{k}_z^2 \pm \left[0.06\bar{E}_{g_0} + 0.061\bar{k}_s^2 + 0.0066\bar{k}_z^2\right]\bar{k}_s \tag{1.359}$$

where $\bar{E}_{g_0} = 0.21\ eV$, $\bar{k}_x$, $\bar{k}_y$ and $\bar{k}_z$ are the units of $10^9\bar{m}^{-1}$

The electron energy spectrum n – type $\bar{k}_z^2 Pb_{1-x}Ge_x\,Te$ under the condition of formation of band tails can be written as

$$\left[\frac{2}{1+Erf(\frac{\bar{E}}{\eta_g})}\right]\theta_0(\bar{E},\eta_g) + \gamma_3(\bar{E},\eta_g)[\bar{E}_{g_0} - 0.195\bar{k}_s^2 - 0.345\bar{k}_z^2] = \left[0.23\bar{k}_s^2 + 0.02\bar{k}_z^2 \pm \left[0.06\bar{E}_{g_0} + 0.061\bar{k}_s^2 + 0.0066\bar{k}_z^2\right]\bar{k}_s + \left[\bar{E}_{g_0} + 0.411\bar{k}_s^2 + 0.377\bar{k}_z^2\right]\left[0.606k_s^2 + 0.722\bar{k}_z^2\right]\right] \tag{1.360}$$

The $E - k_s$ relation in HD QWs of n-type $Pb_{1-x}Ge_xTe$ assumes the form

$$\left[\frac{2}{1+\bar{E}\bar{r}\bar{f}(\frac{\bar{E}}{\eta_g})}\right]\theta_0(\bar{E},\eta_g) + \gamma_3(\bar{E},\eta_g)\left[\bar{E}_{g_0} - 0.195\bar{k}_s^2 - 0.345\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right] = \left[0.23\bar{k}_s^2 + 0.02\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \pm \left[0.06\bar{E}_{g_0} + 0.061\bar{k}_s^2 + 0.0066\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\bar{k}_s + \left[\bar{E}_{g_0} + 0.411\bar{k}_s^2 + 0.377\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\left[0.606\bar{k}_s^2 + 0.722\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right] \tag{1.361}$$

The subband energy ($E_{n_{zHD400}}$) is the lowest positive root of the following equation

$$\left[\frac{2}{1+Erf\left(\frac{\bar{E}_{n_{zHD400}}}{\eta_g}\right)}\right]\theta_0(\bar{E}_{n_{zHD400}},\eta_g) + \gamma_3(\bar{E}_{n_{zHD400}},\eta_g)\left[\bar{E}_{g_0} - 0.345\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right] = \left[0.02\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \pm \left[\bar{E}_{g_0} + 0.377\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\left[0.722\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right] \tag{1.362}$$

The EEM and the DOS function for both the cases should be calculated numerically.

Using (1.31f) and (1.362) we study the entropy numerically.

1.2.14 The entropy in quantum wells (QWs) of HD Zinc and Cadmium diphosphides

The DR of the holes of Cadmium and Zinc diphosphides can approximately be written following Chuiko [166] as

$$\bar{E} = \left[\beta_1 + \frac{\beta_2\beta_3(\bar{k})}{8\beta_4}\right]\bar{k}^2 \pm \left\{\left[\beta_4\beta_3(\bar{k})\left(\beta_5 - \frac{\beta_2\beta_3(\bar{k})}{8\beta_4}\right)k^2\right] + 8\beta_4^2\left(1 - \frac{\beta_3^2(\bar{k})}{4}\right) - \beta_2\left(1 - \frac{\beta_3^2(\bar{k})}{4}\right)\bar{k}^2\right\}^{1/2} \tag{1.363}$$

where $\beta_1, \beta_2, \beta_4$ and β_5 are system constants and $\beta_3(\bar{k}) = \frac{\bar{k}_x^2 + \bar{k}_y^2 - 2\bar{k}_z^2}{\bar{k}^2}$

Under the condition of formation of band tail, the above equation assumes the form

$$\gamma_3(\bar{E}, \eta_g) = \left[\beta_1 + \frac{\beta_2\beta_3(\bar{k})}{8\beta_4}\right]k^2 \pm \left\{\left[\beta_4\beta_3(\bar{k})\left(\beta_5 - \frac{\beta_2\beta_3(\bar{k})}{8\beta_4}\right)\bar{k}^2\right] + 8\beta_4^2\left(1 - \frac{\beta_3^2(\bar{k})}{4}\right) - \beta_2\left(1 - \frac{\beta_3^2(\bar{k})}{4}\right)\bar{k}^2\right\}^{1/2} \tag{1.364}$$

The DR in HD QWs of Zinc and Cadmium diphosphides can be written as

$$\gamma_3(\bar{E}, \eta_g) = \left[\beta_1 + \frac{\beta_2\beta_3(\bar{k})}{8\beta_4}\right]\left[\bar{k}_x^2 + \bar{k}_y^2 + \left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right] \pm \left\{\left[\beta_4\beta_{31}(\bar{k})\left(\beta_5 - \frac{\beta_2\beta_{31}(\bar{k})}{8\beta_4}\right)\left[\bar{k}_x^2 + \bar{k}_y^2 + \left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right] + 8\beta_4^2\left(1 - \frac{\beta_{31}^2(\bar{k})}{4}\right) - \beta_2\left(1 - \frac{\beta_{31}^2(\bar{k})}{4}\right)\left[\bar{k}_x^2 + \bar{k}_y^2 + \left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right\}^{1/2} \tag{1.365}$$

where

$$\beta_{31}(\bar{k}) = \left[\frac{\bar{k}_x^2 + \bar{k}_y^2 - 2\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2}{\left[\bar{k}_x^2 + \bar{k}_y^2 + \left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]}\right]$$

The subband energy $(\bar{E}_{n_{zHD402}})$ is the lowest positive root of the following equation

$$\gamma_3\left(\bar{E}_{n_{zHD401}}, \eta_g\right) = \left[\beta_1 - \frac{\beta_2}{4\beta_4}\right]\left[\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right] \pm \left\{\left[-2\beta_4\left(\beta_5 - \frac{\beta_2}{4\beta_4}\right)\left[\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right]\right\}^{1/2} \tag{1.366}$$

The EEM and the DOS function for both the cases should be calculated numerically.

Using (1.31f) and (1.366) we can study entropy numerically.

Thus, we can summarize the whole mathematical background in the following way.

In this chapter, we have investigated the 3D and 2D entropies in HD bulk and QWs of nonlinear optical materials on the basis of a newly formulated electron dispersion law considering the anisotropies of the effective electron masses, the spin orbit splitting constants and the influence of crystal field splitting within the framework of $\vec{k}\cdot\vec{p}$ formalism. The results for 3D and 2D entropy's for HD bulk and QWs of III–V, ternary and quaternary compounds in accordance with the three and two band models of Kane form a special case of our generalized analysis. We have also studied the entropy in accordance with the models of Stillman et al. and Palik et al., respectively, since these models find use to describe the electron energy spectrum of the aforesaid materials. The 3D and 2D entropy's has also been derived for HD bulk and QWs of II–VI, IV–VI, stressed materials, Te, $n-GaP, p-PtSb_2$, Bi_2Te_3, $n-Ge$, $n-GaSb$, II–V, Lead Germanium Telluride and Zinc and Cadmium Diphosphides compounds by using the models of Hopfield, Dimmock, Seiler, Bouat et al., Rees, Emtage, Kohler, Cardona, Wang et al. Mathur et al., Yamada, Vassilev and Chuiko, respectively, on the basis of the appropriate carrier energy spectra. The well-known expressions of the entropies in the absence of band tails for wide gap materials have been obtained as special cases of our generalized analysis under certain limiting conditions. This indirect test not only exhibits the mathematical compatibility of our formulation but also shows the fact that our simple analysis is a more generalized one, since one can obtain the corresponding results for relatively wide gap materials having parabolic energy bands under certain limiting conditions from our present derivation.

1.3 Result and discussions

Using the appropriate equations and taking the energy band constants as given in Table of appendix (15), the normalized entropy in QWs of HD $CdGeAs_2$ (an example of nonlinear optical materials) have been plotted as a function of film thickness as shown in Figure 1.1 in accordance with the generalized band model ($\delta \neq 0$), three and two band HD models of Kane together with parabolic HD energy bands as shown by curves (a), (c), (d) and (e), respectively. The special case for $\delta = 0$ has also been shown in plot (b) in the same figure to assess the influence of crystal field splitting. The Figure 1.2 exhibits the plots of the normalized entropy in QWs of HD $CdGeAs_2$ as a function of the surface electron concentration per unit area for all cases of Figure 1.1.The Figures 1.3 and 1.5 exhibit the normalized entropy for QWs of HD *InAs and InSb* as a function of film thickness for three and two HD band models of Kane together with HD parabolic energy bands as shown by curves (a), (b) and (c), respectively, in both the figures. The Figures 1.4 and 1.6 show the corresponding

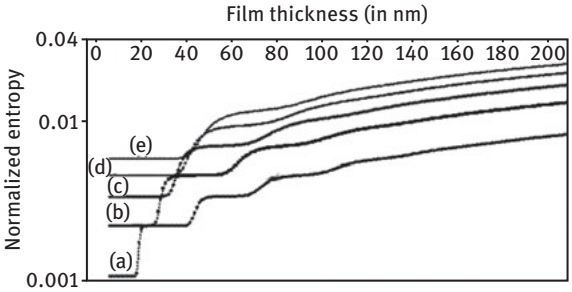

Figure 1.1: Plot of the normalized entropy in UFs of HD $CdGeAs_2$ as a function of film thickness in accordance with (a) the generalized band model ($\delta \neq 0$), (b) $\delta = 0$, (c) the three and (d) the two band models of Kane together with (e) the parabolic energy bands.

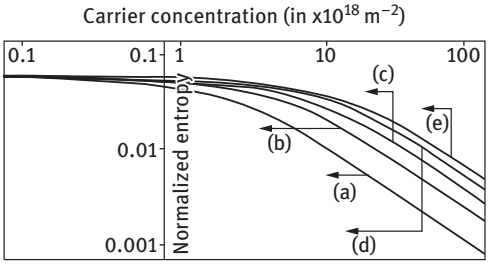

Figure 1.2: Plot of the normalized entropy in UFs of HD $CdGeAs_2$ as a function of carrier concentration for all cases of Figure 1.1.

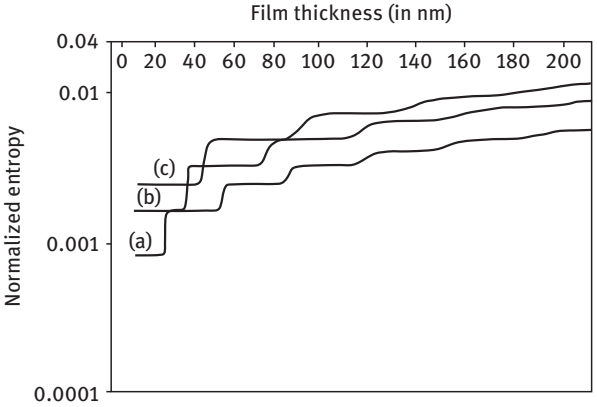

Figure 1.3: Plot of the normalized entropy in UFs of HD InAs as a function of film thickness in accordance with the (a) three and (b) two band models of Kane together with (c) parabolic energy bands.

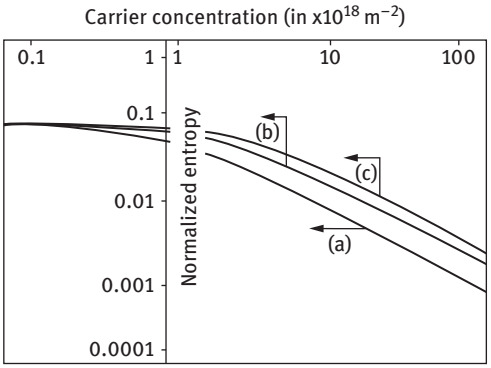

Figure 1.4: Plot of the normalized entropy in UFs of HD InAs as a function of carrier concentration for all the cases of Figure 1.3.

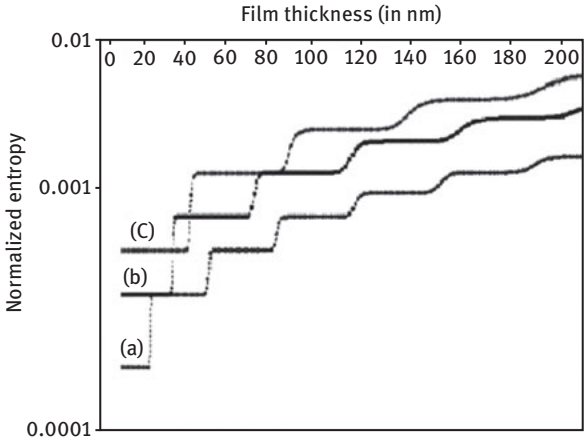

Figure 1.5: Plot of the normalized entropy of UFs of HD InSbas a function of film thickness for all the cases of Figure 1.3.

dependences on the surface electron concentration for QWs of HD *InAs and InSb*. In Figure 1.7, the normalized entropy has been plotted in QWs of HD *CdS* as a function of film thickness for both $\bar{\lambda}_0 = 0$ and $\bar{\lambda}_0 \neq 0$ as shown by curves (b) and (a), respectively, for the purpose of assessing the splitting of the two spin states by the spin orbit coupling and the crystalline field. The Figure 1.8 shows the corresponding carrier statistics dependence of the entropy for all the cases of Figure 1.7. In Figure 1.9, the normalized entropy has been plotted for HD QWs of *PbTe*, *PbSnTe* and HD stressed *InSb* as a function of film thickness in accordance with the appropriate band models as shown by curves (a), (b) and (c), respectively. The Figure 1.10 exhibits the corresponding dependence on the surface electron concentration per

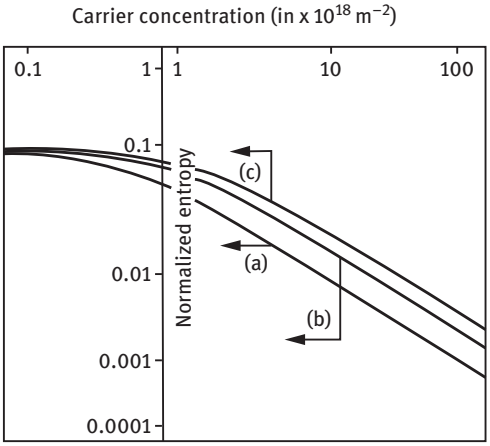

Figure 1.6: Plot of the normalized entropy in UFs of HD InSbas a function of carrier concentration for all the cases of Figure 1.3.

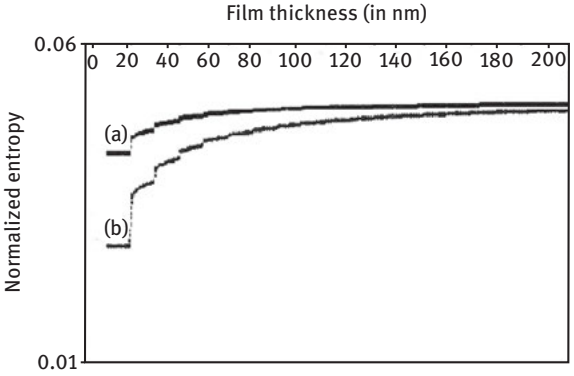

Figure 1.7: Plot of the normalized entropy in UFs of HD CdS as a function of film thickness for (a) $\bar{\lambda}_0 \neq 0$ and (b) $\bar{\lambda}_0 = 0$ in accordance with the model of Hopfield.

unit area. Figure 1.11 demonstrates the plots of the normalized entropy in QWs of HD *GaP*, $PtSb_2$, Bi_2Te_3 and Cadmium Antimonide, respectively, as a function of film thickness. In Figure 1.12, the normalized entropy has been plotted as a function of carrier concentration for all the cases of Figure 1.11.

The influence of 1D quantum confinement is immediately apparent from Figure (1.1), (1.3), (1.5), (1.7), (1.9) and (1.11) since the entropy depends strongly on the thickness of the quantum-confined materials which is in direct contrast with bulk specimens. The entropy increases with increasing film thickness in an oscillatory way with different numerical magnitudes for HD QWs, respectively. It appears from the aforementioned figures that the entropy in HD QWs exhibits spikes for

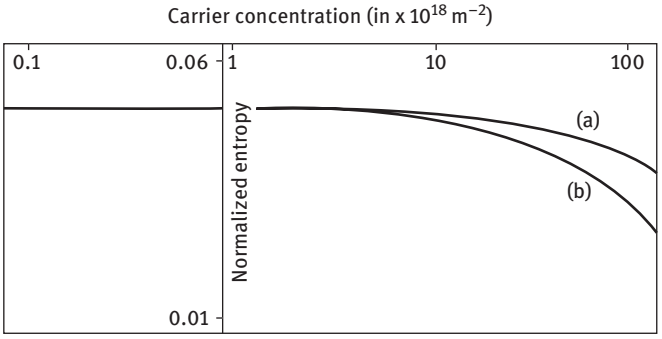

Figure 1.8: Plot of the normalized entropy of UFs of HD CdSas a function of carrier concentration for the cases of Figure 1.7.

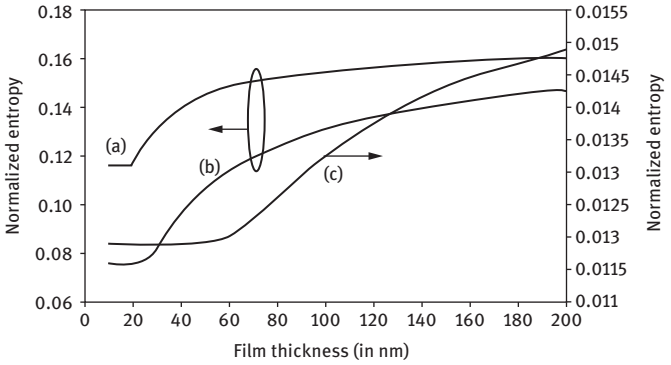

Figure 1.9: Plot of the normalized entropy for UFs of HDs (a) PbTe, (b) PbSnTe and (c) stressed InSbas a function of film thickness.

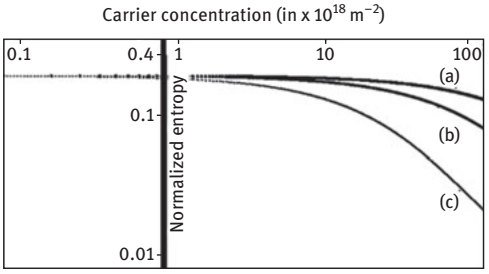

Figure 1.10: Plot of the normalized entropy for UFs of HDs (a) PbTe, (b) PbSnTe and (c) stressed InSbas a function of carrier concentration.

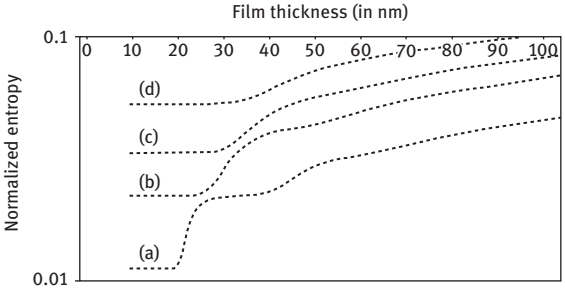

Figure 1.11: Plot of the normalized entropy in HDs QWs of (a) GaP, (b) $PtSb_2$ (c) Bi_2Te_3 and (d) Cadmium Antimonide, respectively, as a function of film thickness.

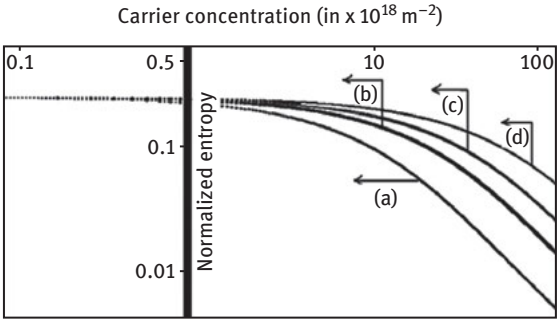

Figure 1.12: Plot of the normalized entropy for HDs QWs of (a) Gap, (b) $PtSb_2$, (c) Bi_2Te_3 and (d) Cadmium Antimonide, respectively, as a function of carrier concentration.

particular values of film thickness which, in turn, is not only the signature of the asymmetry of the wave vector space but also the particular band structure of the specific material. Moreover, the entropy in HD QWs of different compounds can become several orders of magnitude larger than that of the bulk specimens of the same HD materials, which is also a direct signature of quantum confinement. This oscillatory dependence will be less and less prominent with increasing film thickness. It appears from Figure (1.2), (1.4), (1.6), (1.8), (1.10) and (1.12) that the entropy decreases with increasing carrier degeneracy for 1D quantum confinement as considered for the said figures. For relatively high values of carrier degeneracy, the influence of band structure of a specific HD material is large and the plots of entropy differ widely from one another whereas for low values of the carrier degeneracy, they exhibit the converging tendency. For bulk specimens of the same material, the entropy will be found to increase continuously with increasing electron degeneracy in a nonoscillatory manner in an altogether different way.

The appearance of the humps of the respective curves is due to the redistribution of the electrons among the quantized energy levels when the quantum number corresponding to the highest occupied level changes from one fixed value to the

others. With varying electron concentration, a change is reflected in the 2D entropy through the redistribution of the electrons among the quantized levels. Although the 2D entropy varies in various manners with all the variables in all the limiting cases as evident from all the curves of Figures. 1.1 and 1.2, the rates of variations are totally band-structure dependent.The influence of the energy band constants on the entropy in both the cases is apparent for all the materials as considered here.

The normalized 2D entropy for QWs of HD stressed Kane type $n-InSb$ has been plotted in Figures 1.9 and 1.10 as functions of nano-thickness and surface electron concentration, respectively, as shown in plot (a) in the presence of stress while the plot (b) exhibits the same in the absence of stress for the purpose of assessing the influence of stress on the 2D entropy in QWs of HD of stressed $n-InSb$. In the presence of stress, the magnitude of the 2D entropy is being increased as compared with the same under stress free condition. It may be noted that with the advent of modern experimental techniques, it is possible to fabricate quantum-confined structures with an almost defect-free surface. If the direction normal to the film was taken differently from that as assumed in this work, the expressions for the 2D entropy in quasi two-dimensional structures would be different analytically, since the basic dispersion laws of many important materials are anisotropic.

It may be noted that under certain limiting conditions, all the results for all the models as derived here get simplified to have transformed into the well-known expressions of 3D and 2D entropy's. This indirect test not only exhibits the mathematical compatibility of the present formulation but also shows the fact that our simple analysis is a more generalized one, since one can obtain the corresponding results for relatively wide gap 2D materials having parabolic energy bands under certain limiting conditions from the present generalized analysis. Thus, the present investigations cover the study of 2D entropy for QWs of HD nonlinear optical, III–V, ternaries, quaternaries, II–VI, IV–VI, stressed compounds, Te, GaP, $PtSb_2$, Bi_2Te_3, Ge and $GaSb$ having different band structures. One striking understanding as a collateral study as considered here is that, the EEM becomes a function of the size quantum number the Fermi energy and other energy band constants depending on the respective HD 2D dispersion laws as formulated already in the respective theoretical background of this chapter together with the fact that the ***EEMs exists in the band gap, a phenomena which is impossible without the concept of band tailing***. It must be mentioned that a direct research application of the quantized materials is in the area of band structure. The theoretical results as derived in this chapter exhibit the basic qualitative features of 2D entropy for different quantum confined HD materials.

One important concept of this chapter is the presence of poles in the finite complex plane in the dispersion relation of the materials in the absence of band tails creates the complex energy spectrum in the corresponding HD samples. Besides, from the DOS function in this case, it appears that a new forbidden zone has been created in addition to the normal band gap of the semiconductor. If the basic dispersion relation in the absence of band tails contains no poles in the finite complex

plane, the corresponding HD energy band spectrum will be real, although it may be the complicated functions of exponential and error functions and deviate considerably from that in the absence of band tailing.Another important point in this context is the existence of the effective mass within the forbidden zone, which is impossible without the formation of band tails. It is an amazing fact that the study of the carrier transport in HD quantized materials through proper formulation of the Boltzmann transport equationwhich needs in turn, the corresponding HD carrier energy spectra is still one of the open research problems.

It may be noted that with the advent of MBE and other experimental techniques, it is possible to fabricate quantum-confined structures with an almost defect-free surface. In formulating the generalized electron energy spectrum for nonlinear optical materials, we have considered the crystal-field splitting parameter, the anisotropies in the momentum-matrix elements, and the spin-orbit splitting parameters, respectively. In the absence of heavy doping, the crystal field splitting parameter together with the assumptions of isotropic effective electron mass and isotropic spin orbit splitting, our basic relation as given by eq (1.2) converts into eq (1.48). The eq (1.48) is the well-known three-band Kane model and is valid for III–V compounds, in general. It should be used as such for studying the electronic properties of n-InAs where the spin-orbit splitting parameter (Δ) is of the order of band gap ($\bar{E}_{g_0}$). For many important materials $\Delta >> \bar{E}_{g_0}$ and under this inequality, eq (1.48) assumes the form $\bar{E}(1+\bar{E}\bar{E}^{-1}{}_{g_0}) = \hbar^2\bar{k}^2/2\bar{m}_c$ which is the well-known two-band Kane model. Also under the condition, $\bar{E}_{g_0} \to \infty$, the above equation gets simplified to the well-known form of parabolic energy bands as $\bar{E} = \hbar^2\bar{k}^2/2\bar{m}_c$. It is important to note that under certain limiting conditions, all the results for all the models as derived here have transformed into the well-known expression of the 2D entropy for size quantized materials having parabolic bands. We have not considered other types of compounds or external physical variables for numerical computations in order to keep the presentation brief. With different sets of energy band constants, we shall get different numerical values of the HD 2D entropy though the nature of variations of the HD 2D entropy as shown here would be similar for the other types of materials and the simplified analysis of this chapter exhibits the basic qualitative features of the HD 2D entropy for such compounds.

We must note that the study of transport phenomena and the formulation of the electronic properties of HD nano-compounds are based on the dispersion relations in such materials. The theoretical results of our chapter can be used to determine the 2D entropy and the constituent heavily-doped bulk materials in the absence of size effects It is worth remarking that this simplified formulation exhibits the basic qualitative features of HD 2D entropy for nano-materials. The basic objective of this chapter is not solely to demonstrate the influence of quantum confinement on the 2D entropy for HD QWs of nonparabolic materials but also to formulate the appropriate electron statistics in the most generalized form, since the transport and other phenomena in HD nano-materials having different band structures and the

derivation of the expressions of many important electronic properties are based on the temperature-dependent electron statistics in such compounds.

Our method is not at all related to the DOS technique as used in the literature. From the E-k dispersion relation, we can obtain the DOS, but the DOS technique as used in the literature cannot provide the E-k dispersion relation. Therefore, our study is more fundamental than those of the existing literature because the Boltzmann transport equation, which controls the study of the charge transport properties of semiconductor devices, can be solved if and only if the E-k dispersion relation is known. We wish to note that we have not considered the many body effects in this simplified theoretical formalism due to the lack of availability in the literature of proper analytical techniques for including them for the generalized systems as considered in this chapter. Our simplified approach will be useful for the purpose of comparison when methods of tackling the formidable problem after inclusion of the many body effects for the present generalized systems appear. It is worth remarking in this context that from our simple theory under certain limiting conditions we get the well-known result of the entropy for wide gap materials having parabolic energy bands. The inclusion of the said effects would certainly increase the accuracy of the results, although the qualitative features of the 2D entropy in QWs of HD materials discussed in this chapter would not change in the presence of the aforementioned effects. The influence of energy band models and the various band constants on the entropy for different materials can also be studied from all the Figures of this chapter.

The numerical results presented in this chapter would be different for other materials but the nature of variation would be unaltered. The theoretical results as given here would be useful in analyzing various other experimental data related to this phenomenon. Finally, we can write that the analysis as presented in this chapter can be used to investigate, the Burstein Moss shift, the carrier contribution to the elastic constants, the specific heat, screening length, activity coefficient, reflection coefficient, Hall coefficient, plasma frequency, various scattering mechanisms and other different transport coefficients of modern HD nonparabolic quantum confined HD devices operated under different external conditions having varying band structures.

1.4 Open research problems

The problems under these sections of this monograph are by far the most important part for the readers and few open research problems are presented from this chapter till appendix 14. The numerical values of the energy band constants for various materials are given in Table of appendix 15 for the related computer simulations.

(R.1.1) Investigate the entropy for the HD bulk materials whose respective dispersion relations of the carriers in the absence of band tails and any externally applied field are given below:

(a) The electron dispersion law in n-GaP can be written as [167]

$$\bar{E} = \frac{\hbar^2 \bar{k}_s^2}{2m_{\|}^*} + \frac{\hbar^2 \bar{k}_s^2}{2m_{\perp}^*} \mp \frac{\bar{\Delta}}{2} \pm \left[\left(\frac{\bar{\Delta}}{2} \right)^2 + \bar{P}_{\perp} \bar{k}_z^2 + \bar{D}_1 \bar{k}_x^2 \bar{k}_y^2 \right]^{1/2} \tag{R1.1}$$

where $\bar{\Delta} = 335 \bar{m} \bar{e} \bar{V}$, $\bar{P}_1 = 2 \times 10^{-10} \bar{e} \bar{V} \bar{m}$, $\bar{D}_1 = \bar{P}_1 a_1$ and $\bar{a}_1 = 2 \times 10^{-10} \bar{e} \bar{V} \bar{m}$

(b) The dispersion relation for the conduction electrons for IV–VI materials can also be described by the models of Cohen [168], McClure and Choi [169], Bangert et al. [170] and Foley et al. [171], respectively.

(i) In accordance with Cohen [168], the dispersion law of the carriers is given by

$$\bar{E}(1 + \alpha \bar{E}) = \frac{\bar{p}_x^2}{2\bar{m}_1} + \frac{\bar{p}_z^2}{2\bar{m}_3} - \frac{\alpha \bar{E} \bar{p}_y^2}{2\bar{m}'_2} + \left(\frac{\alpha \bar{p}_y^4}{4\bar{m}_2 \bar{m}'} \right) + \frac{\bar{p}_y^2}{2\bar{m}_2} (1 + \alpha \bar{E}) \tag{R1.2}$$

where m_1, m_2 and m_3 are the effective carrier masses at the band-edge along x, y and z directions, respectively, and m'_2 is the effective mass tensor component at the top of the valence band (for electrons) or at the bottom of the conduction band (for holes).

(ii) The carrier energy spectra can be written, following McClure and Choi [169], as

$$\bar{E}(1 + \alpha \bar{E}) = \frac{\bar{p}_x^2}{2\bar{m}_1} + \frac{\bar{p}_y^2}{2\bar{m}_2} + \frac{\bar{p}_z^2}{2\bar{m}_3} + \frac{\bar{p}_y^2}{2\bar{m}_2} \alpha \bar{E} - \frac{\alpha \bar{E} \bar{p}_y^2}{2\bar{m}'_2} + \left(\frac{\alpha \bar{p}_y^4}{4\bar{m}_2 \bar{m}'} \right) (1 + \alpha \bar{E}) \tag{R1.3a}$$

$$\bar{E}(1 + \alpha \bar{E}) = \frac{\bar{p}_x^2}{2\bar{m}_1} + \frac{\bar{p}_y^2}{2\bar{m}_2} + \frac{\bar{p}_z^2}{2\bar{m}_3} + \frac{\bar{p}_y^2}{2\bar{m}_2} \alpha \bar{E} \left\{ 1 - \left(\frac{m_2}{\bar{m}'_2} \right) \right\} + \frac{\bar{p}_y^4 \alpha}{4\bar{m}_2 \bar{m}'_2} - \frac{\alpha \bar{p}_x^2 \bar{p}_y^2}{4\bar{m}_1 \bar{m}_2} - \frac{\alpha \bar{p}_y^2 \bar{p}_z^2}{4\bar{m}_2 \bar{m}_3} \tag{R1.3b}$$

(iii) In accordance with Bangert and Kastner [170], the dispersion relation is given by

$$\Gamma(\bar{E}) = \bar{F}_1(\bar{E}) k_s^2 + \bar{F}_2(\bar{E}) k_z^2 \tag{R1.4}$$

where $\Gamma(\bar{E}) \equiv 2\bar{E}$, $\bar{F}_1(\bar{E}) \equiv \frac{\bar{R}_1^2}{\bar{E} + \bar{E}_{g0}} + \frac{\bar{S}_1^2}{\bar{E} + \Delta'_c} + \frac{\bar{Q}_1^2}{\bar{E} + \bar{E}_{g0}}$,

$$\bar{F}_2(\bar{E}) \equiv \frac{2\bar{C}_5^2}{\bar{E} + \bar{E}_{g0}} + \frac{(\bar{S}_1 + \bar{Q}_1)^2}{\bar{E} + \Delta''_c}$$

$\bar{R}_1^2 = 2.3 \times 10^{-19} (eVm)^2$, $\bar{C}_1^2 = 0.83 \times 10^{-19} (eVm)^2$, $\bar{Q}_1^2 = 1.3 \bar{R}_1^2$, $\bar{S}_1^2 = 4.6 \bar{R}_1^2$, $\Delta'_c = 3.07 eV$ $\Delta''_c = 3.028 eV$ and $g_v = 4$. It may be noted that under the $\bar{S}_1 = 0$, $\bar{Q}_1 = 0$, $\bar{R}_1^2 \equiv \frac{\hbar^2 \bar{E}_{g0}}{\bar{m}_{\perp}^*}$, $\bar{C}_5^2 \equiv \frac{\hbar^2 \bar{E}_{g0}}{2\bar{m}_{\|}^*}$, (R1.4) assumes the form $\bar{E}(1 + \alpha \bar{E}) = \frac{\hbar^2 \bar{k}_s^2}{2\bar{m}_{\perp}^*} + \frac{\hbar^2 \bar{k}_z^2}{2\bar{m}_{\|}^*}$ which is the simplified Lax model.

(iv) The carrier energy spectrum of IV–VI materials in accordance with Foley et al. [171] can be written as

$$\bar{E} + \frac{\bar{E}_{g_0}}{2} = \bar{E}_-(\bar{k}) + \left[\left[\bar{E}_+(\bar{k}) + \frac{\bar{E}_g}{2}\right]^2 + \bar{P}_\perp^2 \bar{k}_s^2 + \bar{P}_\parallel^2 \bar{k}_z^2\right]^{1/2} \tag{R1.5}$$

where $\bar{E}_+ = (\bar{k}) = \frac{\hbar^2 \bar{k}_s^2}{2\bar{m}_\perp^+} + \frac{\hbar^2 \bar{k}_z^2}{2\bar{m}_\parallel^+}$, $E_- = (k) = \frac{\hbar^2 k_s^2}{2m_\perp^-} + \frac{\hbar^2 k_z^2}{2m_\parallel^-}$ represents the contribution from the interaction of the conduction and the valance band edge states with the more distant bands and the free electron term, $\frac{1}{\bar{m}_\perp^\pm} = \frac{1}{2}\left[\frac{1}{\bar{m}_{tc}} \pm \frac{1}{\bar{m}_{tv}}\right]$, $\frac{1}{\bar{m}_\parallel^\pm} = \frac{1}{2}\left[\frac{1}{\bar{m}_{1c}} \pm \frac{1}{\bar{m}_{1v}}\right]$

For n-PbTe $\bar{P}_\perp = 4.61 \times 10^{-10} eVm$, $\bar{P}_\parallel = 4.61 \times 10^{-10} eVm$, $\frac{\bar{m}_0}{\bar{m}_{tv}} = 10.36$, $\frac{\bar{m}_0}{\bar{m}_{tv}} = 0.75$, $\frac{\bar{m}_0}{\bar{m}_{tc}} = 11.36$, $\frac{\bar{m}_0}{\bar{m}_{1c}} = 1.20$ *and* $\bar{g}_v = 4$ The hole energy spectrum of p-type zero-gap Materials (e.g. HgTe) is given by [172]

$$\bar{E} = \frac{\hbar^2 \bar{k}^2}{2\bar{m}_v} + \frac{3e}{128\varepsilon_\infty}\bar{k} - \left(\frac{2\bar{E}_B}{\pi}\right) ln\left|\frac{\bar{k}}{\bar{k}_0}\right| \tag{R1.6}$$

Where $\bar{m}_v^*$ is the effective mass of the hole at the top of the valence band,

$$\bar{E}_B \equiv \frac{\bar{m}_0 e^2}{2\hbar^2 \varepsilon_\infty^2} \; and \; \bar{k}_o \equiv \frac{\bar{m}_0 e^2}{2\hbar^2 \varepsilon_\infty^2}.$$

(c) The conduction electrons of n-GaSb obey the following two dispersion relations:

(i) In accordance with the model of Seiler et al. [173]

$$\bar{E} = \left[-\frac{\bar{E}_{g_0}}{2} + \frac{\bar{E}_{g_0}}{2}[1 + \alpha_4 \bar{k}^2] + \frac{\bar{E}_{g_0}}{2}\left[1 + 4\frac{\hbar^2 \bar{k}^2}{2\bar{m}'_c}\frac{\bar{f}_1(\bar{E})}{\bar{E}_{g_0}}\right]\right. \tag{R1.7}$$

where $\alpha_4 \equiv 4\bar{P}(\bar{E}_{g_0} + \frac{2}{3}\Delta)[\bar{E}_{g_0}(\bar{E}_{g_0} + \Delta)]^{-1}$, P is the isotropic momentum matrix element, $\bar{f}_1(\bar{k}) \equiv \bar{k}^{-2}[\bar{k}_x^2 \bar{k}_y^2 + \bar{k}_y 2\bar{k}_z^2 + \bar{k}_z^2 \bar{k}_x^2]$ represents the warping of the Fermi surface, $\bar{f}_2(\bar{k}) \equiv [\{\bar{k}^{-2}(\bar{k}_x^2 \bar{k}_y^2 + \bar{k}_y^2 \bar{k}_z^2 + \bar{k}_z^2 \bar{k}_x^2) - 9\bar{k}_x^2 \bar{k}_y^2 \bar{k}_z^2\}^{1/2} \bar{k}^{-1}]$ represents the inversion asymmetry splitting of the conduction bandand $\bar{\varsigma}_0, \bar{\nu}_0$ and $\bar{\omega}_0$ represent the constants of the electron spectrum in this case.

(ii) In accordance with the model of Zhang et al. [174]

$$\bar{E} = [\bar{E}_2^{(1)} + \bar{E}_2^{(2)} \bar{K}_{4,1}]\bar{k}^2 + [\bar{E}_4^{(1)} + \bar{E}_4^{(2)} \bar{K}_{4,1}]\bar{k}^4 + \bar{k}^6[\bar{E}_6^{(1)} + \bar{E}_6^{(2)} \bar{K}_{4,1} + \bar{E}_6^{(3)} \bar{k}_{6,1} \tag{R1.8}$$

where

$$\bar{K}_{4,1} \equiv \frac{5}{4}\sqrt{21}\left[\frac{\bar{k}_x^4+\bar{k}_y^4+\bar{k}_z^4}{k^4}\right], \bar{K}_{6,1} \equiv \sqrt{\frac{639639}{32}}\left[\frac{\bar{k}_x^2\bar{k}_y^2\bar{k}_z^2}{k^6}+\frac{1}{22}\left(\frac{\bar{k}_x^2\bar{k}_y^2\bar{k}_z^2}{k^6}-\frac{3}{5}\right)-\frac{1}{105}\right]$$

the coefficients are in eV, the values of k are $10\left(\frac{\bar{a}}{2\pi}\right)$ times those of k in atomic units (a is the lattice constant), $\bar{E}_2^{(1)} = 1.0239620$, $\bar{E}_2^{(2)} = 0$, $\bar{E}_4^{(1)} = -1.1320772$, $\bar{E}_4^{(2)} = 0.05658$, $\bar{E}_6^{(1)} = 1.1072073, \bar{E}_6^{(2)} = -0.1134024$ *and* $\bar{E}_6^{(3)} = -0.0072275$.

(d) In addition to the well-known band models of III–V materials as discussed in this monograph, the conduction electrons of such compounds obey the following three dispersion relations:

(i) In accordance with the model of Rossler [175]

$$\bar{E} = \frac{\hbar^2\bar{k}^2}{2\bar{m}^*}\alpha_{10}\bar{k}_4 + \beta_{10}\left[[\bar{k}_x^2\bar{k}_y^2+\bar{k}_y^2\bar{k}_z^2+\bar{k}_z^2\bar{k}_x^2] \pm \gamma_{10}[\bar{k}^{-2}(\bar{k}_x^2\bar{k}_y^2+\bar{k}_y^2\bar{k}_z^2+\bar{k}_z^2\bar{k}_x^2) - 9\bar{k}_x^2\bar{k}_y^2\bar{k}_z^2\}\right]^{1/2} \tag{R1.9}$$

where $\bar{\alpha}_{10} = \bar{\alpha}_{11} + \bar{\alpha}_{12}\bar{k}$, $\bar{\beta}_{10} = \bar{\beta}_{11} + \bar{\beta}_{12}\bar{k}$ *and* $\bar{\gamma}_{10} = \bar{\gamma}_{11} + \bar{\gamma}_{12}\bar{k}$ in which, $\bar{\alpha}_{11} = -2132 \times 10^{-40} eVm^4$, $\bar{\alpha}_{12} = 9030 \times 10^{-50} eVm^5$, $\bar{\beta}_{11} = -2493 \times 10^{-40} eVm^4$, $\bar{\beta}_{12} = 12594 \times 10^{-50} eVm^5$,

$\bar{\gamma}_{11} = 30 \times 10^{-30} eVm^3$ *and* $\bar{\gamma}_{12} = 154 \times 10^{-42} eVm^4$.

(ii) In accordance with Johnson and Dickey [176], the electron energy spectrum assumes the form

$$\bar{E} = -\frac{\bar{E}_{g_0}}{2\bar{m}_v} + \frac{\hbar^2\bar{k}^2}{2}\left[\frac{1}{\bar{m}_o}+\frac{1}{\bar{m}_{\gamma b}}\right]\frac{\bar{E}_{g_0}}{2}\left[1+4\frac{\hbar^2\bar{k}^2}{2\bar{m}'_c}\frac{\bar{f}_1(\bar{E})}{\bar{E}_{g_0}}\right]^{1/2}$$

where

$$\frac{\bar{m}_o}{m'_c} \equiv P_2\left[\frac{\bar{E}_{g_0}+\frac{2\Delta}{3}}{\bar{E}_{g_0}(\bar{E}_{g_0}+\Delta)}\right], f_1(\bar{E}) \equiv \frac{(\bar{E}_{g_0}+\Delta)(E+\bar{E}_{g_0}+\frac{2\Delta}{3})}{\left(\bar{E}_{g_0}+\frac{2\Delta}{3}\right)(E+\bar{E}_{g_0}+\Delta)}, \bar{m}'_c = 0.139\bar{m}_0 \text{ and}$$

$$\bar{m}_{\gamma b} = \left[\frac{1}{\bar{m}'_c} - \frac{2}{m_0}\right]$$

(iii) In accordance with Agafonov et al. [177], the electron energy spectrum can be written as

$$\bar{E} = -\frac{\eta-\bar{E}_{g_0}}{2}\left[1-\frac{\hbar^2\bar{k}^2}{2\bar{\eta}\bar{m}^*}\left\{\frac{\bar{D}\sqrt{3}-3\bar{B}}{2\left(\frac{\hbar^2}{2\bar{m}^*}\right)}\right\}\left[\frac{\bar{k}_x^4+\bar{k}_y^4+\bar{k}_z^4}{\bar{k}^4{}_c}\right]^{1/2}\right. \tag{R1.10}$$

where

$$\bar{\eta} \equiv \left(\bar{E}_{g_0}^2 + \frac{8}{3}\bar{P}^2\bar{k}^2\right)^{1/2},\ \bar{B} \equiv -21\frac{\hbar^2}{2\bar{m}_0}$$

and

$$\bar{D} \equiv -40\left(\frac{\hbar^2}{2\bar{m}_0}\right)$$

(e) The energy spectrum of the carriers in the two higher valance bands and the single lower valance band of Te can, respectively, be expressed as [179]

$$\bar{E} = \bar{A}_{10}\bar{k}_z^2 + \bar{B}_{10}\bar{k}_s^2 \pm [\Delta_{10}^2 + (\beta_{10}\bar{k}_z)^2]^{1/2} \text{ and } \bar{E} = \Delta_{||} + \bar{A}_{10}\bar{k}_z^2 + \bar{B}_{10}k_s^2 \pm \beta_{10}\bar{k}_z \quad \text{(R1.11)}$$

where $\bar{E}$ is the energy of the hole as measured from the top of the valance and within it,
$\bar{A}_{10} = 3.77 \times 10^{-19} eVm^2$, $\bar{B}_{10} = 3.57 \times 10^{-19} eVm^2$, $\Delta_{10} = 0.628eV$, $(\bar{B}_{10})^2 = 6 \times 10^{-20}$ $(eVm)^2$ and $\Delta_{||} = 1004 \times 10^{-5} eV$ are the spectrum constants.

(f) The dispersion relation in graphite can be written following Brandt [180] as

$$\bar{E} = \frac{1}{2}[\bar{E}_2 + \bar{E}_3] \pm \left[\frac{1}{4}(\bar{E}_2 - \bar{E}_3)^2 + \eta_2^2 k^2\right]^{1/2} \quad \text{(R1.12)}$$

where

$$\bar{E}_2 \equiv \bar{\Delta} - 2\bar{\gamma}_1 \cos\phi_0, \phi_0 \equiv \frac{\bar{c}_6\bar{k}_z}{2},\ \bar{E}_3 \equiv 2\bar{\gamma}_2\cos^2\phi_0$$

and $\eta_2 \equiv \left(\frac{\sqrt{3}}{2}\right)\bar{a}_6(\bar{\gamma}_0 + 2\bar{\gamma}_4\cos\phi_0)$ in which the band constants are $\bar{\Delta}$, $\bar{\gamma}_0$, $\bar{\gamma}_1$, $\bar{\gamma}_2$, $\bar{\gamma}_4$, $\bar{\gamma}_5$, $\bar{a}_6$ and $\bar{c}_6$, respectively.

(g) The dispersion relation of the holes in p- InSb can be written in accordance with Cunningham [181–185] as

$$\bar{E} = \bar{c}_4(1 + \gamma_4\bar{f}_4)\bar{k}^2 \pm \frac{1}{3}\left[2\sqrt{2}\sqrt{\bar{c}_4}\sqrt{16 + 5\gamma_4}\sqrt{\bar{E}_4\bar{g}_4\bar{k}}\right] \quad \text{(R1.13)}$$

where

$$\bar{c}_4 \equiv \frac{\hbar^2}{2\bar{m}_0} + \theta_4,\ \theta_4 \equiv 4.7\frac{\hbar^2}{2\bar{m}_0}, \gamma_4 \equiv \frac{\bar{b}_4}{\bar{c}_4}, \bar{b}_4 \equiv \frac{3}{2}\bar{b}_5 + 2\theta_4, \bar{b}_5 \equiv 2.4\frac{\hbar^2}{2\bar{m}_0},$$

$$\bar{f}_4 \equiv \frac{1}{4}[\sin^2 2\theta + \sin^4\theta\sin^2 2\phi],$$

θ is measured from the positive z- axis, ϕ is measured from positive x-axis, $\bar{g}_4 \equiv \sin\theta[\cos^2\theta + \frac{1}{4}\sin^4\theta\sin^2 2\phi]$ *and* $\bar{E}_4 = 5\times10^{-4}eV$

(h) The energy spectrum of the valance bands of CuClin accordance with Yekimovet. Al. [183] can be written as

$$\bar{E}_h = (\gamma_6 - 2\gamma_7)\frac{\hbar^2\bar{k}^2}{2\bar{m}_0} \tag{R1.14}$$

and

$$\bar{E}_{l,s} = (\gamma_6 + \gamma_7)\frac{\hbar^2\bar{k}^2}{2\bar{m}_0} - \frac{\Delta_1}{2} \pm \left[\frac{\Delta_1^2}{4} + \gamma_7\Delta_1\frac{\hbar^2\bar{k}^2}{2\bar{m}_0} + 9\left(\frac{\gamma_7\hbar^2\bar{k}^2}{2\bar{m}_0}\right)^2\right]^{1/2} \tag{R1.15}$$

where

$$\gamma_6 = 0.53,\ \gamma_7 = 0.07,\ \Delta_1 = 70meV.$$

(i) In the presence of stress, χ_6 along <001> and <111> directions, the energy spectra of the holes in Materials having diamond structure valance bands can be, respectively, expressed following Roman [184] et al. as

$$\bar{E} = \bar{A}_6\bar{k}^2 \pm [\bar{B}_7^2 + \delta_6^2 + \bar{B}_7\delta_6(2\bar{k}_z^2 - \bar{k}_s^2)]^{1/2} \tag{R1.16}$$

and

$$\bar{E} = \bar{A}_6\bar{k}^2 \pm \left[\bar{B}_7^2\bar{k}^4 + \delta_7^2 + \frac{\bar{D}_6}{\sqrt{3}}\delta_7(2\bar{k}_z^2 - \bar{k}_s^2)\right]^{1/2} \tag{R1.17}$$

where $\bar{A}_6$, $\bar{B}_7$, $\bar{D}_6$ and $\bar{C}_6$ are inverse mass band parameters in which $\delta_6 \equiv \bar{l}_7(\bar{S}_{11} - \bar{S}_{12})\chi_6$,, $\bar{S}_{ij}$ are the usual elastic compliance constants, $\bar{B}_7^2 \equiv (\bar{B}_7^2 + \frac{\bar{c}_6^2}{5})$ *and* $\delta_7 \equiv (\frac{\bar{d}_g\bar{S}_{44}}{2\sqrt{3}})\chi_6$. For gray tin, $\bar{d}_8 = -4.1eV$, $\bar{l}_7 = -2.3eV$, $\bar{A}_6 = 19.2\frac{\hbar^2}{2\bar{m}_0}$, $\bar{B}_7 = 26.3\frac{\hbar^2}{2\bar{m}_0}$, $\bar{D}_6 = 31\frac{\hbar^2}{2\bar{m}_0}$ *and* $\bar{c}_6^2 = -1112\frac{\hbar^2}{2\bar{m}_0}$.

(R. 1.2) Investigate the entropy for bulk specimens of the heavily–doped materials in the presences of Gaussian, exponential, Kane, Halperian, Lax and Bonch-Burevich types of band tails [37] for all systems whose unperturbed carrier energy spectra are defined in R1.1.

(R. 1.3) Investigate the entropy for QWs of all the HD materials as considered in R1.2.

(R. 1.4) Investigate the entropy for HD bulk specimens of the negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field.

(R. 1.5) Investigate the entropy for the QWs of HD negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field.

(R. 1.6) Investigate the entropy for the multiple QWs of HD materials whose unperturbed carrier energy spectra are defined in R1.1

(R. 1.7) Investigate the entropy for all the appropriate HD low dimensional systems of this chapter in the presence of finite potential wells.

(R. 1.8) Investigate the entropy for all the appropriate HD low dimensional systems of this chapter in the presence of parabolic potential wells.

(R. 1.9) Investigate the entropy for all the appropriate HD systems of this chapter forming quantum rings.

(R 1.10) Investigate the entropy for all the above appropriate problems in the presence of elliptical Hill and quantum square rings.

(R. 1.11) Investigate the entropy for parabolic cylindrical HD low dimensional systems in the presence of an arbitrarily oriented alternating electric field for all the HD materials whose unperturbed carrier energy spectra are defined in R1.1.

(R. 1.12) Investigate the entropy for HD low dimensional systems of the negative refractive index and otheradvanced optical materials in the presence of an arbitrarily oriented alternating electric field and nonuniform light waves.

(R. 1.13) Investigate the entropy for triangular HD low dimensional systems of the negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field in the presence of strain.

(R. 1.14) Investigate the entropy in HD QWs of nonparabolic materials as discussed in this chapter in the presence of nonuniform magnetic field.

(R. 1.15) Investigate the entropy for all the problems of (R1.14) in the presence of arbitrarily oriented magnetic field.

(R. 1.16) Investigate the entropy for all the problems of (R1.14) in the presence of alternating electric field.

(R. 1.17) Investigate the entropy for all the problems of (R1.14) in the presence of alternating magnetic field.

(R. 1.18) Investigate the entropy for all the problems of (R1.14) in the presence of crossed electric field and quantizing magnetic fields.

(R. 1.19) Investigate the entropy for all the problems of (R1.14) in the presence of crossed alternating electric field and alternating quantizing magnetic fields.

(R. 1.20) Investigate the entropy for HD QWs of the negative refractive index, organic and magnetic materials in the presence of nonuniform electric field.

(R. 1.21) Investigate the entropy for HD QWs of the negative refractive index, organic and magnetic materials in the presence of alternating time dependent nonuniform magnetic field.

(R. 1.22) Investigate the entropy for HD QWs of the negative refractive index, organic and magnetic materials in the presence of in the presence of crossed alternating electric field and alternating quantizing nonuniform magnetic fields.

(R. 1.23) a) Investigate the entropy for HD low dimensional systems of the negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field considering many body effects.

b) Investigate all the appropriate problems of this chapter for a Dirac electron.

(R. 1.24) investigate all the appropriate problems of this chapter by including the many body, image force, broadening and hot carrier effects, respectively.

(R. 1.25) Investigate all the appropriate problems of this chapter by removing all the mathematical approximations and establishing the respective appropriate uniqueness conditions.

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2 The entropy in nanowires of heavily doped materials

To be the best, I must extract the best from myself.

2.1 Introduction

It is well known that in nanowires (NWs), the restriction of the motion of the carriers along two directions may be viewed as carrier confinement by two infinitely deep one-dimensional (1D) rectangular potential wells, along any two orthogonal directions leading to quantization of the wave vectors along the said directions, allowing 1D carrier transport [1]. With the help of modern experimental techniques, such1D quantized structures have been experimentally realized and enjoy an enormous range of important applications in the realm of nanoscience in the quantum regime. They have generated much interest in the analysis of nano-structured devices for investigating their electronic, optical and allied properties [2–4]. Examples of such new applications are based on the different transport properties of ballistic charge carriers which include quantum resistors [5–10], resonant tunneling diodes and band filters [11, 12], quantum switches [13], quantum sensors [14–16], quantum logic gates [17–18], quantum transistors and sub tuners [19–21], heterojunction FETs [22], high-speed digital networks [23], high-frequency microwave circuits [24], optical modulators [25], optical switching systems [26, 27], and other devices.

In this chapter through Sections 2.2.1–2.2.14 we have investigated the entropy's in NWs of heavily doped (HD) nonlinear optical, III–V, II–VI, stressed Kane type, Te, GaP, $PtSb_2$, Bi_2Te_3, Ge, GaAs, II–V, lead germanium telluride and zinc and cadmium phosphides respectively. Section 2.3 contains the summary and conclusions pertaining to this chapter. Section 2.4 presents 19 open research problems.

2.2 Theoretical background

2.2.1 The entropy in NWs of HD nonlinear optical materials

The dispersion relation of 1D electrons in this case can be written following (1.32) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{||}\bar{T}_{21}(\bar{E},\eta_g)} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}^*_{||}\bar{T}_{22}(\bar{E},\eta_g)} + \frac{\hbar^2\bar{k}_x{}^2}{2\bar{m}^*_{||}\bar{T}_{21}(\bar{E},\eta_g)} = 1 \tag{2.1}$$

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where $\bar{n}_z(=1,2,3,.....)$, $\bar{d}_z$ are the size quantum number and the nanothickness along the z-direction respectively, $\bar{n}_y(=1,2,3,.....)$ and $\bar{d}_y$ are the size quantum number and the nanothickness along the y-direction respectively

The 1D DOS function per sub-band is given by

$$\bar{N}_{1D}(\bar{E}) = \frac{2\bar{g}_v}{\pi}\frac{\partial \bar{k}_x}{\partial \bar{E}} \tag{2.2}$$

The complex sub-band energy ($\bar{E}'_{1HDNW}$) can be expressed in this case as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{||}T_{21}(\bar{E}'_{1HDNW},\eta_g)} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}^*_{\perp}\bar{T}_{22}(\bar{E}'_{1HDNW},\eta_g)} = 1 \tag{2.3}$$

The EEM in this case in given by

$$\bar{m}^*(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g) = \frac{\hbar^2}{2}\left[\text{Real part of}\frac{\partial}{\partial(\bar{E}_{F1HDNW})}[\bar{T}_{1HDNW}(\bar{E},\bar{n}_y,\bar{n}_z,\eta_g)]^2\right] \tag{2.4}$$

where,

$$\bar{T}_{1HDNW}(\bar{E},\bar{n}_y,\bar{n}_z,\eta_g) = \left[\left[1-\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{||}\bar{T}_{21}(\bar{E},\eta_g)} - \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}^*_{\perp}\bar{T}_{22}(\bar{E},\eta_g)}\right]\frac{2\bar{m}^*_{\perp}\bar{T}_{22}(\bar{E},\eta_g)}{\hbar^2}\right]^{1/2}$$

and $\bar{E}_{F1HDNW}$ is the Fermic energy in this case

Thus, we observe that the EEM is the function of size quantum numbers in both the directions and the Fermi energy due to the combined influence of the crystal filed splitting constant and the anisotropic spin-orbit splitting constants respectively. Besides it is a function of η_g due to which the EEM exists in the band gap, which is otherwise impossible.

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right)\text{Real part of}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{\max}}}[\bar{T}_{1HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)+\bar{T}_{2HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)] \tag{2.5}$$

and

$$\bar{T}_{2HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{T}_{1HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)]$$

Using (2.5) and (1.31f) we can find the entropy in this case.

In the absence of bandtails, for electron motion along x-direction only, the 1D electron dispersion law in this case can be written following (1.2) as

$$\gamma(\bar{E}) = \bar{f}_1(\bar{E})k_x^2 + \bar{f}_1(\bar{E})(\pi\bar{n}_y/\bar{d}_y)^2 + \bar{f}_2(\bar{E})(\pi\bar{n}_z/\bar{d}_z)^2 \tag{2.6}$$

The sub-band energy($\bar{E}'_1$) are given by the equation

$$\gamma(\bar{E}_1{}') = f_1(\bar{E}_1{}')(\pi\bar{n}_y/\bar{d}_y)^2 + f_2(\bar{E}_1{}')(\pi\bar{n}_z/\bar{d}_z)^2 \tag{2.7}$$

The electron concentration per unit length can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{t}_1(\bar{\mathrm{E}}_{F1d},\bar{\mathrm{n}}_y,\bar{\mathrm{n}}_z) + \bar{t}_2(\bar{\mathrm{E}}_{F1d},\bar{\mathrm{n}}_y,\bar{\mathrm{n}}_z)] \tag{2.8}$$

where $\bar{E}_{F1d}$ is the Fermic energy in this case,

$$t_1(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z) \equiv [\gamma(\bar{E}_{F1d}) - \bar{f}_1(\bar{E}_{F1d})(\pi\bar{n}_y/\bar{d}_y)^2 - \bar{f}_2(\bar{E}_{F1d})(\pi\bar{n}_z/\bar{d}_z)^2]^{1/2}[\bar{f}_1(\bar{E}_{F1d})]^{-1/2}$$

and

$$\bar{t}_2(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}} L(r)[\bar{t}_1(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)]$$

using (1.44) and (2.8), we can find entropy in this case.

2.2.2 The entropy in NWsof HD III–V materials

(i) Three-band model of Kane

The dispersion relation of 1D electrons in this case can be written following (1.55) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2\bar{k}_x{}^2}{2\bar{m}_c} = \bar{T}_{31}(\bar{E},\eta_g) + i\bar{T}_{31}(\bar{E},\eta_g) \tag{2.9}$$

The sub-band energy ($\bar{E}'_{2HDNW}$) in this case can be expressed as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} = \bar{T}_{31}(\bar{E}'_{2HDNW},\eta_g) + i\bar{T}_{31}(\bar{E}'_{2HDNW},\eta_g) \tag{2.10}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW},\eta_g) = \bar{m}_c[\bar{T}_{31}{}'(\bar{E}_{F1HDNW},\eta_g)] \tag{2.11}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right)\mathrm{Re}al\ Part\ of \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{T}_{3HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g) + \bar{T}_{4HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)] \tag{2.12}$$

where

$$\bar{T}_{3HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \left[\left[\bar{T}_{31}(\bar{E}_{F1HDNW}, \eta_g) + \bar{i}\bar{T}_{31}(\bar{E}_{F1HDNW}, \eta_g) - \frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} - \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}\right]\frac{2\bar{m}_c}{\hbar^2}\right]^{1/2}$$

where

$$\bar{T}_{4HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{T}_{3HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)]$$

Using (1.31f) and (2.12) we can investigate the entropy in this case.

In the absence of doping, 1D electron dispersion law is given by

$$\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c} + \bar{G}_2(\bar{n}_y, \bar{n}_z) = \bar{I}_{11}(\bar{E}) \tag{2.13}$$

where

$$\bar{G}_2(\bar{n}_y, \bar{n}_z) \equiv (\hbar^2\pi^2/2\bar{m}_c)[(\bar{n}_y/\bar{d}_y)^2 + (\bar{n}_z/\bar{d}_z)^2]$$

The sub-band energy $\bar{E}'_2$ can be written as

$$\bar{G}_2(\bar{n}_y, \bar{n}_z) = \bar{I}_{11}(\bar{E}'_2) \tag{2.14}$$

The electron statistics in this case can be written as

$$\bar{n}_{1D} = \frac{2\bar{g}_v\sqrt{2\bar{m}_c}}{\pi\hbar}\sum_{n_y=1}^{\bar{n}_{y\max}}\sum_{n_z=1}^{\bar{n}_{z\max}}[\bar{t}_3(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) + \bar{t}_4(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)] \tag{2.15}$$

where

$$\bar{t}_3(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) \equiv [\bar{I}_{11}(\bar{E}_{F1d}) - \bar{G}_2(\bar{n}_y, \bar{n}_z)]^{1/2}$$

and

$$\bar{t}_4(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{t}_3(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)]$$

Thus using (1.44) and (2.15), we can study the entropy in this case.

(ii) Two band model of Kane

The dispersion relation under heavy doping of 1D electrons in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c}+\frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}+\frac{\hbar^2\bar{k}_x{}^2}{2\bar{m}_c}=\gamma_2(\bar{E},\eta_g) \tag{2.16}$$

The sub-band energy ($\bar{E}'_{3HDNW}$) in this case can be expressed as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c}+\frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}=\gamma_2(\bar{E}'_{3HDNW},\eta_g) \tag{2.17}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW},\eta_g)=\bar{m}_c[\gamma_2{}'(\bar{E}_{F1HDNW},\eta_g)] \tag{2.18a}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{T}_{7HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)+\bar{T}_{8HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)] \tag{2.18b}$$

where

$$\bar{T}_{7HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\left[\left[\gamma_2(\bar{E}_{F1HDNW},\eta_g)-\frac{\bar{}h^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c}-\frac{\bar{}h^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}\right]\frac{2\bar{m}_c}{\bar{}h^2}\right]^{1/2}$$

and

$$\bar{T}_{8HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{T}_{7HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)]$$

Thus using (1.44) and (2.18b) we can study the entropy in this case.

The expression of 1D dispersion relation, for NWs of III-V materials whose energy band structures are defined by the two-band model of Kane in the absence of band tailing assumes the form

$$\bar{E}(1+\alpha\bar{E})=\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c}+\bar{G}_2(\bar{n}_y,\bar{n}_z) \tag{2.19}$$

In this case, the quantized energy $\bar{E}'_3$ is given by

$$\bar{E}'_3=(2\alpha)^{-1}\left[-1+\sqrt{1+4\alpha\bar{G}_2(\bar{n}_y,\bar{n}_z)}\right] \tag{2.20}$$

The carrier statistics in the case can be expressed as

$$\bar{n}_{1D}=\frac{2\bar{g}_v}{\pi}\frac{\sqrt{2\bar{m}_c}}{\hbar}\sum_{\bar{n}y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{t}_5(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)+\bar{t}_6(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.21}$$

where,

$$\bar{t}_5(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) \equiv [\bar{E}_{F1d}(1 + \alpha\bar{E}_{F1d}) - \bar{G}_2(\bar{n}_y, \bar{n}_z)]^{1/2}$$

and

$$\bar{t}_6(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{t}_5(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)]$$

Thus using (1.44) and (2.21) we can study the entropy in this case.

(iii) Parabolic energy bands

The dispersion relation of 1D electrons under the condition of heavy doping this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2\bar{k}_x{}^2}{2\bar{m}_c} = \gamma_3(\bar{E}, \eta_g) \tag{2.22}$$

The sub-band energy ($\bar{E}'_{5HDNW}$) in this case can be expressed as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} = \gamma_3(\bar{E}'_{5HDNW}, \eta_g) \tag{2.23}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW}, \eta_g) = \bar{m}_c[\gamma_3{}'(\bar{E}_{F1HDNW}, \eta_g)] \tag{2.24a}$$

Thus the carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right) \sum_{\bar{n}y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \left[\bar{T}_{9HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) + \bar{T}_{10HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)\right] \tag{2.24b}$$

where,

$$\bar{T}_{9HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \left[\left[\gamma_3(\bar{E}_{F1HDNW}, \eta_g) - \frac{\bar{h}^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} - \frac{\bar{h}^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}\right]\frac{2\bar{m}_c}{\bar{h}^2}\right]^{1/2},$$

and

$$T_{10HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{T}_{9HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)]$$

Thus using (1.44) and (2.24b) we can study the entropy in this case.

The expression of 1D dispersion relation, for NWs of III-V materials whose energy band structures are defined by parabolic isotropic energy bands in the absence of band tailing assumes that

$$\bar{E} = \frac{\hbar^2 \bar{k}_x^2}{2\bar{m}_c} + \bar{G}_2(\bar{n}_y, \bar{n}_z) \tag{2.25}$$

In this case, the quantized energy $\bar{E}'_7$ is given by

$$\bar{E}'_7 = \bar{G}_2(\bar{n}_y, \bar{n}_z) \tag{2.26}$$

The carrier statistics in the case can be expressed as

$$\bar{n}_{1D} = \frac{2\bar{g}_v\sqrt{2\bar{m}_c \pi \bar{k}_B \bar{T}}}{h} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{\frac{-1}{2}}(\eta_{67}), \tag{2.27}$$

where

$$\eta_{67} = \left[\frac{\bar{E}_{F1d-}(\bar{E}'_7 + \bar{W} - \bar{h}\bar{\nu})}{\bar{k}_B \bar{T}}\right]$$

Using(1.44) and (2.27), we can write

$$\bar{G} = \left(\frac{\pi^2 \bar{k}_B}{3\bar{e}}\right)\left[\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{\frac{-1}{2}}(\eta_{67})\right]^{-1} \cdot \left[\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{\frac{-3}{2}}(\eta_{67})\right] \tag{2.28}$$

Under the condition of non degeneracy, (2.28) get transformed into the well-known expression as given in the preface.

(iv) The Model of Stillman et al.

The dispersion relation of 1D electrons under heavy doping in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2 \bar{k}_x^{\,2}}{2\bar{m}_c} = \theta_4(\bar{E}, \eta_g) \tag{2.29}$$

where,

$$\theta_4(\bar{E}, \eta_g) = \bar{I}_{12}(\bar{E}, \eta_g)$$

The sub-band energy ($\bar{E}'_{9HDNW}$) in this case can be expressed as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} = \theta_4(\bar{E}'_{9HDNW}, \eta_g) \tag{2.30}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1HDNW},\eta_g)=\bar{m}_c[\theta_4{}'(\bar{E}_{F1HDNW},\eta_g)] \tag{2.31a}$$

The carrier statistics canbe written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{T}_{11HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)+\bar{T}_{12HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)] \tag{2.31b}$$

where,

$$\bar{T}_{11HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\left[\left[\theta_4(\bar{E}_{F1HDNW},\eta_g)-\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c}-\frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}\right]\frac{2\bar{m}_c}{\hbar^2}\right]^{1/2}$$

Thus using (1.31f) and (2.31b) we can study the entropy in this case.

The expression of 1D dispersion relation for NWs of III–V materials whose energy band structures are defined by the model of Stillman et al in the absence of band tailing assumes the form

$$\bar{I}_{12}(\bar{E})=\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c}+\bar{G}_2(\bar{n}_y,\bar{n}_z) \tag{2.32}$$

In this case, the quantized energy $\bar{E}'_9$ is given by

$$\bar{I}_{12}(\bar{E}'_9)=\bar{G}_2(\bar{n}_y,\bar{n}_z) \tag{2.33}$$

The carrier statistics in the case can be expressed as

$$\bar{n}_{1D}=\frac{2\bar{g}_v}{\pi}\frac{\sqrt{2\bar{m}_c}}{\hbar}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{P}_9(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)+\bar{Q}_9(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.34}$$

where

$$\bar{P}_9(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)\equiv[\bar{I}_{12}(\bar{E}_{F1d})-\bar{G}_2(\bar{n}_y,\bar{n}_z)]^{1/2}$$

and

$$\bar{Q}_9(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)\equiv\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{P}_9(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)]$$

Thus using (1.44) and (2.34), we can study the entropy in this case.

(v) The Model of Palik et al.

The dispersion relation of 1D electrons in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2\bar{k}_x{}^2}{2\bar{m}_c} = \theta_5(\bar{E}, \eta_g) \tag{2.35}$$

where

$$\theta_5(\bar{E}, \eta_g) = \bar{I}_{13}(\bar{E}, \eta_g)$$

The sub-band energy ($\bar{E}'_{10HDNW}$) in this case can be expressed as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} = \theta_5(\bar{E}'_{10HDNW}, \eta_g) \tag{2.36}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW}, \eta_g) = \bar{m}_c[\theta_5{}'(\bar{E}_{F1HDNW}, \eta_g)] \tag{2.37a}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{T}_{13HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) + \bar{T}_{14HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)] \tag{2.37b}$$

where

$$\bar{T}_{13HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \left[\left[\theta_5(\bar{E}_{F1HDNW}, \eta_g) - \frac{\bar{}h^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\bar{}h^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}\right]\frac{2\bar{m}_c}{\bar{}h^2}\right]^{1/2}$$

and

$$\bar{T}_{14HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{T}_{13HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)]$$

Thus, using (1.31f) and (2.37b), we can investigate the entropy in this case.

The expression of 1D dispersion relation for NWs of III–V materials whose energy band structures are defined by the model of Palik et al in the absence of band tailing assumes the form

$$\bar{I}_{13}(\bar{E}) = \frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c} + \bar{G}_2(\bar{n}_y, \bar{n}_z) \tag{2.38}$$

In this case, the quantized energy $\bar{E}'_{10}$ is given by

$$\bar{I}_{13}(\bar{E}'_{10}) = \bar{G}_2(\bar{n}_y, \bar{n}_z) \tag{2.39}$$

The carrier statistics in the case can be expressed as

$$\bar{n}_{1D} = \frac{2\bar{g}_v}{\pi}\frac{\sqrt{2\bar{m}_c}}{\hbar}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\left[\bar{P}_{11}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)+\bar{Q}_{12}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)\right] \tag{2.40}$$

where

$$\bar{P}_{11}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z) \equiv \left[\bar{I}_{13}(\bar{E}_{F1d})-\bar{G}_2(\bar{n}_y,\bar{n}_z)\right]^{1/2}$$

and

$$\bar{Q}_{12}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{P}_{11}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)\right]$$

Using (1.44) and (2.40), we can study the entropy in this case.

2.2.3 The entropy in nanowires of HD II–VI materials

The 1D electron dispersion law in NW of HD II–VI materials can be written following (1.141) as

$$\gamma_3(\bar{E},\eta_g) = \bar{a}'_0\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\pm\bar{\lambda}_0\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}^*_{||}} \tag{2.41}$$

The sub-band energy ($\bar{E}'_{13HDNW}$) in this case can be expressed as

$$\gamma_3(\bar{E}'_{13HDNW},\eta_g) = \bar{a}'_0\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\pm\bar{\lambda}_0\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2} \tag{2.42}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW},\eta_g) = \bar{m}^*_{||}\gamma'_3(\bar{E}_{F1HDNW},\eta_g) \tag{2.43}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\left[\bar{T}_{17HDNW}(\bar{E}_{F1HDNW},\bar{n}_x,\bar{n}_y,\eta_g)+\bar{T}_{18HDNW}(\bar{E}_{F1HDNW},\bar{n}_x,\bar{n}_y,\eta_g)\right] \tag{2.44}$$

Where,

$$\bar{T}_{17HDNW}(\bar{E}_{F1HDNW},\bar{n}_x,\bar{n}_y,\eta_g) = \left[\left[\gamma_3(\bar{E}_{F1HDNW},\eta_g)-\bar{a}'_0\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right.\right.$$

$$\mp \bar{\lambda}_0 \left[\left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)^2 + \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 \right]^{1/2} \left] \left(\frac{2\bar{m}^*_{\|}}{\hbar^2} \right) \right]^{1/2}$$

and

$$\bar{T}_{18HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) [T_{17HDNW}(E_{F1HDNW}, n_x, n_y, \eta_g)]$$

Using (1.31f) and (2.44), we can study the entropy in this case.

The 1D dispersion relation for NWs of II–VI materials in the absence of band-tails can be written as

$$\bar{E} = \bar{b}'_0 \bar{k}_z^2 + \bar{G}_{3,\pm}(\bar{n}_x, \bar{n}_y) \tag{2.45}$$

where,

$$\bar{G}_{3,\pm}(\bar{n}_x, \bar{n}_y) \equiv \left[\bar{a}'_0 \left\{ \left(\frac{\pi \bar{n}_x}{\bar{d}_x} \right)^2 + \left(\frac{\pi \bar{n}_y}{\bar{d}_y} \right)^2 \right\} \pm \bar{\lambda}_0 \left\{ \left(\frac{\pi \bar{n}_x}{\bar{d}_x} \right)^2 + \left(\frac{\pi \bar{n}_y}{\bar{d}_y} \right)^2 \right\}^{1/2} \right]$$

The 1D electron statistics can be written as

$$\bar{n}_{1D} = \frac{\bar{g}_v \sqrt{2\bar{m}^*_{\|} \pi \bar{k}_B \bar{T}}}{\bar{h}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{\frac{-1}{2}}(\eta_{68,\pm}), \eta_{68,\pm} = (\bar{k}_B \bar{T})^{-1} [\bar{E}_{F1d} - [\bar{G}_{3,\pm}(\bar{n}_x, \bar{n}_y)]] \tag{2.46}$$

Thus using (1.44) and (2.46) we can study the entropy in this case.

2.2.4 The entropy in nanwires of HD IV–VI materials

(i) Dimmock Model

The 1D electron dispersion law in NW of HD IV–VI materials can be expressed following (1.174) as

$$\gamma_2(\bar{E}, \eta_g) + \alpha\gamma_3(\bar{E}, \eta_g) \left(\frac{\hbar^2}{2\bar{x}_4} \left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)^2 + \frac{\hbar^2}{2\bar{x}_5} \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 \right) + \alpha\gamma_3(\bar{E}, \eta_g) \frac{\hbar^2}{2\bar{x}_6} k_z^2$$
$$- (1 + \alpha\gamma_3(\bar{E}, \eta_g)) \left(\frac{\hbar^2}{2\bar{x}_1} \left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)^2 + \frac{\hbar^2}{2\bar{x}_2} \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 \right)$$
$$- \alpha \left(\frac{\hbar^2}{2\bar{x}_1} \left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)^2 + \frac{\hbar^2}{2\bar{x}_2} \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 \right)$$

$$
\begin{aligned}
&-\alpha\left(\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\frac{\hbar^2}{2\bar{x}_6}\bar{k}_z^2\\
&-(1+\alpha\gamma_3(\bar{E},\eta_g))\frac{\hbar^2}{2\bar{x}_3}\bar{k}_z^2\\
&-\alpha\frac{\hbar^2}{2\bar{x}_3}\bar{k}_z^2\left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\\
&-\alpha\frac{\hbar^4\bar{k}_z^4}{4\bar{x}_3\bar{x}_6}=\frac{\hbar^2}{2\bar{m}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{m}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\frac{\hbar^2}{2\bar{m}_3}\bar{k}_z^2
\end{aligned}
\tag{2.47}
$$

Equation (2.47) can be written as

$$
\bar{k}_z=\bar{T}_{36}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y) \tag{2.48}
$$

where

$$
\begin{aligned}
\bar{T}_{36}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)&=[(2\bar{C}_{22})^{-1}[-\bar{B}_{HD}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)\\
&+\sqrt{\bar{B}^2{}_{HD}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)+4\bar{C}_{22}\bar{A}_{HD}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)}\,]]^{1/2}\\
\bar{C}_{22}=\left(\bar{\alpha}\frac{\hbar^4}{4\bar{x}_3\bar{x}_6}\right),\ \bar{B}_{HD}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)&=\left[\bar{\alpha}\left(\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\frac{\hbar^2}{2\bar{x}_6}\right.\\
&+(1+\bar{\alpha}\gamma_3(\bar{E},\eta_g))\frac{\hbar^2}{2\bar{x}_3}-\bar{\alpha}\gamma_3(\bar{E},\eta_g)\frac{\hbar^2}{2\bar{x}_6}\\
&\left.+\frac{\hbar^2}{2\bar{m}_3}+\bar{\alpha}\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\right]
\end{aligned}
$$

and

$$
\begin{aligned}
\bar{A}_{HD}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)=&\left[-\left[\frac{\bar{}h^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\bar{}h^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\gamma_2(\bar{E},\eta_g)+\alpha\gamma_3(\bar{E},\eta_g)\right.\\
&\left(\frac{\bar{}h^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\bar{}h^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\\
&-\alpha\left(\frac{\bar{}h^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\bar{}h^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\left(\frac{\bar{}h^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\bar{}h^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\\
&\left.-(1+\alpha\gamma_3(\bar{E},\eta_g))\left(\frac{\bar{}h^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\bar{}h^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\right]
\end{aligned}
$$

The sub-band energy ($\bar{E}'_{14HDNW}$) in this case can be expressed as

$$0 = \bar{T}_{36}(\bar{E}'_{14HDNW}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{2.49}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\frac{\partial}{\partial \bar{E}}[\bar{T}^2_{36}(\bar{E}_{F1HDNW}, \eta_g, \bar{n}_x, \bar{n}_y)] \tag{2.50}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\bar{T}_{36HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) + \bar{T}_{37HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g)] \tag{2.51}$$

where

$$\bar{T}_{36HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) = \bar{T}_{36}(\bar{E}_{F1HDNW}, n_x, n_y, \eta_g)$$

and

$$\bar{T}_{37HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{T}_{36HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g)]$$

thus using (1.31f) and (2.51) we can study the entropy in this case.

The 1D electron dispersion law in NW of IV–VI materials in the absence of band tails can be expressed as

$$\begin{aligned}
&\bar{E}(1+\alpha\bar{E}) + \alpha\bar{E}\left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right) + \alpha\bar{E}\frac{\hbar^2}{2\bar{x}_6}\bar{k}_z^2 \\
&\quad - (1+\alpha\bar{E})\left(\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right) - \alpha\left(\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right) \\
&\quad \left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right) - \alpha\left(\frac{\hbar^2}{2\bar{x}_1}(\frac{\bar{n}_x\pi}{\bar{d}_x})^2 + \frac{\hbar^2}{2\bar{x}_2}(\frac{\bar{n}_y\pi}{\bar{d}_y})^2\right) \\
&\quad \frac{\hbar^2}{2x_6}k_z^2 - (1+\alpha\bar{E})\frac{\hbar^2}{2\bar{x}_3}\bar{k}_z^2 - \alpha\frac{\hbar^2}{2\bar{x}_3}k_z^2\left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right) \\
&\quad - \alpha\frac{\hbar^4\bar{k}_z^4}{4\bar{x}_3\bar{x}_6} = \frac{\hbar^2}{2\bar{m}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \frac{\hbar^2}{2\bar{m}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \frac{\hbar^2}{2\bar{m}_3}\bar{k}_z^2
\end{aligned} \tag{2.52}$$

Equation (2.52) can be written as

$$\bar{k}_z = \bar{T}_{40}(\bar{E}, \bar{n}_x, \bar{n}_y) \tag{2.53}$$

where

$$\bar{T}_{40}(\bar{E},\bar{n}_x,\bar{n}_y)=\left[(2\bar{C}_{22})^{-1}\left[-\bar{B}_0(\bar{E},\bar{n}_x,\bar{n}_y)+\sqrt{\bar{B}^2{}_0(\bar{E},\bar{n}_x,\bar{n}_y)+4\bar{C}_{22}\bar{A}_0(\bar{E},\bar{n}_x,\bar{n}_y)}\right]\right]^{1/2}$$

where

$$\bar{B}_0(\bar{E},\bar{n}_x,\bar{n}_y)=\left[\alpha\left(\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\frac{\hbar^2}{2\bar{x}_6}+(1+\alpha\bar{E})\frac{\hbar^2}{2\bar{x}_3}-\alpha\bar{E}\frac{\hbar^2}{2\bar{x}_6}\right.$$
$$\left.+\frac{\hbar^2}{2\bar{m}_3}+\alpha\frac{\hbar^2}{2\bar{x}_3}\left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\right]$$

and

$$\bar{A}_0(\bar{E},\bar{n}_x,\bar{n}_y)=\left[-\left[\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^2\right.$$
$$\bar{E}(1+\alpha\bar{E})+\alpha\bar{E}\left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)$$
$$-\alpha\left(\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\left(\frac{\hbar^2}{2\bar{x}_4}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_5}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)$$
$$\left.-(1+\alpha\bar{E})\left(\frac{\hbar^2}{2\bar{x}_1}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\frac{\hbar^2}{2\bar{x}_2}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right)\right]$$

The sub-band energy ($\bar{E}'_{20}$)in this case can be expressed as

$$0=\bar{T}_{40}(\bar{E}'_{20},\bar{n}_x,\bar{n}_y) \tag{2.54}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{T}^2_{40}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)] \tag{2.55}$$

The carrier statistics assumes the form

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\bar{T}_{40}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)+\bar{T}_{41}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)] \tag{2.56}$$

where

$$\bar{T}_{41}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{T}_{40}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)]$$

Thus using (1.44) and (2.56), we can study the entropy in this case.

(ii) Bangert and Kastner Model

The dispersion relation of the conduction electrons in bulk specimens of IV–VI materials in accordance with the model of Bangert and Kastner is given by

$$\omega_1(\bar{E})k_s^2 + \omega_2(\bar{E})k_z^2 = 1 \tag{2.57a}$$

where

$$\omega_1(\bar{E}) = (2\bar{E})^{-1}\left[\frac{(\bar{R})^2}{\bar{E}_{g_0}(1+\alpha_1\bar{E})} + \frac{(\bar{S})^2}{\Delta_c{}'(1+\alpha_2\bar{E})} + \frac{(\bar{Q})^2}{\Delta''_c(1+\alpha_3\bar{E})}\right]$$

and

$$\omega_2(\bar{E}) = (2\bar{E})^{-1}\left[\frac{(\bar{A})^2}{\bar{E}_{g0}(1+\alpha_1\bar{E})} + \frac{(\bar{S}+\bar{Q})^2}{\Delta''_c(1+\alpha_3\bar{E})}\right], (\bar{\mathrm{R}})^2 = 2.3\times10^{-10}(\bar{e}\bar{v})^2, (\bar{S})^2 = 4.6(\bar{\mathrm{R}})^2$$

$$\alpha_1 = \frac{1}{\bar{\mathrm{E}}_{g_0}}, \alpha_2 = \frac{1}{\bar{\Delta}_c{}'}, \alpha_3 = \frac{1}{\bar{\Delta}''_c},$$

$$\bar{\Delta}''_c = 3.28\bar{e}\bar{V}, \bar{\Delta}'_c = 3.07\bar{e}\bar{V}, \ (\bar{Q})^2 = 1.3(\bar{\mathrm{R}})^2, \ (\bar{A})^2 = 0.8\times10^{-4}(\bar{e}\bar{V}\bar{m}^2)$$

The electron energy spectrum in HD IV–VI materials in accordance with this model can be expressed by using the methods as given in chapter 1 as

$$\begin{aligned}2\bar{I}(4) = \bar{k}_s^2\Bigg[&\{\bar{c}_1(\bar{\alpha}_1,\bar{E},\bar{E}_{g_0}) - i\bar{D}_1(\bar{\alpha}_1,\bar{E},\bar{E}_{g_0})\}\frac{(\bar{R})^2}{\bar{E}_{go}} + \{\bar{c}_2(\bar{\alpha}_2,\bar{E},\bar{E}_{g_0}) - i\bar{D}_2(\bar{\alpha}_2,\bar{E},\bar{E}_{g_0})\}\frac{(\bar{S})^2}{\bar{\Delta}'_c}\\ &+ \{\bar{c}_3(\bar{\alpha}_3,\bar{E},\bar{E}_g) - i\bar{D}_3(\bar{\alpha}_3,\bar{E},\bar{E}_{g_0})\}\frac{(\bar{Q})^2}{\bar{\Delta}''_c}\Bigg] + \bar{k}_z^2\Bigg[\frac{2(\bar{A})}{\bar{E}_{go}}\{\bar{c}_1(\bar{\alpha}_1,\bar{E},\bar{E}_g) - i\bar{D}_1(\bar{\alpha}_1,\bar{E},\bar{E}_{g_0})\}\\ &+ \frac{(\bar{S}+\bar{Q})^2}{\bar{\Delta}''_c}\{\bar{c}_3(\bar{\alpha}_3,\bar{E},\bar{E}_{g_0}) - i\bar{D}_3(\bar{\alpha}_3,\bar{E},\bar{E}_{g_0})\}\end{aligned} \tag{2.57b}$$

where

$$\alpha_1 = \frac{1}{\bar{E}_{g_0}}, \alpha_2 = \frac{1}{\bar{\Delta}'_c}, \ \alpha_3 = \frac{1}{\bar{\Delta}''_c},$$

$$\bar{c}_1(\bar{\alpha}_1,\bar{E},\bar{E}_{g_0}) = \left[\frac{2}{\alpha_i\eta_g\sqrt{\pi}}\right]\exp(-\bar{u}_i^2)\times\left[\sum_{\bar{p}=1}^{\infty}\{\exp(-\bar{p}^2/4)(\sinh(\bar{p}\bar{u}_i))\}\bar{p}^{-1}\right]$$

$$\bar{D}_1(\bar{\alpha}_1, \bar{E}, \bar{E}_{g_0}) = \left[\frac{\sqrt{\pi}}{\alpha_1 \eta_g}\right] exp(-\bar{u}_i^2)$$

Therefore (2.57b) can be written as,

$$\bar{F}_1(\bar{E}, \eta_g)\bar{k}_s^2 + \bar{F}_2(\bar{E}, \eta_g)\bar{k}_z^2 = 1 \tag{2.57c}$$

where,

$$\bar{F}_1(\bar{E}, \eta_g)[2\gamma_0(\bar{E}, \eta_g)]^{-1}\left[\frac{(\bar{R})}{\bar{E}_g}\{\bar{c}_1(\bar{\alpha}_1, \bar{E}, \bar{E}_{g_0}) - i\bar{D}_1(\bar{\alpha}_1, \bar{E}, \bar{E}_{g_0})\}\right.$$
$$+ \frac{(\bar{S})}{\Delta'_c}\{\bar{c}_2(\bar{\alpha}_2, \bar{E}, \bar{E}_g) - i\bar{D}_2(\bar{\alpha}_2, \bar{E}, \bar{E}_{g_0})\}$$
$$\left. + \frac{(\bar{Q})}{\Delta'_c}\{\bar{c}_3(\bar{\alpha}_3, \bar{E}, \bar{E}_{g_0}) - i\bar{D}_3(\bar{\alpha}_3, \bar{E}, \bar{E}_{g_0})\}\right]$$

and

$$\bar{F}_2(\bar{E}, \eta_g)\left[2\gamma_0(\bar{E}, \eta_g)\right]^{-1}\left[\frac{2(\bar{A})}{\bar{E}_{g_0}}\{\bar{c}_1(\bar{\alpha}_1, \bar{E}, \bar{E}_g) - i\bar{D}_1(\bar{\alpha}_1, \bar{E}, \bar{E}_{g_0})\}\right.$$
$$\left. + \frac{(\bar{S} + \bar{Q})}{\Delta'_c}\{\bar{c}_3(\bar{\alpha}_3, \bar{E}, \bar{E}_g) - i\bar{D}_3(\bar{\alpha}_3, \bar{E}, \bar{E}_{g_0})\}\right]$$

Since $\bar{F}_1(\bar{E}, \eta_g)$ and $\bar{F}_2(\bar{E}, \eta_g)$ are complex, the energy spectrum is also complex in the presence of Gaussian band tails.

Following (2.57c), the 1D dispersion relation in NW of IV–VI materials in accordance with the present model can be written as

$$\bar{F}_1(\bar{E}, \eta_g)\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right] + \bar{F}_2(\bar{E}, \eta_g)\bar{k}_z^2 = 1 \tag{2.58}$$

The (2.58) can be written as

$$\bar{k}_z = \bar{T}_{60}(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{2.59}$$

where

$$\bar{T}_{60}(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \left[\left[1 - \bar{F}_1(\bar{E}, \eta_g)\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right][\bar{F}_2(\bar{E}, \eta_g)]^{-1}\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{15HDNW}$) in this case can be expressed as

$$0 = \bar{T}_{60}(\bar{E}'_{15HDNW}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{2.60}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\frac{\partial}{\partial \bar{E}}[\bar{T}^2_{60}(\bar{E}_{F1HDNW}, \eta_g, \bar{n}_x, \bar{n}_y)] \tag{2.61}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} [\bar{T}_{50HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g)(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) + \bar{T}_{51HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g)] \tag{2.62}$$

where,

$$\bar{T}_{50HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) = T_{40}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g)$$

and

$$\bar{T}_{51HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[T_{50HDNW}(\bar{E}_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g)]$$

Thus, using (1.31f) and (2.66), we can study the entropy in this case.

The 1D dispersion relation in the absence of band tailing can be written in this case following (2.57a) as

$$\omega_1(\bar{E})\left[\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right] + \omega_2(\bar{E})\bar{k}_z^2 = 1 \tag{2.63}$$

Then (2.63) can be written as

$$\bar{k}_z = \bar{T}_{61}(\bar{E}, \bar{n}_x, \bar{n}_y) \tag{2.64}$$

where,

$$\bar{T}_{61}(\bar{E}, \bar{n}_x, \bar{n}_y) = \left[\left[1 - \omega_1(\bar{E})\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right][\omega_2(\bar{E})]^{-1}\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{21}$) in this case can be expressed as

$$0 = \bar{T}_{61}(\bar{E}'_{21}, \bar{n}_x, \bar{n}_y) \tag{2.65}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{T}_{61}^{2}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)] \tag{2.66}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\bar{T}_{61}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)+\bar{T}_{62}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)] \tag{2.67}$$

where

$$\bar{T}_{62}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)=\sum_{\bar{r}=1}^{\bar{S}}\bar{L}(\bar{r})[T_{61}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)]$$

Using (1.44) and (2.67), we can study the entropy in this case.

2.2.5 The entropy in nanowiresof HD stressed Kane-type materials

The 1D dispersion relation in this case can be written following (1.206) as

$$\bar{P}_{11}(\bar{E},\eta_g)\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2+\bar{Q}_{11}(\bar{E},\eta_g)\left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2+\bar{S}_{11}(\bar{E},\eta_g)\bar{k}_z^2=1 \tag{2.68}$$

Then (2.68) can be written as

$$\bar{k}_z=\bar{T}_{70}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y) \tag{2.69}$$

where

$$\bar{T}_{70}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)=\left[\left[1-\bar{P}_{11}(\bar{E},\eta_g)\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2+\bar{Q}_{11}(\bar{E},\eta_g)\left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right][\bar{S}_{11}(\bar{E},\eta_g)]^{-1}\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{30HDNW}$) in this case can be expressed as

$$0=\bar{T}_{70}(\bar{E}'_{30HDNW},\eta_g,\bar{n}_x,\bar{n}_y) \tag{2.70}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_x,\bar{n}_y)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{T}_{70}^{2}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_x,\bar{n}_y)] \tag{2.71}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right) \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} [\bar{T}_{70HDNW}(\bar{\mathrm{E}}_{F1HDNW}, \bar{\mathrm{n}}_x, \bar{\mathrm{n}}_y, \eta_g) + \bar{T}_{71HDNW}(\bar{\mathrm{E}}_{F1HDNW}, \bar{\mathrm{n}}_x, \bar{\mathrm{n}}_y, \eta_g)] \tag{2.72}$$

where

$$\bar{T}_{70HDNW}(\bar{\mathrm{E}}_{F1HDNW}, \bar{\mathrm{n}}_x, \bar{\mathrm{n}}_y, \eta_g) = \bar{T}_{70HDNW}(\bar{\mathrm{E}}_{F1HDNW}, \bar{\mathrm{n}}_x, \bar{\mathrm{n}}_y, \eta_g)$$

and

$$\bar{T}_{71HDNW}(\bar{\mathrm{E}}_{F1HDNW}, \bar{\mathrm{n}}_x, \bar{\mathrm{n}}_y, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{T}_{70HDNW}(\bar{\mathrm{E}}_{F1HDNW}, \bar{\mathrm{n}}_x, \bar{\mathrm{n}}_y, \eta_g)]$$

Thus, using (1.31f) and (2.72), we can study the entropy in this case.

In the absence of band tailing,1D dispersion relation in this case assumes the form

$$\bar{k}_z = \bar{t}_{70}(\bar{E}, \bar{n}_x, \bar{n}_y) \tag{2.73}$$

where

$$\bar{t}_{70}(\bar{E}, \bar{n}_x, \bar{n}_y) = \left[\left[\bar{c}_0(\bar{E})\left[1 - \left(\frac{\pi\bar{n}_x}{\bar{d}_x\bar{a}_0(\bar{E})}\right)^2 - \left(\frac{\pi\bar{n}_y}{\bar{d}_y\bar{b}_0(\bar{E})}\right)^2\right]\right]^{1/2}\right]$$

The sub-band energy ($\bar{E}'_{42}$) in this case can be expressed as

$$0 = \bar{t}_{60}(\bar{E}'_{42}, \bar{n}_x, \bar{n}_y) \tag{2.74}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1d}, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{t}^2_{60}(\bar{E}_{F1d}, \bar{n}_x, \bar{n}_y)] \tag{2.75}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right) \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} [\bar{t}_{60}(\bar{E}_{F1d}, \bar{n}_x, \bar{n}_y) + \bar{t}_{61}(\bar{E}_{F1d}, \bar{n}_x, \bar{n}_y)] \tag{2.76}$$

where

$$\bar{t}_{61}(\bar{E}_{F1d}, \bar{n}_x, \bar{n}_y) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{t}_{60}(\bar{E}_{F1d}, \bar{n}_x, \bar{n}_y)]$$

Thus, using (1.44) and (2.76), we can study the ENTROPY in this case.

2.2.6 The entropy in nanowires of HD Te

The 1D dispersion relation may be written in this case following (1.235) as

$$\bar{k}_x = \bar{t}_{72}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{2.77}$$

where

$$\bar{t}_{72}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) = \left[-\left(\frac{\bar{n}_y \pi}{\bar{d}_y}\right)^2 + \psi_{5HD}(\bar{E}, \eta_g) - \psi_6 \left(\frac{\pi \bar{n}_z}{\bar{d}_z}\right)^2 \pm \psi_7 \left[\psi_{8HD}^2(\bar{E}, \eta_g) - \left(\frac{\pi \bar{n}_z}{\bar{d}_z}\right)^2\right]^{1/2}\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{31HDNW}$) in this case can be expressed as

$$0 = \bar{t}_{72}(\bar{E}'_{31HDNW}, \eta_g, \bar{n}_y, \bar{n}_z) \tag{2.78}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW}, \eta_g, \bar{n}_y, \bar{n}_z) = \frac{\hbar^2}{2} \frac{\partial}{\partial \bar{E}} [\bar{t}_{72}^2(\bar{E}_{F1HDNW}, \eta_g, \bar{n}_y, \bar{n}_z)] \tag{2.79}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right) \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{t}_{72HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) + \bar{t}_{73HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)] \tag{2.80}$$

where

$$\bar{t}_{72HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \bar{t}_{72HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)$$

and

$$\bar{t}_{73HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) [\bar{t}_{72HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)]$$

Thus, using (1.31f) and (2.80), we can study the entropy in this case.

In the absence of band tailing the 1D dispersion relation in this case assumes the form

$$\bar{k} = \bar{H}_{70}(\bar{E}, \bar{n}_y, \bar{n}_z) \tag{2.81}$$

where

$$\bar{H}_{70}(\bar{E},\bar{n}_y,\bar{n}_z)=\left[-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\psi_5(\bar{E})-\psi_6\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\pm\psi_7\left[\psi_8^2(\bar{E})-\left(\frac{\pi\bar{n}_z}{d_z}\right)^2\right]^{1/2}\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{44}$) in this case can be expressed as

$$0=\bar{H}_{70}(\bar{\mathrm{E}}'_{44},\bar{\mathrm{n}}_y,\bar{\mathrm{n}}_z) \tag{2.82}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{H}_{70}^2(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.83}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2g_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{H}_{70}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)+\bar{H}_{71}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.84}$$

where

$$\bar{H}_{71}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)=\sum_{\bar{r}=1}^{\bar{s}}L(r)[\bar{H}_{70}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)]$$

Thus, using (1.44) and (2.84), we can study the entropy in this case.

2.2.7 The entropy in nanowires of HD gallium phosphide

The 1D dispersion relation may be written in this case following (1.253) as

$$\bar{k}_x=\bar{u}_{70}(\bar{E},\bar{n}_y,\bar{n}_z,\eta_g) \tag{2.85}$$

where

$$\bar{u}_{70}(\bar{E},\bar{n}_y,\bar{n}_z,\eta_g)=\left[-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\bar{t}_{11}\gamma_3(\bar{E},\eta_g)+\bar{t}_{21}-\bar{t}_{31}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-\bar{t}_{41}\left[\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\bar{t}_5^2(\bar{E},\eta_g)\right]^{1/2}\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{32HDNW}$) in this case can be expressed as

$$0=\bar{u}_{70}(\bar{E}'_{32HDNW},\eta_g,\bar{n}_y,\bar{n}_z) \tag{2.86}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{32HDNW},\eta_g,\bar{n}_y,\bar{n}_z)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{u}_{70}^2(\bar{E}_{32HDNW},\eta_g,\bar{n}_y,\bar{n}_z)] \tag{2.87}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{u}_{70HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)+\bar{u}_{71HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)] \tag{2.88}$$

where,

$$\bar{u}_{70HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\bar{u}_{70HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)$$

and

$$\bar{u}_{71HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{u}_{70HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)]$$

By using (1.31f) and (2.88), we can find the entropy in this case.

In the absence of band tailing the 1D dispersion relation in this case can be written using (1.260) as

$$\bar{k}_x=\bar{X}_{71}(\bar{\mathrm{E}},\bar{\mathrm{n}}_y,\bar{\mathrm{n}}_z) \tag{2.89}$$

where

$$\bar{X}_{71}(\bar{\mathrm{E}},\bar{\mathrm{n}}_y,\bar{\mathrm{n}}_z)=\left[-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\bar{t}_{42}(\bar{\mathrm{E}},\mathrm{n}_z)\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{46}$) in this case can be expressed as

$$0=\bar{X}_{71}(\bar{E}'_{46},\bar{n}_y,\bar{n}_z) \tag{2.90}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}\left[\bar{X}_{71}^2(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)\right] \tag{2.91}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\left[\bar{X}_{71}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)+\bar{X}_{72}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)\right] \tag{2.92}$$

where

$$\bar{X}_{72}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} L(r)[\bar{X}_{71}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)]$$

By using (1.44) and (2.92), we can find the entropy in this case.

2.2.8 The entropy in nanowires of HD platinum antimonide

The 1D dispersion relation may be written in this case following (1.275) as

$$\bar{k}_x = \bar{V}_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \bar{\eta}_g) \tag{2.93}$$

where

$$\bar{V}_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \bar{\eta}_g) = \left[- \left(\frac{\bar{n}_y \pi}{d_y} \right)^2 + \bar{A}_{60}(\bar{E}, \bar{\eta}_g, \bar{n}_y) \right]^{1/2}$$

The sub-band energy ($\overline{E'}_{34HDNW}$) in this case can be expressed as

$$0 = \bar{V}_{70}(\bar{E'}_{34HDNW}, \bar{\eta}_g, \bar{n}_y, \bar{n}_z) \tag{2.94}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1HDNW}, \bar{\eta}_g, \bar{n}_y, \bar{n}_z) = \frac{\hbar^2}{2} \frac{\partial}{\partial \bar{E}} [\bar{V}_{70}^2(\bar{E}_{F1HDNW}, \bar{\eta}_g, \bar{n}_y, \bar{n}_z)] \tag{2.95}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi} \right) \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \left[\bar{V}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) + \bar{V}_{71HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) \right] \tag{2.96}$$

where

$$\bar{V}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \bar{V}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)$$

and

$$\bar{V}_{71HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\bar{V}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)]$$

By using (1.31f) and (2.96), we can find the entropy in this case.

In the absence of band tailing the 1D dispersion relation in this case can be written using (1.278) as

$$\bar{k}_x = \bar{D}_{71}(\bar{E}, \bar{n}_y, \bar{n}_z) \tag{2.97}$$

where

$$\bar{D}_{71}(\bar{E}, \bar{n}_y, \bar{n}_z) = \left[-\left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 + \bar{t}_{44}(\bar{E}, n_z) \right]^{1/2}$$

The sub-band energy($(\overline{E}' 48)$) in this case can be expressed as

$$0 = \bar{D}_{71}(\bar{E}'_{48}, \bar{n}_y, \bar{n}_z) \tag{2.98}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) = \frac{\hbar^2}{2} \frac{\partial}{\partial \bar{E}} [\bar{D}_{71}^2(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)] \tag{2.99}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi} \right) \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{D}_{71}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) + \bar{D}_{72}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)] \tag{2.100a}$$

where

$$\bar{D}_{72}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) [\bar{D}_{71}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)]$$

Using (1.44) and (2.100a), we can find the entropy in this case.

2.2.9 The entropy in nanowires of HD bismuth telluride

The dispersion relation in this case can be written following (1.285) as

$$\bar{k}_x = \bar{J}_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{2.100b}$$

where

$$\bar{J}_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) = \left[\left[\gamma_2(\bar{E}, \eta_g) - \omega_2 \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 - \omega_3 \left(\frac{\bar{n}_z \pi}{\bar{d}_z} \right)^2 - 2\omega_4 \frac{\bar{n}_y \bar{n}_z \pi^2}{\bar{d}_y \bar{d}_z} \right] (\omega_1)^{-1} \right]^{1/2}$$

The sub-band energy ($\bar{E}'_{50HDNW}$) in this case can be expressed as

$$0 = \bar{J}_{70}(\bar{E}'_{50HDNW}, \eta_g, \bar{n}_y, \bar{n}_z) \tag{2.101}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{J}_{70}^{2}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)] \tag{2.102}$$

The carrier statistics which can, in turn, be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{J}_{70HDNW}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)+\bar{J}_{71HDNW}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)] \tag{2.103}$$

where

$$\bar{J}_{70HDNW}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)=\bar{J}_{70HDNW}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)$$

and

$$\bar{J}_{71HDNW}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{J}_{70HDNW}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)]$$

Using (1.31f) and (2.103), we can find the entropy in this case.

In the absence of band tailing the 1D dispersion relation in this case can be written using (1.278) as

$$\bar{k}_x=\bar{B}_{71}(\bar{E},\bar{n}_y,\bar{n}_z) \tag{2.104}$$

where

$$\bar{B}_{71}(\bar{E},\bar{n}_y,\bar{n}_z)=\left[\left[\bar{E}(1+\alpha\bar{E})-\omega_2\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2-\omega_3\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2-2\omega_4\frac{\bar{n}_y\bar{n}_z\pi^2}{\bar{d}_y\bar{d}_z}\right](\omega_1)^{-1}\right]^{1/2}$$

The sub-band energy ($E'50$) in this case can be expressed as

$$0=\bar{B}_{71}(\bar{E}'_{50},\bar{n}_y,\bar{n}_z) \tag{2.105}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{B}^{2}{}_{71}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.106}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{B}_{71}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)+\bar{B}_{72}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.107}$$

where

$$\bar{B}_{72}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{B}_{71}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)]$$

Using (1.44) and (2.107), we can find the entropy in this case.

2.2.10 The entropy in nanowires of HD germanium

(a) Model of Cardona et al

The dispersion relation in accordance with this model in the present case can be written following (1.306b) as

$$\bar{k}_x = \bar{L}_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{2.108}$$

where

$$\bar{L}_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) = \left[\left[\gamma_2(\bar{E}, \eta_g) + \alpha\left[\frac{\hbar^2}{2\bar{m}^*_{||}}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]^2 - (1 + 2\alpha\gamma_3(\bar{E}, \eta_g))\frac{\hbar^2}{2\bar{m}^*_{||}}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\left(\frac{2\bar{m}^*_{||}}{\hbar^2}\right)\right]^{1/2}$$

The sub-band energy ($\overline{E'}_{52HDNW}$) in this case can be expressed as

$$0 = \bar{L}_{70}(\bar{E}'_{52HDNW}, \eta_g, \bar{n}_y, \bar{n}_z) \tag{2.109}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}'_{F1HDNW}, \eta_g, \bar{n}_y, \bar{n}_z) = \frac{\hbar^2}{2}\frac{\partial}{\partial \bar{E}}[\bar{L}^2_{70}(\bar{E}'_{F1HDNW}, \eta_g, \bar{n}_y, \bar{n}_z)] \tag{2.110}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2g_v}{\pi}\right)\sum_{\bar{n}y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}z=1}^{\bar{n}_{z\max}}[\bar{L}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) + \bar{L}_{71HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)] \tag{2.111}$$

where

$$\bar{L}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \bar{L}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)$$

and

$$\bar{L}_{71HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{L}_{70HDNW}(\bar{E}_{F1HDNW}, \bar{n}_y, \bar{n}_z, \eta_g)]$$

In the absence of band tailing the 1D dispersion relation in this case can be written using (1.278) as

$$\bar{k}_x = \bar{B}_{77}(\bar{E}, \bar{n}_y, \bar{n}_z) \tag{2.112}$$

where

$$\bar{B}_{77}(\bar{E}, \bar{n}_y, \bar{n}_z) = \left[\left[\bar{E}(1+\alpha\bar{E}) + \alpha\left[\frac{\hbar^2}{2\bar{m}^*_{||}}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]^2 - (1+2\alpha\bar{E})\frac{\hbar^2}{2m^*_{||}}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\left(\frac{2\bar{m}^*_{||}}{\hbar^2}\right)\right]^{1/2}$$

The sub-band energy ($\bar{E}'60$) in this case can be expressed as

$$0 = \bar{B}_{77}(\bar{E}'_{60}, \bar{n}_y, \bar{n}_z) \tag{2.113}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) = \frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{B}^2_{77}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)] \tag{2.114}$$

The carrier statistics can be written as

$$\bar{n}_{1D} = \left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{B}_{77}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) + \bar{B}_{78}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)] \tag{2.115}$$

where

$$\bar{B}_{78}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) = \sum_{\bar{r}=1}^{\bar{s}} L(r)[\bar{B}_{77}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)]$$

Using (1.44) and (2.115), we can study the entropy in this case.

(b) Model of Wang et al.

The dispersion relation in accordance with this model in the present case can be written following (1.326) as

$$\bar{k}_x = \beta_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{2.116}$$

where

$$\beta_{70}(\bar{E}, \bar{n}_y, \bar{n}_z, \eta_g) = \left[-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \frac{2\bar{m}^*_{\perp}}{\hbar^2}\left[\alpha_8 - \alpha_9\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 - \alpha_{10}\left[\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^4 + \alpha_{11}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + \alpha_{12}(\bar{E}, \eta_g)\right]^{1/2}\right]\right]^{1/2}$$

The sub-band energy ($\overline{E'}_{54HDNW}$) in this case can be expressed as

$$0 = \beta_{70}(\bar{E}'_{54HDNW}, \eta_g, \bar{n}_y, \bar{n}_z) \tag{2.117}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\beta_{70}^2(\bar{E}_{F1HDNW},\eta_g,\bar{n}_y,\bar{n}_z)] \tag{2.118}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\beta_{70HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)+\beta_{71HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)] \tag{2.119}$$

where

$$\beta_{70HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\beta_{70}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)$$

and

$$\beta_{71HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\beta_{70HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)]$$

Using (1.31f) and (2.119), we can study the entropy in this case.

In the absence of band tailing the 1D dispersion relation in this case can be written using (1.278) as

$$\bar{k}_x=\bar{P}_{77}(\bar{E},\bar{n}_y,\bar{n}_z) \tag{2.120}$$

where

$$\bar{P}_{77}(\bar{E},\bar{n}_y,\bar{n}_z)=\left[\left[\bar{I}_1(\bar{E},\bar{n}_z)-\frac{\hbar^2}{2\bar{m}_2^{*}}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\left(\frac{2\bar{m}_1^{*}}{\hbar^2}\right)\right]^{1/2}$$

The sub-band energy ($\bar{E}'_{2HDNW}$) in this case can be expressed as

$$0=\bar{P}_{77}(\bar{E}'_{80},\bar{n}_y,\bar{n}_z) \tag{2.121}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)=\frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\bar{P}_{77}^2(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.122}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{P}_{77}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)+\bar{P}_{78}(\bar{E}_{F1d},\bar{n}_y,\bar{n}_z)] \tag{2.123}$$

where

$$\bar{P}_{77}(\bar{E},\bar{n}_y,\bar{n}_z)=\left[\left[\bar{I}_1(\bar{E},\bar{n}_z)-\frac{\hbar^2}{2\bar{m}_2^*}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\left(\frac{2\bar{m}_1^*}{\hbar^2}\right)\right]^{1/2}$$

Using (1.44) and (2.123), we can study the entropy in this case.

2.2.11 The entropy in nanowires of HD galium antimonide

The dispersion relation of the 1D electrons in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c}+\frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}+\frac{\hbar^2\bar{k}_x{}^2}{2\bar{m}_c}=\bar{I}_{36}(\bar{E},\eta_g) \tag{2.124}$$

The sub-band energy $(\overline{E'}_{100HDNW})$ in this case can be expressed as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c}+\frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2m_c}=\bar{I}_{36}(\overline{E'}_{100HDNW},\eta_g) \tag{2.125}$$

The EEM in this case is given by

$$\bar{m}^*(\overline{E'}_{F1HDNW},\eta_g)=\bar{m}_c[\bar{I}_{36}{}'(\overline{E'}_{F1HDNW},\eta_g)] \tag{2.126}$$

The carrier statistics can be written as

$$\bar{n}_{1D}=\left(\frac{2\bar{g}_v}{\pi}\right)\sum_{\bar{n}y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}z=1}^{\bar{n}_{z\max}}[\bar{R}_{7HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)+\bar{R}_{8HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)] \tag{2.127}$$

where

$$\bar{R}_{7HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\left[\left[\bar{I}_{36}(\bar{E}_{F1HDNW},\eta_g)(\bar{E}_{F1HDNW},\eta_g)-\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c}-\frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c}\right]\frac{2\bar{m}_c}{\hbar^2}\right]^{1/2}$$

and

$$\bar{R}_{8HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{R}_{7HDNW}(\bar{E}_{F1HDNW},\bar{n}_y,\bar{n}_z,\eta_g)]$$

Using (1.31f) and (2.127), we can study the entropy in this case.

The expression of 1D dispersion relation, for NWs of GaSb whose energy band structures in the absence of band tailing assumes the form

$$\bar{I}_{36}(\bar{E}) = \frac{\hbar^2 \bar{k}_x^2}{2\bar{m}_c} + \bar{G}_2(\bar{n}_y, \bar{n}_z) \tag{2.128}$$

In this case, the quantized energy $\overline{E'}_{101}$ is given by

$$\bar{I}_{36}(\overline{E'}_{101}) = \bar{G}_2(\bar{n}_y, \bar{n}_z) \tag{2.129}$$

The carrier statistics in the case can be expressed as

$$\bar{n}_{1D} = \frac{2\bar{g}_v}{\pi} \frac{\sqrt{2\bar{m}_c}}{\hbar} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} [\bar{R}_{101}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) + \bar{R}_{102}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)] \tag{2.130}$$

where

$$\bar{R}_{101}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) \equiv [\bar{I}_{36}(\bar{E}_{F1d}) - \bar{G}_2(\bar{n}_y, \bar{n}_z)]^{1/2}$$

and

$$\bar{R}_{102}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z) \equiv \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) [\bar{R}_{101}(\bar{E}_{F1d}, \bar{n}_y, \bar{n}_z)]$$

Thus, using (1.44) and (2.160), we can study the entropy in this case.

2.2.12 The entropy in nanowires of HD II–V materials

The DR of the 1D holes in II-V compounds can be expressed as

$$\gamma_3(\bar{E}, \eta_g) = \bar{A}_{10} \left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)^2 + \bar{A}_{11} \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 + \bar{A}_{12} \bar{k}_z^2 + \bar{A}_{13} \left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)$$
$$\pm \left[\left(\bar{A}_{14} \left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)^2 + \bar{A}_{15} \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 + \bar{A}_{16} \bar{k}_z^2 + \bar{A}_{17} \left(\frac{\bar{n}_x \pi}{\bar{d}_x} \right)^2 \right)^2 + \bar{A}_{18} \left(\frac{\bar{n}_y \pi}{\bar{d}_y} \right)^2 + \bar{A}_{19}^2 \right]^{1/2} \tag{2.131}$$

where the numerical values of the energy band constants are given in Appendix A.

The sub-band energy ($\bar{E}_{n_{zHD401}}$) is the lowest positive root of the following equation

$$\gamma_3(\bar{E}_{n_{zHD401}}, \eta_g) = \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right) \pm \left[\left(\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right)^2 + \bar{A}_{19}^2\right]^{1/2} \tag{2.132}$$

(2.132) can be expressed as

$$\bar{k}_x = \Delta_{27}(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{2.133}$$

where

$$\Delta_{27}(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = [(\bar{A}_{12}^2 - \bar{A}_{16}^2)^{-1}[[\Delta_{21}(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y)\bar{A}_{12} + \bar{A}_{16}\Delta_{22}(\bar{n}_x, \bar{n}_y)]$$
$$+ [[\Delta_{21}(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y)\bar{A}_{12} + \bar{A}_{16}\Delta_{22}(\bar{n}_x, \bar{n}_y)]^2 - (\bar{A}_{12}^2 - \bar{A}_{16}^2)\Delta_{25}(\bar{n}_x, \bar{n}_y, \bar{E}, \eta_g)]^{1/2}$$

$$\Delta_{21}(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \left[\gamma_3(\bar{E}, \eta_g) - \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 - \bar{A}_{11}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 - \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right],$$

$$\Delta_{22}(\bar{n}_x, \bar{n}_y) = \left[\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{15}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right], \Delta_{25}(\bar{n}_x, \bar{n}_y, \bar{E}, \eta_g)$$
$$= \Delta_{21}^2(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) - \Delta_{24}(\bar{n}_x, \bar{n}_y)],$$

$$\Delta_{24}(\bar{n}_x, \bar{n}_y) = [\Delta_{22}^2(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) + \Delta_{23}(\bar{n}_y)]$$

and

$$\Delta_{23}(\bar{n}_y) = \left[\bar{A}_{18}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{19}^2\right]$$

The DOS function in this case can be written as

$$\bar{N}_{1DHD\Gamma}(\bar{E}, \eta_g) = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\Delta'_{27}(\bar{E}, \bar{n}_x, \bar{n}_y, \eta_g)\bar{H}(\bar{E} - \bar{E}_{200HDNW}) \tag{2.134}$$

In (2.164), $\bar{E}'_{200HDNW}$ is the sub-band energy and in this case can be expressed as

$$0 = \Delta_{27}(\bar{E}'_{200HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) \tag{2.135}$$

The EEM in this case is given by

$$\bar{m}^*(\overline{E'}_{F1HDNW}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\Delta_{27}^2(E'_{F1HDNW}, \eta_g, \bar{n}_x, \bar{n}_y)] \tag{2.136}$$

The carrier statistics in this case can be written as

$$\bar{n}_{1D} = \left(\frac{\bar{g}_v}{\pi}\right) \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \left[\Delta_{27}(E'_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g) \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) \left[\Delta_{27}(E'_{F1HDNW}, \bar{n}_x, \bar{n}_y, \eta_g)\right]\right] \tag{2.137}$$

Thus, using (1.31f) and (2.137), we can study the entropy in this case.

In the absence of band-tailing, the 1D hole energy spectrum in this case assumes the form

$$\bar{E} = \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{11}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{12}\bar{k}_z^2 + \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)$$
$$\pm \left[\left(\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{15}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{16}\bar{k}_z^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right)^2 + \bar{A}_{18}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{19}^2\right]^{1/2} \tag{2.138}$$

The subband energy ($\bar{E}'_{300}$) is the lowest positive root of the following equation

$$\bar{E}'_{300} = \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right) \pm \left[\left(\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right)^2 + \bar{A}_{19}^2\right]^{1/2} \tag{2.139}$$

(2.139) can be expressed as

$$\bar{k}_z = \Delta_{271}(\bar{E}, \eta_g, \bar{n}_y) \tag{2.140}$$

where

$$\Delta_{271}(\bar{E}, \bar{n}_x, \bar{n}_y) = [(\bar{A}_{12}^2 - \bar{A}_{16}^2)^{-1}[[\Delta_{211}(\bar{E}, \bar{n}_x, \bar{n}_y)\bar{A}_{12} + \bar{A}_{16}\Delta_{22}(\bar{n}_x, \bar{n}_y)]$$
$$+ [[\Delta_{211}(\bar{E}, \bar{n}_x, \bar{n}_y)\bar{A}_{12} + \bar{A}_{16}\Delta_{22}(\bar{n}_x, \bar{n}_y)]^2 - (\bar{A}_{12}^2 - \bar{A}_{16}^2)\Delta_{251}(\bar{n}_x, \bar{n}_y, \bar{E})]^{1/2}$$

$$\Delta_{211}(\bar{E}, \bar{n}_x, \bar{n}_y) = \left[\bar{E} - \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 - \bar{A}_{11}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 - \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right],$$

$$\Delta_{22}(\bar{n}_x, \bar{n}_y) = \left[\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{15}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right],$$

$$\Delta_{251}(\bar{n}_x, \bar{n}_y, \bar{E}) = \Delta_{211}^2(\bar{E}, \bar{n}_x, \bar{n}_y) - \Delta_{24}(\bar{n}_x, \bar{n}_y)],$$

$$\Delta_{24}(\bar{n}_x, \bar{n}_y) = [\Delta_{22}^2(\bar{E}, \bar{n}_x, \bar{n}_y) + \Delta_{23}(\bar{n}_y)] \text{ and } \Delta_{23}(\bar{n}_y) = \left[\bar{A}_{18}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{19}^2\right]$$

The DOS function in this case can be written as

$$\bar{N}_{1D\Gamma}(\bar{E}) = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\Delta'_{271}(\bar{E},\bar{n}_x,\bar{n}_y)\bar{H}(\bar{E}-\bar{E}_{300HDNW}) \tag{2.141}$$

In (2.171), $\bar{E}'_{300}$ is the sub-band energy in this case which can be expressed as

$$0 = \Delta_{271}(\bar{E}'_{300},\bar{n}_x,\bar{n}_y) \tag{2.142}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}_{F1d},\eta_g,\bar{n}_x,\bar{n}_y) = \frac{\hbar^2}{2}\frac{\partial}{\partial\bar{E}}[\Delta^2_{271}(\overline{E'}_{F1d},\bar{n}_x,\bar{n}_y)] \tag{2.143}$$

The DOS function in this case can be written as

$$\bar{n}_{1D} = \left(\frac{\bar{g}_v}{\pi}\right)\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\left[\Delta_{271}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\Delta_{271}(\bar{E}_{F1d},\bar{n}_x,\bar{n}_y)\right]\right] \tag{2.144}$$

Using (1.44) and (2.144) we can study the entropy in this case.

2.2.13 Entropy in nanowires of HD lead germanium telluride

The 1D electron energy spectrum in n-type $Pb_{1-x}Ge_xTe$ under the condition of formation of band tails can be written as

$$\begin{aligned}
&\left[\frac{2}{1+\left(\frac{\bar{E}}{\bar{\eta}_g}\right)}\right]\theta_0(\bar{E},\eta_g)+\gamma_3(\bar{E},\eta_g)\left[\bar{E}_{go}-0.195\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]-0.345\bar{k}_z^2\right]\\
&=\left[0.23\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]-0.02\bar{k}_z^2\right]\\
&\pm\left[0.06\bar{E}_{go}+0.061\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]-0.0066\bar{k}_z^2\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2}\\
&+\left[\bar{E}_{go}+0.0411\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right.\\
&\left.+0.377\bar{k}_z^2\right]\left[0.606\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+0.722\bar{k}_z^2\right]\right]
\end{aligned} \tag{2.145}$$

The subband energy ($\bar{E}_{n_{zHD500}}$) is the lowest positive root of the following equation

$$\left[\frac{2}{1+Erf\left(\frac{\bar{E}_{n_{zHD500}}}{\eta_g}\right)}\right]\theta_0(\bar{E}_{n_{zHD500}},\eta_g)+\gamma_3(\bar{E}_{n_{zHD500}},\eta_g)[\bar{E}_{go}-0.195\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]$$
$$=\left[0.23\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]-0.02\bar{k}_z^2\right]$$
$$\pm[0.06\bar{E}_{go}+0.061\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2}$$
$$+\left[\bar{E}_{go}+0.0411\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right]\left[0.606\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right]\Bigg] \tag{2.146}$$

The EEM and the DOS function for both the cases should be calculated numerically.

Using (1.31f) and (2.145), we can study the entropy numerically.

The 1D dispersion law of n-type $Pb_{1-x}Ge_xTe$ with $x=0.01$ in the absence of band-tails can be expressed as

$$\left[\bar{E}-0.606\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]-0.722\bar{k}_z^2\right]$$
$$\left[\bar{E}+\bar{E}_{go}+0.411\left[(\frac{\bar{n}_x\pi}{\bar{d}_x})^2-(\frac{\bar{n}_y\pi}{\bar{d}_y})^2\right]+0.377\bar{k}_z^2\right]$$
$$=\left[0.23\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]+0.02\bar{k}_z^2\right.$$
$$\left.\pm\left[0.06\bar{E}_{go}+0.061\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]+0.0066\bar{k}_z^2\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2}\right. \tag{2.147}$$

The sub-band energy $\bar{E}_{500}$ in this can be written as

$$\left[\bar{E}_{500}-0.606\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\left[\bar{E}_{500}+\bar{E}_{go}+0.411\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right]\right.$$
$$=\left[0.23\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\pm\left[0.06\bar{E}_{go}+0.061\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2\right.\right.\right.$$
$$\left.\left.\left.-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2-\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2} \tag{2.148}$$

Using (1.44) and (2.147) we can study the entropy numerically.

2.2.14 Entropy in nanowires of HD zinc and cadmium diphosphides

The DR in HD NWs of zinc and cadmium diphosphides can be written as

$$\gamma_3(\bar{E},\eta_g)=\left[\beta_1+\frac{\beta_2\beta_{31}(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right]\left[\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$
$$\pm\left\{\left[\beta_4\beta_{31}(\bar{k}_x,\bar{n}_y,\bar{n}_z)\left(\beta_5-\frac{\beta_2\beta_{31}(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right)\left[\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right]\right.$$
$$\left.+8{\beta_4}^2\left(1-\frac{{\beta_{31}}^2(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{4}\right)-\beta_2\left(1-\frac{{\beta_{31}}^2(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{4}\right)\left[\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right\}^{1/2} \tag{2.149}$$

where

$$\beta_{31}(\bar{k}_x,\bar{n}_y,\bar{n}_z)=\left[\frac{\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2-2\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2}{\left[\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]}\right]$$

The sub-band energy $\bar{E}_{n_{zHD600}}$ in this case assumes the form

$$\gamma_3(\bar{E}_{n_{zHD600}},\eta_g)=\left[\beta_1+\frac{\beta_2\beta_{31}(0,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right]\left[\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$
$$\pm\left\{\left[\beta_4\beta_{31}(0,\bar{n}_y,\bar{n}_z)\left(\beta_5-\frac{\beta_2\beta_{31}(0,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right)\left[\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right]\right.$$
$$\left.+8{\beta_4}^2\left(1-\frac{{\beta_{31}}^2(0,\bar{n}_y,\bar{n}_z)}{4}\right)-\beta_2\left(1-\frac{{\beta_{31}}^2(0,\bar{n}_y,\bar{n}_z)}{4}\right)\left[\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right\}^{1/2} \tag{2.150}$$

where

$$\beta_{31}(0,\bar{n}_y,\bar{n}_z)=\left[\frac{\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2-2\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)}{\left[\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]}\right]$$

The EEM and the DOS function should be obtained numerically.

Using (1.31f) and (2.149) we can study the entropy numerically.

The 1D DR in NWs of zinc and cadmium diphosphides in the absence of band-tails can be written as

$$\begin{aligned}\bar{E}=&\left[\beta_1+\frac{\beta_2\beta_{311}(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right]\left[\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\\&\pm\left\{\left[\beta_4\beta_{311}(\bar{k}_x,\bar{n}_y,\bar{n}_z)\left(\beta_5-\frac{\beta_2\beta_{311}(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right)\left[\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right]\right.\\&+8\beta_4{}^2\left(1-\frac{\beta_{311}^2(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{4}\right)-\beta_2\left(1-\frac{\beta_{311}^2(\bar{k}_x,\bar{n}_y,\bar{n}_z)}{4}\right)\\&\left.\left[\bar{k}_x^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right\}^{1/2}\end{aligned}\tag{2.151}$$

The subband energy ($\bar{E}_{700}$) is the lowest positive root of the following equation

$$\begin{aligned}\bar{E}_{700}=&\left[\beta_1+\frac{\beta_2\beta_{311}(0,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right]\left[\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\\&\pm\left\{\left[\beta_4\beta_{311}(0,\bar{n}_y,\bar{n}_z)\left(\beta_5-\frac{\beta_2\beta_{311}(0,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right)\left[\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right]\right.\\&\left.+8\beta_4{}^2\left(1-\frac{\beta_{311}^2(0,\bar{n}_y,\bar{n}_z)}{4}\right)-\beta_2\left(1-\frac{\beta_{311}^2(0,\bar{n}_y,\bar{n}_z)}{4}\right)\left[\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right\}^{1/2}\end{aligned}\tag{2.152}$$

The EEM and the DOS function for both the cases should be calculated numerically.

Using (1.44) and (2.151), we can study the entropy numerically.

2.3 Results and discussion

Figures 2.1–2.12 exhibits the dependences of the normalized entropy in HD NWs of all the materials as considered in Chapter 1 in accordance with all the band models and obtained by using the appropriate equations as formulated in this chapter.

From Figure 2.1 it appears that the entropy in HD NWs of $CdGeAs_2$ for all the models of the same material exhibit quantized variations with increasing film thickness. For a range of film thickness, the dependence exhibit trapezoidal variations and for higher values of film thickness, the length and width of the trapezoid increases. From Figure 2.2, it appears that the entropy decreases with increasing carrier concentration per unit length and the value of the entropy is least for the generalized band model and greatest for the parabolic band model of the same. From Figure 2.3, we observe that the entropy for HD NWs of InAs exhibits the lowest value in accordance with the three-band model of Kane model of the same whereas for parabolic energy bands it exhibits the highest value. It is apparent from plot (a) of Figure. 2.3 that the influence of the energy band gap is to reduce the value of the entropy as

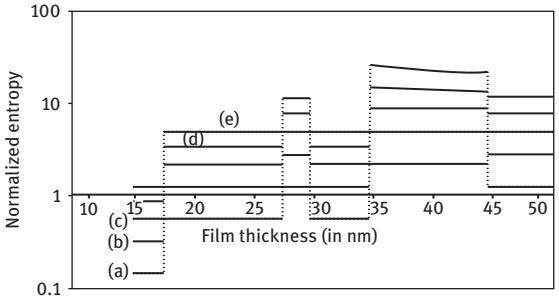

Figure 2.1: Plot of the normalized entropy for HD NWs of $CdGeAs_2$ as a function of film thickness for all cases of Figure 1.1.

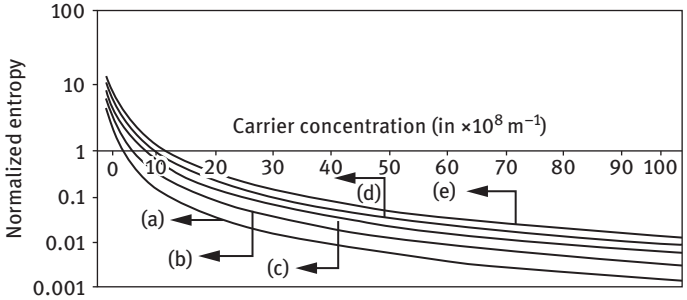

Figure 2.2: Plot of the normalized entropy for HD NWs of quantum wires of $CdGeAs_2$,as a function of carrier concentration for all cases of Figure 1.1.

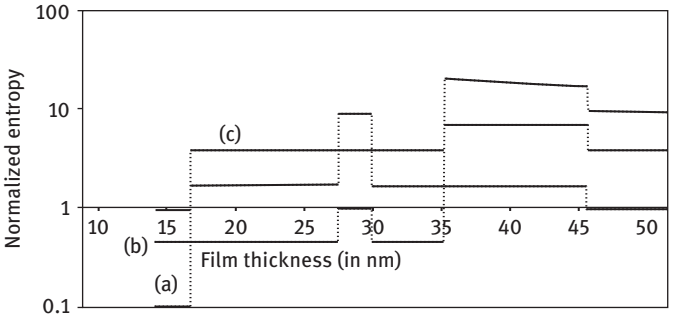

Figure 2.3: Plot of the normalized entropy for HD NWs of InAs as a function of film thickness for all cases of Figure 1.3.

compared with parabolic energy bands, and the influence of spin orbit splitting constant is to reduce the entropy further in the whole range of thickness as compared with two-band model of Kane. From Figure 2.4, we observe that entropy decreases with increasing concentration and the value of entropy in accordance with all the band models differs widely as concentration increases. Figures 2.5 and 2.6 exhibit the plot of the entropy for HD NWs of InSb as functions of thickness and concentration respectively. Nature of these two figures does not differ as compared with the plot of entropy in HD NWs of InAs as given in Figures 2.3 and 2.4, respectively. Important point to note here is that although the nature of the plots is same, the exact numerical values of the entropy are determined by the numerical values of the energy band constants of InSb and InAs, respectively. From Figure 2.7, we observe that the influence of the splitting of the two spin states by the spin orbit coupling and the crystalline field enhances the numerical values of the entropy in HD NWs of CdS as compared with $\bar{\lambda}_0 = 0$. Besides, trapezoidal variations of entropy in HD NWs of CdS with respect to thickness as appearing from Figure 2.7 are found to be perfect. From Figure 2.8, we observe that entropy decreases with increasing carrier concentration per unit length and by comparing it with Figure 1.8 as the corresponding plot for HD NWs of CdS, we can state that although entropy decreases with increasing carrier degeneracy in the latter case the nature and rate of decrement with increasing concentration are totally different in the HD NWs of CdS. From Figure 2.9, we observe that the entropy for HD NWs of PbTe, PbSnTe and stressed InSb in accordance with the appropriate band models exhibit quantum steps and trapezoidal variations in the whole range of thickness as considered with widely different numerical values as apparent from thisfigure. From Figure 2.10, the entropy decreases with increasing carrier degeneracy for HD NWs of PbTe,PbSnTe and stressed InSb respectively. Figure 2.11 exhibits the plots of the normalized entropy in HD NWs of (a) GaP, (b) $PtSb_2$, (c)Bi_2Te_3,and (d)cadmium antimonide, respectively, as a function of normalized film thickness.

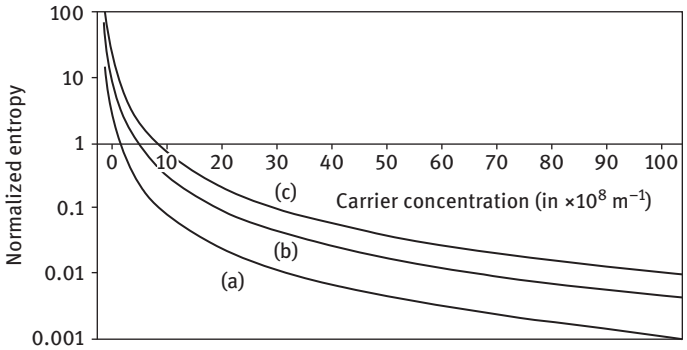

Figure 2.4: Plot of the normalized entropy for HD NWs of InAs as a function of carrier concentration for all cases of Figure 1.4.

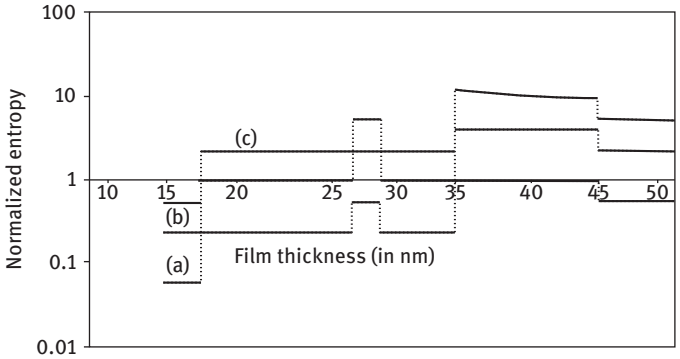

Figure 2.5: Plot of the normalized entropy for HD NWs of InSb as a function of film thickness for all cases of Figure 1.3.

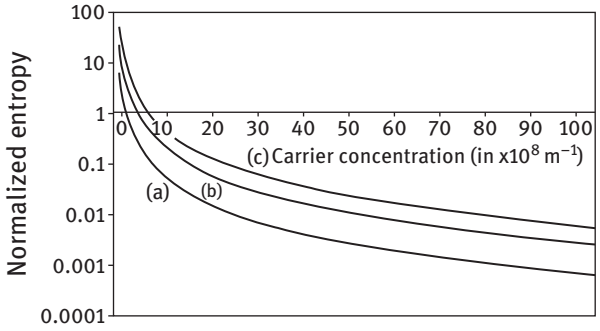

Figure 2.6: Plot of the normalized entropy for HD NWs of InSb as a function of carrier concentration for all cases of Figure 1.3.

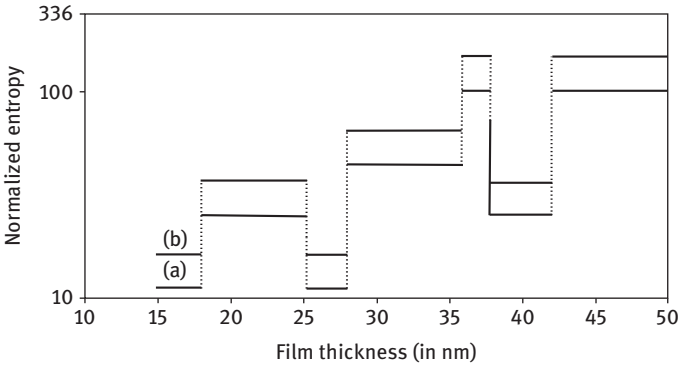

Figure 2.7: Plot of the normalized entropy for HD NWs of CdS as a function of film thickness for all cases of Figure 1.7.

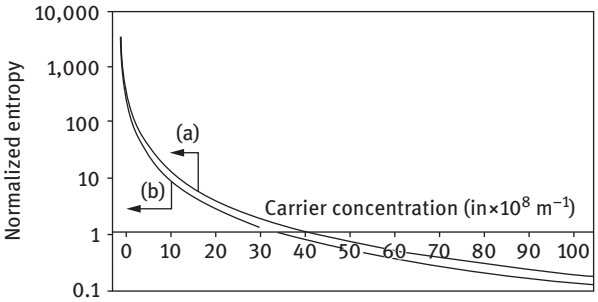

Figure 2.8: Plot of the normalized entropy for HD NWs of CdS as a function of carrier concentration for all cases of Figure 1.7.

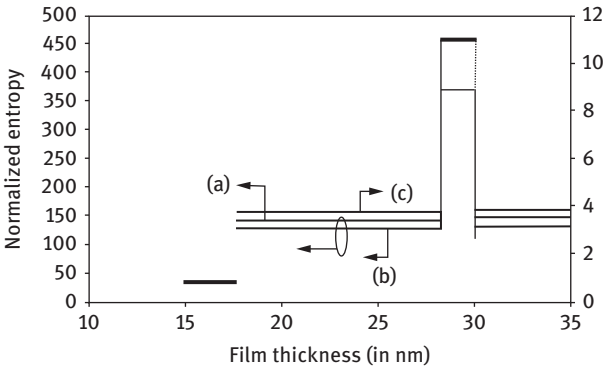

Figure 2.9: Plot of the normalized entropy in HD NWs of (a) PbTe, (b) PbSnTe and (c) stressed InSb as a function of film thickness.

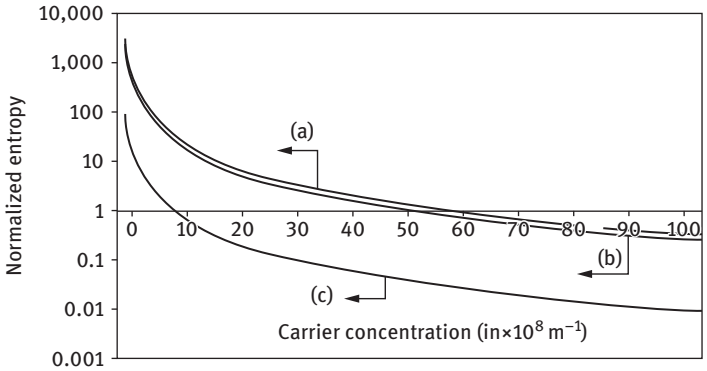

Figure 2.10: Plot of the normalized entropy in HD NWs of (a) PbTe, (b) PbSnTe and (c) stressed InSb as a function of carrier concentration.

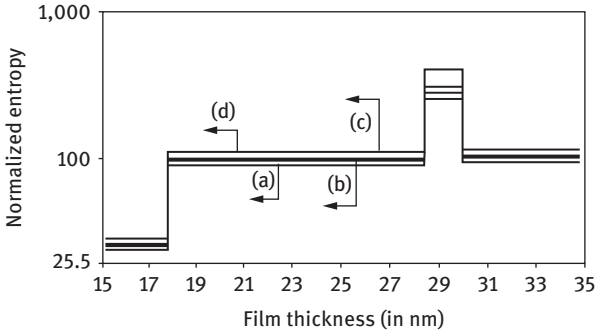

Figure 2.11: Plot of the normalized entropy in HD NWs of (a) GaP, (b) $PtSb_2$, (c) Bi_2Te_3, and (d) cadmium antimonide respectively, as a function of film thickness.

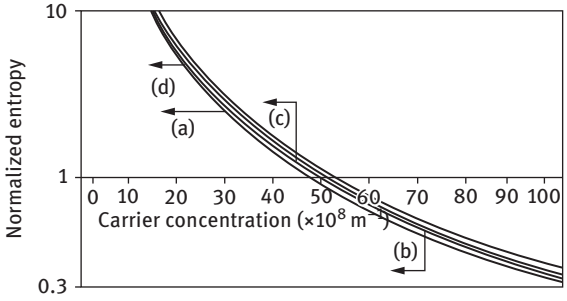

Figure 2.12: Plot of the normalized entropy for HD NWs of (a) GaP, (b) $PtSb_2$, (c) Bi_2Te_3, and (d) cadmium antimonide respectively, as a function of carrier concentration.

The influence of 2D quantum confinement appears from Figures 2.1, 2.3, 2.5, 2.7, 2.9 and 2.11, respectively since the entropy depends strongly on the thickness of the quantum-confined materials which is in direct contrast with bulk specimens. The entropy increases with increasing film thickness in an oscillatory way with different numerical magnitudes. It appears from the aforementioned figures that the entropy in HD NWs exhibits spikes for particular values of film thickness which, in turn, is not only the signature of the asymmetry of the wave vector space but also the particular band structure of the specific material. Moreover, the entropy in HD NWs of different compounds can become several orders of magnitude larger than that of the bulk specimens of the same materials, which is also a direct signature of quantum confinement. This oscillatory dependence will be less and less prominent with increasing film thickness.

It appears from Figures. (2.2), (2.4), (2.6), (2.8), (2.10) and (2.12) that the entropy decreases with increasing carrier degeneracy for 1D quantum confinement as considered for the said Figures. For relatively high values of carrier degeneracy, the influence of band structure of a specific 1D material is large and the plots of entropy differ widely from one another whereas for low values of the carrier degeneracy, they exhibit the converging tendency. For bulk specimens of the same material, the entropy will be found to decrease continuously with increasing electron degeneracy in a non-oscillatory manner in an altogether different way.

For HD NWs, the entropy increases with increasing film thickness in a step like manner for all the appropriate Figures. The appearance of the discrete jumps in the Figures for HD NWs is due to the redistribution of the electrons among the quantized energy levels when the size quantum number corresponding to the highest occupied level changes from one fixed value to the others. With varying thickness, a change is reflected in the entropy through the redistribution of the electrons among the size-quantized levels. It should be noted that although, the entropy varies in various manners with all the variables in all the cases as evident from all the Figures, the rates of variations are totally band- structure dependent. The two different signatures of 2D and 1D quantization of the carriers of in HD NWs of all the materials as considered here are apparent from all the appropriate plots, values of entropy for NWs differ as compared with HD QWs and the nature of variations of the entropy also changes accordingly.

2.4 Open research problems

(R2.1) Investigate the entropy for NWs of all of the HD materials in the presences of Gaussian, exponential, Kane, Halperian, Lax and Bonch-Burevich types of band tails for all systems whose unperturbed carrier energy spectra are defined in R1.1.

(R2.2) Investigate the entropy in the presence of strain for NWs of all of the HD materials of the negative refractive index, organic, magnetic and other advanced optical materials.

(R2.3) Investigate the entropy for the NWs of HD negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field.

(R2.4) Investigate the entropy for the multiple NWs of HD materials whose unperturbed carrier energy spectra are defined in R1.1.

(R2.5) Investigate the entropy for all the appropriate HD 1D of this chapter in the presence of finite potential wells.

(R2.6) Investigate the entropy for all the appropriate HD 1D systems of this chapter in the presence of parabolic potential wells.

(R2.7) Investigate the entropy for HD 1D systems of the negative refractive index and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field and non-uniform light waves and in the presence of strain.

(R2.8) Investigate the entropy for triangular HD 1D systems of the negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field in the presence of strain.

(R2.9) Investigate the entropy for all the problems of (R1.1) in the presence of arbitrarily oriented magnetic field.

(R2.10) Investigate the entropy for all the problems of (R1.1) in the presence of alternating electric field.

(R2.11) Investigate the entropy for all the problems of (R1.1) in the presence of alternating magnetic field.

(R2.12) Investigate the entropy for all the problems of (R1.1) in the presence of crossed electric field and quantizing magnetic fields.

(R2.13) Investigate the entropy for all the problems of (R1.1) in the presence of crossed alternating electric field and alternating quantizing magnetic fields.

(R2.14) Investigate the entropy for HD NWs of the negative refractive index, organic and magnetic materials.

(R2.15) Investigate the entropy for HD NWs of the negative refractive index, organic and magnetic materials in the presence of alternating time dependent magnetic field.

(R2.16) Investigate the entropy for HD NWs of the negative refractive index, organic and magnetic materials in the presence of in the presence of crossed alternating electric field and alternating quantizing magnetic fields.

(R2.17) (a) Investigate the entropy for HD NWs of the negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field considering many body effects.

(b) Investigate all the appropriate problems of this chapter for a Dirac electron.

(R2.18) Investigate all the appropriate problems of this chapter by including the many body, image force, broadening and hot carrier effects, respectively.

(R2.19) Investigate all the appropriate problems of this chapter by removing all the mathematical approximations and establishing the respective appropriate uniqueness conditions.

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3 Entropy in quantum box of heavily doped materials

A person is measured by not what he says or does, but by what he becomes.

3.1 Introduction

It is well known that as the dimension of the QWs increases from 1D to 3D, the degree of freedom of the free carriers decreases drastically and the density-of-states function changes from the Heaviside step function in OWs to the Dirac's delta function in quantum box (QB) [1].

QBs can be used for visualizing and tracking molecular processes in cells using standard fluorescence microscopy [2–4]. They display minimal photobleaching [5], thus allowing molecular tracking over prolonged periods and consequently, single molecule can be tracked by using optical fluorescence microscopy [6]. The salient features of quantum dot lasers [7] include low threshold currents, higher power, and great stability as compared with the conventional one, and the QBs find extensive applications in nanorobotics [8], neural networks [9], and high-density memory or storage media [10]. QBs are also used in nanophotonics [11] because of their theoretically high quantum yield and have been suggested as implementations of Q-bits for quantum information processing [12]. QBs also find applications in diode lasers [13], amplifiers [14], and optical sensors [15]. High-quality QBs are well suited for optical encoding [16] because of their broad excitation profiles and narrow emission spectra. The new generations of QBs have far-reaching potential for the accurate investigations of intracellular processes at the single-molecule level, high-resolution cellular imaging, long-term in vivo observation of cell trafficking, tumor targeting, and diagnostics [17]. QB nanotechnology is one of the most promising candidates for use in solid-state quantum computation [18]. It may also be noted that QBs are being used in single electron transistors [19], photovoltaic devices [20], photoelectrics [21], ultrafast all-optical switches and logic gates [22], organic dyes [23], and other types of nano devices [24–29].

In this chapter in Sections 3.2.1–3.2.14, we have investigated the entropy in QBs of HD nonlinear optical, III–V, II–VI, stressed Kane-type, Te, GaP, $PtSb_2$, Bi_2Te_3, Ge, GaSb, II–V, lead germanium telluride, zinc and cadmium diphosphides, respectively. Section 3.3 contains the result and discussions pertaining to this chapter. Section 3.4 presents 22 open research problems.

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3.2 Theoretical background

3.2.1 Entropy in QB of HD nonlinear optical materials

The dispersion relation in this case can be written following (2.1) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{||}\bar{T}_{21}(\bar{E}_{1QBHD},\eta_g)}+\frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}^*_{\perp}\bar{T}_{22}(\bar{E}_{1QBHD},\eta_g)}+\frac{\hbar^2(\bar{n}_x\pi/\bar{d}_x)^2}{2\bar{m}^*_{||}\bar{T}_{21}(\bar{E}_{1QBHD},\eta_g)}=1 \tag{3.1}$$

where $\bar{E}_{1QBHD}$ is the totally quantized energy in this case.

The total density-of-states function in this case is given by

$$\bar{N}_{0DT}(\bar{E})=\frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-\bar{E}_{1QBHD}) \tag{3.2}$$

where, $\delta'(\bar{E}-\bar{E}_{1QBHD})$ is the Dirac's Delta function.

Using (3.2) and Fermi–Dirac occupation probability factor, the total electron concentration can be written as

$$\bar{n}_{0D}=\frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\,\text{Re}\,al\,Part\,of\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{31HD}) \tag{3.3}$$

where

$$\eta_{31HD}\equiv(\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD}-\bar{E}_{1QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.3) we can study the entropy in this case.

For the purpose of comparison we shall also study the entropy in the absence of band tails in this case.

Let $\bar{E}_{n_i}$ $(i=\bar{x},\bar{y}\,and\,\bar{z})$ be the quantized energy levels due to infinitely deep potential well along ith-axis with $\bar{n}_i(=1,2,3,\ldots)$ as the size quantum numbers. Therefore, from (1.2), one can write

$$\gamma(\bar{E}_{n_x})=\bar{f}_1(\bar{E}_{n_x})\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 \tag{3.4}$$

$$\gamma(\bar{E}_{n_y})=\bar{f}_1(\bar{E}_{n_y})\left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2 \tag{3.5}$$

$$\gamma(\bar{E}_{n_z})=\bar{f}_2(\bar{E}_{n_z})\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 \tag{3.6}$$

From (1.2), the totally quantized energy $(\bar{E}_{QD1})$ can be expressed as

$$\gamma(\bar{E}_{QD1}) = \bar{f}_1(\bar{E}_{QD1})\left[\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right] + \bar{f}_2(\bar{E}_{QD1})\left[\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right] \tag{3.7}$$

The total density-of-states function in this case is given by

$$\bar{N}_{0DT}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\delta'(\bar{E}-\bar{E}_{QD1}) \tag{3.8}$$

The total electron concentration in this case can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{31}) \tag{3.9}$$

where

$$\eta_{31} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0D} - \bar{E}_{QD1})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.9), we can find the entropy in this case.

3.2.2 Entropy in QB of HD III–V materials

The dispersion relation of the conduction electrons of III–V materials are described by the models of Kane (both three and two bands together with parabolic energy band), Stillman et al. and Palik et al., respectively. For the purpose of complete and coherent presentation, the entropy in QBs of HD III–V compounds have also been investigated in accordance with the aforementioned different dispersion relations for relative comparison as follows:

(a) The three-band model of Kane

The dispersion relation in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_x\pi/\bar{d}_x)^2}{2\bar{m}_c} = \bar{T}_{44}(\bar{E}_{2QBHD}, \eta_g) \tag{3.10}$$

where

$$\bar{T}_{44}(\bar{E}_{2QBHD}, \eta_g) = \bar{T}_{31}(\bar{E}_{2QBHD}, \eta_g) + i\bar{T}_{31}(\bar{E}_{2QBHD}, \eta_g)$$

and $\bar{E}_{2QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\,\mathrm{Re}\,al\,Part\,of\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{31}) \tag{3.11}$$

where

$$\eta_{32\,HD} \equiv (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F0\,DHD} - \bar{E}_{2QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.11) we can study the entropy in this case.

The quantized energy levels ($\bar{E}_{n_x}, \bar{E}_{n_y}$ and $\bar{E}_{n_z}$ along x, y, and z directions, respectively) in the absence of band tails in QBs of III–V materials in accordance with the three-band model of Kane can be expressed as

$$\bar{I}_{11}(\bar{E}_{n_x}) = \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\pi \bar{n}_x}{\bar{d}_x}\right)^2 \tag{3.12}$$

$$\bar{I}_{11}(\bar{E}_{n_y}) = \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\pi \bar{n}_y}{\bar{d}_y}\right)^2 \tag{3.13}$$

and

$$\bar{I}_{11}(\bar{E}_{n_z}) = \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\pi \bar{n}_z}{\bar{d}_z}\right)^2 \tag{3.14}$$

The totally quantized energy $(\bar{E}_{QD2})$ in this case assumes the form

$$\bar{I}_{11}(\bar{E}_{QD2}) = \frac{\hbar^2\pi^2}{2\bar{m}_c}\left[\left(\frac{\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y}{\bar{d}_y}\right)^2 + \left(\frac{\bar{n}_z}{\bar{d}_z}\right)^2\right] \tag{3.15}$$

The electron concentration in this case is given by

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}x_{\max}}\sum_{\bar{n}_y=1}^{\bar{n}y_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}z_{\max}} \bar{F}_{-1}(\eta_{32}) \tag{3.16}$$

where

$$\eta_{32} \equiv (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F0D} - \bar{E}_{QD2})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.16) we can study the entropy in this case.

(b) The two band model of Kane

The dispersion relation in this case can be written following (2.24) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_x\pi/\bar{d}_x)^2}{2\bar{m}_c} = \gamma_2(\bar{E}_{3\,QBHD}, \eta_g) \tag{3.17}$$

and

$\bar{E}_{3QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{33\,HD}) \tag{3.18}$$

where

$$\eta_{33\,HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{3QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.18) we can find the entropy in this case.

For two-band model of Kane in the absence of bandtails, $\bar{E}_{n_z}$ obeys the equation

$$\bar{E}_{n_z}(1+\alpha\bar{E}_{n_z}) = \frac{\hbar^2\pi^2}{2\bar{m}_c}\left(\frac{\bar{n}_z}{\bar{d}_z}\right)^2 \tag{3.19}$$

The totally quantized energy $(\bar{E}_{QD3})$ in this case is given by

$$\bar{E}_{QD3}(1+\alpha\bar{E}_{QD3}) = \frac{\hbar^2\pi^2}{2\bar{m}_c}\left[\left(\frac{\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y}{\bar{d}_y}\right)^2 + \left(\frac{\bar{n}_z}{\bar{d}_z}\right)^2\right] \tag{3.20}$$

The electron concentration in this case is given by

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{33}) \tag{3.21}$$

where

$$\eta_{33} \equiv (\bar{k}_B\bar{T})^{-1}[(\bar{E}_{F0D} - \bar{E}_{QD3})]$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.21), we can find the entropy in this case.

(c) The parabolic energy bands

The dispersion relation in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_x\pi/\bar{d}_x)^2}{2\bar{m}_c} = \gamma_3(\bar{E}_{4QBHD}, \eta_g) \tag{3.22}$$

and $\bar{E}_{4QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{34\,HD}) \tag{3.23}$$

where

$$\eta_{34HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{4QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.23) we can find the entropy in this case.

In the absence of bandtails, the expressions for $\Delta\bar{n}_{0D}$, $\bar{E}_{n_z}$ and total electron concentration $(\bar{n}_{0D})$, for QBs of wide-gap materials can, respectively, be written as

$$\Delta\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\bar{F}_{-1}(\eta') \tag{3.24}$$

$$\bar{E}_{n_z} = \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \tag{3.25}$$

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta') \tag{3.26}$$

where,

$$\eta' \equiv (\bar{k}_B\bar{T})^{-1}\left[\bar{E}_{F0D} - \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.26) we can find the entropy in this case.

(d) The Model of Stillman et al.

The dispersion relation of the electrons in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_x\pi/\bar{d}_x)^2}{2\bar{m}_c} = \theta_4(\bar{E}_{5QBHD}, \eta_g) \tag{3.27}$$

and $\bar{E}_{5QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{35\,HD}) \tag{3.28}$$

where

$$\eta_{35\,HD} \equiv (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{5QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.28) we can find the entropy in this case.

In the absence of band tails, $\bar{E}_{n_z}$ obeys the equation

$$(\hbar^2/2\bar{m}_c)(\pi\bar{n}_z/\bar{d}_z)^2 \equiv \bar{I}_{12}(\bar{E}_{n_z}) \tag{3.29}$$

$\bar{E}_{QD5}$ in this case can be defined as

$$\bar{I}_{12}(\bar{E}_{QD5}) = \frac{\hbar^2\pi^2}{2\bar{m}_c}\left[\left(\frac{\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y}{\bar{d}_y}\right)^2 + \left(\frac{\bar{n}_z}{\bar{d}_z}\right)^2\right] \tag{3.30}$$

The electron concentration in this case is given by

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{35}) \tag{3.31}$$

where

$$\eta_{35} \equiv (\bar{k}_B \bar{T})^{-1}[(\bar{E}_{F0D} - \bar{E}_{5\,QDS})]$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.31), we can find the entropy in this case.

(e) The model of Palik et al.

The dispersion relation of the electrons in this case can be written as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_x\pi/\bar{d}_x)^2}{2\bar{m}_c} = \theta_5(\bar{E}_{6QBHD}, \eta_g) \tag{3.32}$$

and $\bar{E}_{6QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{36\,HD}) \tag{3.33}$$

where

$$\eta_{35} \equiv (\bar{k}_B \bar{T})^{-1}[(\bar{E}_{F0DHD} - \bar{E}_{6QBHD})]$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.33), we can study the entropy in this case.

In the absence of band tails, $\bar{E}_{n_z}$ and $\bar{E}_{QD7}$ are defined by the following equations:

$$\bar{I}_{13}(\bar{E}_{n_z}) = \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 \tag{3.34}$$

$$\bar{I}_{13}(\bar{E}_{QD7}) = \frac{\hbar^2}{2\bar{m}_c}\left[\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2 + \left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right] \tag{3.35}$$

The electron concentration in this case is given by

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{37}) \tag{3.36}$$

where

$$\eta_{37} \equiv \frac{(\bar{E}_{F0D} - \bar{E}_{5QDS})}{\bar{k}_B\bar{T}}$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.36), we can study the entropy in this case.

3.2.3 Entropy in QB of HD II–VI materials

The 0D electron dispersion law in QB of HD II–VI materials can be written following (2.56) as

$$\gamma_3(\bar{E}_{7QBHD}, \eta_g) = \overline{a'}_0\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right] \pm \bar{\lambda}_0\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2} + \frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}^*_{\|}} \tag{3.37}$$

where $\bar{E}_{7QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{37HD}) \tag{3.38}$$

where

$$\eta_{37HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0\,DHD} - \bar{E}_{7\,QBHD})$$

Using (1.31f) and (3.38), we can study the entropy in this case.

In the absence of band tails the totally quantized energy $\bar{E}_{QD10,\pm}$ in this case can be expressed as

$$\bar{E}_{QD10,\pm} = \overline{a'}_0 \left[\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right] + \frac{1}{2\bar{m}^*_{\|}}\left(\frac{\hbar\pi\bar{n}_z}{\bar{d}_z}\right)^2 \pm \bar{\lambda}_0 \left[\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right]^{1/2} \tag{3.39}$$

The electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{40,\pm}) \tag{3.40}$$

where

$$\eta_{40,\pm} \equiv \frac{1}{\bar{k}_B\bar{T}}[\bar{E}_{F0D} - \bar{E}_{QD10,\pm}]$$

Using (1.44) and (3.40), we can study the entropy in this case.

3.2.4 Entropy in QBof HD IV–VI materials

(a) Dimmock Model

In this case, the dispersion relation of the electrons can be written following (2.65) as

$$\frac{\bar{n}_z\pi}{\bar{d}_z} = \bar{T}_{36}(\bar{E}_{8QBHD}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{3.41}$$

where $\bar{E}_{8QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{38HD}) \tag{3.42}$$

where

$$\eta_{38HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{8QBHD})$$

Using (1.31f) and (3.42), we can study the entropy in this case.

In the absence of band tailing, the electron dispersion relation in this case can be written following (2.71) as

$$\frac{\bar{n}_z\pi}{\bar{d}_z} = \bar{T}_{40}(\bar{E}_{QD11}, \bar{n}_x, \bar{n}_y) \tag{3.43}$$

where $\bar{E}_{QD11}$ is the totally quantized energy in this case.

The electron concentration per band can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} [\bar{F}_{-1}(\eta_{41})] \tag{3.44}$$

where

$$\eta_{41} \equiv \frac{1}{\bar{k}_B \bar{T}} [\bar{E}_{F0D} - \bar{E}_{QD11}]$$

Using (1.44) and (3.44), we can study the entropy in this case.

(b) Bangert and Kastner Model

The electron dispersion relation in this case is given by following (2.77) as

$$\frac{\bar{n}_z \pi}{\bar{d}_z} = \bar{T}_{60}(\bar{E}_{9QBHD}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{3.45}$$

where $\bar{E}_{9QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{39HD}) \tag{3.46}$$

where

$$\eta_{39\,HD} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0DHD} - \bar{E}_{9QBHD})$$

Using (1.31f) and (3.46), we can study the entropy in this case.

In the absence of bandtails following (2.83) the dispersion relation is given by

$$\frac{\bar{n}_z \pi}{\bar{d}_z} = \bar{T}_{61}(\bar{E}_{12QD}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{3.47}$$

where $\bar{E}_{12QD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{42}) \tag{3.48}$$

where

$$\eta_{42} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0D} - \bar{E}_{12QD})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.48), we can study the entropy in this case.

3.2.5 Entropy in QB of HD stressed Kane-type materials

The electron dispersion relation in this case is given by following (2.89) as

$$\frac{\bar{n}_z \pi}{\bar{d}_z} = \bar{T}_{70}(\bar{E}_{10\,QBHD}, \eta_g, \bar{n}_x, \bar{n}_y) \tag{3.49}$$

where $\bar{E}_{10QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{40\,HD}) \tag{3.50}$$

where

$$\eta_{40HD} \equiv (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{10QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.50) we can study the entropy in this case.

In the absence of band-tails, the totally quantized energy $\bar{E}_{QD23}$ in this case assumes the form

$$\left(\frac{\pi \bar{n}_x}{\bar{d}_x}\right)^2 [\bar{a}_0(\bar{E}_{QD23})]^{-2} + \left(\frac{\pi \bar{n}_y}{\bar{d}_y}\right)^2 [\bar{b}_0(\bar{E}_{QD23})]^{-2} + \left(\frac{\pi \bar{n}_z}{\bar{d}_z}\right)^2 [\bar{c}_0(\bar{E}_{QD23})]^{-2} = 1 \tag{3.51}$$

The electron concentration is given by

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{53}) \tag{3.52}$$

where

$$\eta_{53} \equiv (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F0D} - \bar{E}_{QD23})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.52), we can study the entropy in this case.

3.2.6 Entropy in QB of HD Te

The 0D dispersion relation may be written in this case as

$$\frac{\bar{n}_x \pi}{\bar{d}_x} = \bar{T}_{72}(\bar{E}_{11QBHD}, \bar{n}_x, \bar{n}_y, \eta_g) \tag{3.53}$$

where $\bar{E}_{11QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written a

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{42HD}) \tag{3.54}$$

where

$$\eta_{42HD} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0DHD} - \bar{E}_{12QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.54) we can study the entropy in this case.

In the absence of doping, the totally quantized energy can be written as

$$\bar{E}_{QD14,\pm} = \psi_1 \left(\frac{\pi \bar{n}_z}{\bar{d}_z} \right) + \psi_2 \left[\left(\frac{\pi \bar{n}_x}{\bar{d}_x} \right)^2 + \left(\frac{\pi \bar{n}_y}{\bar{d}_y} \right)^2 \right] \pm \left[\psi_3^2 \left(\frac{\pi \bar{n}_z}{\bar{d}_z} \right)^2 + \psi_4^2 \left[\left(\frac{\pi \bar{n}_x}{\bar{d}_x} \right)^2 + \left(\frac{\pi \bar{n}_y}{\bar{d}_y} \right)^2 \right] \right]^{1/2} \tag{3.55}$$

The electron concentration is given by

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{44,\pm}) \tag{3.56}$$

where

$$\eta_{44,\pm} \equiv (\bar{E}_{F0D} - \bar{E}_{QD14,\pm}) / (\bar{k}_B \bar{T})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.56) we can study the entropy in this case.

3.2.7 Entropy in QB of HD gallium phosphide

The 0D dispersion relation may be written in this case following (2.109) as

$$\frac{\bar{n}_x \pi}{\bar{d}_x} = \bar{u}_{70}(\bar{E}_{14\,QBHD}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{3.57}$$

where $\bar{E}_{14QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{44HD}) \tag{3.58}$$

where

$$\eta_{44HD} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0DHD} - \bar{E}_{14QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.58), we can study the entropy in this case.

In the absence of doping, the totally quantized energy ($\bar{E}_{QD16}$) in this case can be written as

$$\begin{aligned}\bar{E}_{QD16} = {} & \frac{\hbar^2}{2\bar{m}^*_{\perp}} \left[\left(\frac{\pi \bar{n}_x}{\bar{d}_x} \right)^2 + \left(\frac{\pi \bar{n}_y}{\bar{d}_y} \right)^2 \right] + \frac{\hbar^2}{2\bar{m}^*_{||}} \left[\left(\frac{\pi \bar{n}_x}{\bar{d}_x} \right)^2 + \left(\frac{\pi \bar{n}_y}{\bar{d}_y} \right)^2 + \left(\frac{\pi \bar{n}_z}{\bar{d}_z} \right)^2 \right] \\ & - \left[\frac{\hbar^4 \bar{k}_0^2}{\bar{m}^{*2}_{||}} \left[\left(\frac{\pi \bar{n}_x}{\bar{d}_x} \right)^2 + \left(\frac{\pi \bar{n}_y}{\bar{d}_y} \right)^2 + \left(\frac{\pi \bar{n}_z}{\bar{d}_z} \right)^2 \right] + |V_G|^2 \right]^{1/2} + |V_G|\end{aligned} \tag{3.59}$$

The electron concentration assumes the form

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_{x=1}}^{\bar{n}_{x\max}} \sum_{\bar{n}_{y=1}}^{\bar{n}_{y\max}} \sum_{\bar{n}_{z=1}}^{\bar{n}_{z\max}} [\bar{F}_{-1}(s\eta_{46})] \tag{3.60}$$

where

$$\eta_{46} \equiv \frac{1}{\bar{k}_B \bar{T}} (\bar{E}_{F0D} - \bar{E}_{QD16})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.60), we can study the entropy in this case.

3.2.8 Entropy in QB of HD platinum antimonide

The 0D dispersion relation may be written in this case following (2.119) as

$$\frac{\bar{n}_x \pi}{\bar{d}_x} = \bar{V}_{70}(\bar{E}_{15QBHD}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{3.61}$$

where $\bar{E}_{15QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_{x=1}}^{\bar{n}_{x\max}} \sum_{\bar{n}_{y=1}}^{\bar{n}_{y\max}} \sum_{\bar{n}_{z=1}}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{45HD}) \tag{3.62}$$

where

$$\eta_{45HD} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0DHD} - \bar{E}_{15QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.62), we can study the entropy in this case.

In the absence of band tailing the 0D dispersion relation in this case can be written using (2.124) as

$$\frac{\bar{n}_x \pi}{\bar{d}_x} = \bar{D}_{71}(\bar{E}_{QD17}, \bar{n}_y, \bar{n}_z) \tag{3.63}$$

where $\bar{E}_{1QD17}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{50}) \tag{3.64}$$

where

$$\eta_{50} \equiv (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F0D} - \bar{E}_{QD17})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.64) we can study the entropy in this case.

3.2.9 Entropy in QB of HD bismuth telluride

The dispersion relation in this case can be written as

$$\frac{\bar{n}_x \pi}{\bar{d}_x} = \bar{J}_{70}(\bar{E}_{18\,QBHD}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{3.65}$$

where $\bar{E}_{18QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{48\,HD}) \tag{3.66}$$

where

$$\eta_{48HD} \equiv (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{18QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.66), we can study the entropy in this case.

The dispersion relation of the conduction electrons in Bi_2Te_3 in the absence of doping can be written as

$$\bar{E}(1 + \alpha \bar{E}) = \frac{\hbar^2}{2\bar{m}_0}(\alpha_{11}\bar{k}_x^{\,2} + \alpha_{22}\bar{k}_y^{\,2} + \alpha_{33}\bar{k}_z^{\,2} + 2\alpha_{23}\bar{k}_y\bar{k}_z) \tag{3.67}$$

where $\alpha_{11}, \alpha_{22}, \alpha_{33}$ and α_{23} are spectrum constants.

The totally quantized energy $\bar{E}_{QD33}$ can be written as

$$\bar{E}_{QD33}(1+\alpha\bar{E}_{QD33}) = \frac{\hbar^2}{2\bar{m}_0}\left[\alpha_{11}\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \alpha_{22}\left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2 + \alpha_{33}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + 2\alpha_{23}\left(\frac{\pi^2\bar{n}_y\bar{n}_z}{\bar{d}_y\bar{d}_z}\right)\right] \tag{3.68}$$

The hole concentration is given by

$$\bar{p}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[1+\exp(\eta_{62})]^{-1} \tag{3.69}$$

where

$$\eta_{62} = \frac{1}{\bar{k}_B\bar{T}}[\bar{E}_{F0D} - \bar{E}_{QD33}]$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.69), we can study the entropy in this case.

3.2.10 Entropy in QB of HD germanium

(a) Model of Cardona et al.

The dispersion relation in accordance with this model in the present case can be written following (2.138) as

$$\frac{\bar{n}_x\pi}{\bar{d}_x} = \bar{L}_{70}(\bar{E}_{20QBHD}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{3.70}$$

where $\bar{E}_{20QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{50HD}) \tag{3.71}$$

where

$$\eta_{50HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{20QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.71) we can study the entropy in this case.

In the absence of doping the totally quantized energy $\bar{E}_{QD30}$ in this case can be written as

$$\bar{E}_{QD30} = -\frac{\bar{E}_{g_0}}{2} + \frac{\hbar^2}{2\bar{m}^*_{\|}}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + \left[\frac{\bar{E}^2_{g_0}}{4} + \bar{E}_{g_0}\left(\frac{\hbar^2}{2\bar{m}^*_{\perp}}\right)\left\{\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right\}\right]^{1/2} \tag{3.72}$$

The electron concentration assumes the form

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}[\bar{F}_{-1}(\eta_{42})] \tag{3.73}$$

where

$$\eta_{42} \equiv \frac{1}{\bar{k}_B\bar{T}}(\bar{E}_{F0D} - \bar{E}_{QD30})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.73) we can study the entropy in this case.

(b) Model of Wang and Ressler

The dispersion relation in accordance with this model in the present case can be written following (2.148) as

$$\frac{\bar{n}_x\pi}{\bar{d}_x} = \beta_{70}(\bar{E}_{24QBHD}, \bar{n}_y, \bar{n}_z, \eta_g) \tag{3.74}$$

where $\bar{E}_{24QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}[\bar{F}_{-1}(\eta_{54HD})] \tag{3.75}$$

where

$$\eta_{54HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{24QDBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.75) we can study the entropy in this case.

In the absence of doping, the totally quantized energy E_{QD40} in this case is given by

$$\bar{E}_{QD40} = \frac{\bar{h}^2}{2\bar{m}^*_{\|}}\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 + \frac{\bar{h}^2}{2\bar{m}^*_{\perp}}\left\{\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right\} - \bar{c}_1\left(\frac{\bar{h}^2}{2\bar{m}^*_{\perp}}\right)\left\{\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right\}$$
$$- \bar{d}_{11}\left(\frac{\bar{h}^2}{2\bar{m}^*_{\perp}}\right)\left\{\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right\}\left(\frac{\bar{h}^2}{2\bar{m}^*_{\|}}\right)\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 - e_1\left(\frac{\bar{h}^2}{2\bar{m}^*_{\|}}\right)^2\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^4 \tag{3.76}$$

The electron concentration assumes the form

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{\max}}}[\bar{F}_{-1}(\eta_{50})] \tag{3.77}$$

where

$$\eta_{50} \equiv \frac{1}{\bar{k}_B\bar{T}}(\bar{E}_{F0D} - \bar{E}_{QD40})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.77) we can study the entropy in this case.

3.2.11 The entropy in quantum box (QB) of HD gallium antimonide

The dispersion relation of the 0D electrons in this case can be written following (2.158) as

$$\frac{\hbar^2(\bar{n}_z\pi/\bar{d}_z)^2}{2\bar{m}_c} + \frac{\hbar^2(\bar{n}_y\pi/\bar{d}_y)^2}{2\bar{m}_c} + \frac{\hbar^2(\frac{\bar{n}_x\pi}{\bar{d}_x})^2}{2\bar{m}_c} = \bar{I}_{36}(\bar{E}_{30QBHD}, \eta_g) \tag{3.78}$$

where $\bar{E}_{30QBHD}$ is the totally quantized energy in this case.

The total electron concentration can be written as

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{\max}}}[\bar{F}_{-1}(\eta_{60HD})] \tag{3.79}$$

where

$$\eta_{60HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD} - \bar{E}_{30QBHD})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.79) we can study the entropy in this case.

In the absence of band tails, the dispersion relation in this case can be written as

$$\bar{E} = \alpha_9\bar{k}^2 + \frac{\bar{E}_{g1}}{2}\left[\sqrt{1+\alpha_{10}\bar{k}^2} - 1\right] \tag{3.80}$$

where $\alpha_9 = \frac{\hbar^2}{2\bar{m}_0}$ and $\alpha_{10} = \left(\frac{(2\hbar^2)}{(\bar{E}_{g1})}\right)\left[\frac{1}{\bar{m}_c} - \frac{1}{\bar{m}_0}\right]$

From (3.80), we get

$$\bar{k}^2 = \frac{\bar{E}}{\alpha_9} + \alpha_{11} - [\alpha_{12}\bar{E} + \alpha_{13}]^{1/2} \tag{3.81}$$

where

$$\alpha_{11} = \frac{\bar{E}_{g1}^2}{8\alpha_9^2}\left[\alpha_{10} + \frac{4\alpha_9}{\bar{E}_{g1}}\right],\ \bar{\alpha}_{12} = \left(\frac{\bar{E}_{g1}^2}{\alpha_9^3}\right),\ \alpha_{13} = \frac{\bar{E}_{g1}^4}{64\alpha_9^4}\left[\alpha_{10}^2 + \frac{10\alpha_9^2}{\bar{E}_{g1}^2} - \frac{8\alpha_9\alpha_{10}}{\bar{E}_{g1}}\right]$$

The totally quantized energy $\bar{E}_{QD60}$ assumes the form

$$\bar{E}_{QD60} = \alpha_9\left[\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2 + \left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^4\right] + \frac{\bar{E}_{g1}}{2}\left[\sqrt{1 + \alpha_{10}\left[\left(\frac{\pi\bar{n}_x}{\bar{d}_x}\right)^2 + \left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2 + \left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]} - 1\right] \tag{3.82}$$

The electron concentration is given by

$$\bar{n}_{0D} = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{70}) \tag{3.83}$$

where

$$\eta_{70} \equiv (\bar{E}_{F0D} - \bar{E}_{QD60})/(\bar{k}_B\bar{T})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.83) we can study the entropy in this case.

3.2.12 The entropy in quantum box (QB) of HD II–V materials

The DR of the holes in QDs of HD II–V compounds can be expressed as

$$\gamma_3(\bar{E}_{100QBHD}, \eta_g) = \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{11}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{12}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^{22} \pm \left[\left(\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{15}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{16}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right)^2 + \bar{A}_{18}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right) + \bar{A}_{19}^2\right]^{1/2} \tag{3.84}$$

where $\bar{E}_{100QBHD}, \eta_g$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_D = \frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\delta(\bar{E} - \bar{E}_{100QBHD,\pm}) \tag{3.85}$$

The electron concentration can be expressed as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{601HD}) \tag{3.86}$$

where

$$\eta_{601HD} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0DHD} - \bar{E}_{10QBHD,\pm})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.86) we can study the entropy in this case.

In the absence of band-tailing, the 0D hole energy spectrum in this case assumes the form

$$\bar{E}_{QD70,\pm} = \bar{A}_{10}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{11}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{12}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \bar{A}_{13}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^{22}$$
$$\pm \left[\left(\bar{A}_{14}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \bar{A}_{15}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \bar{A}_{16}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \bar{A}_{17}\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)\right)^2 + \bar{A}_{18}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right) + \bar{A}_{19}^2\right]^{1/2} \tag{3.87}$$

where $\bar{E}_{QD70,\pm}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{0DT}(\bar{E}) = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \delta(\bar{E} - \bar{E}_{QB70HD,\pm}) \tag{3.88}$$

The electron concentration can be expressed as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{602HD}) \tag{3.89}$$

where

$$\eta_{602HD} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0D} - \bar{E}_{QD70,\pm})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.89) we can study the entropy in this case.

3.2.13 The entropy in quantum box (QB) of HD lead germanium telluride

The 0D electron energy spectrum in n-type $Pb_{1-x}Ge_xTe$ under the condition of formation of band tails can be written as

$$\left[\frac{2}{1+Erf\left(\frac{\bar{E}_{101QBHD,\pm}}{\eta_g}\right)}\right]\theta_0(\bar{E}_{101QBHD,\pm},\eta_g)+\gamma_3(\bar{E}_{101QBHD,\pm},\eta_g)$$

$$\left[\bar{E}_{go}-0.195\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]-0.345\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right.$$

$$=\left[0.23\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]+0.02\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$

$$\pm\left[0.06\bar{E}_{go}+0.061\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]+0.0066\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2}$$

$$+\left[\bar{E}_{go}+0.411\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]+0.377\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$

$$\left.\left[0.606\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]+0.722\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right] \tag{3.90}$$

where $\bar{E}_{101QBHD,\pm}$ is the quantized energy in this case.

The DOS function is given by

$$\bar{N}_{0DT}(\bar{E})=\frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{max}}}\delta(\bar{E}-\bar{E}_{101QBHD,\pm}) \tag{3.91}$$

The electron concentration can be expressed as

$$\bar{n}_{0D}=\frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{max}}}\bar{F}_{-1}(\eta_{603HD}) \tag{3.92}$$

where

$$\eta_{603HD}\equiv(\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD}-\bar{E}_{101QBHD,\pm})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.92) we can study the entropy in this case.

The 0D dispersion law of n-type $Pb_{1-x}Ge_xTe$ with x = 0.01 in the absence of band-tails can be expressed as

$$\left[\bar{E}_{QD70,\pm} - 0.606\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right] - 0.722\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$

$$\left[\bar{E}_{QD71,\pm} + \bar{E}_{go} + 0.411\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right] + 0.377\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$

$$\left[0.23\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right] + 0.02\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 \pm \left[0.06\bar{E}_{go} + 0.061\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]\right.\right.$$

$$\left.\left. + 0.0066\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2\right]^{1/2} \tag{3.93}$$

where $\bar{E}_{QD71,\pm}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{0DT}(\bar{E}) = \frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\delta'(\bar{E} - \bar{E}_{QD71,\pm}) \tag{3.94}$$

The electron concentration can be expressed as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{604HD}) \tag{3.95}$$

where

$$\eta_{604HD} \equiv (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0D} - \bar{E}_{QD71,\pm})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.44) and (3.95) we can study the entropy in this case.

3.2.14 The entropy in quantum box (QB) of HD zinc and cadmium diphosphides

The DR in HD QDs of Zinc and Cadmium diphosphides can be written as

$$\gamma_3(\bar{E}_{102QBHD,\pm}, \eta_g) = \left[\beta_1 + \frac{\beta_2\beta_{31}(\bar{n}_x, \bar{n}_y, \bar{n}_z)}{8\beta_4}\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$

$$\pm\left\{\left[\beta_4\beta_{31}(\bar{n}_x, \bar{n}_y, \bar{n}_z)\left(\beta_5 - \frac{\beta_2\beta_{31}(\bar{n}_x, \bar{n}_y, \bar{n}_z)}{8\beta_4}\right)\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right]\right.$$

$$+8\beta_4{}^2\left(1-\frac{\beta_{31}{}^2(\bar{n}_x,\bar{n}_y,\bar{n}_z)}{4}\right)-\beta_2\left(1-\frac{\beta_{31}{}^2(\bar{n}_x,\bar{n}_y,\bar{n}_z)}{4}\right)\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\Bigg\}^{1/2} \tag{3.96}$$

where

$$\beta_{31}(\bar{n}_x,\bar{n}_y,\bar{n}_z)=\left[\frac{(\frac{\bar{n}_x\pi}{\bar{d}_x})^2+(\frac{\bar{n}_y\pi}{\bar{d}_y})^2-2(\frac{\bar{n}_z\pi}{\bar{d}_z})^2}{\left[(\frac{\bar{n}_x\pi}{\bar{d}_x})^2+(\frac{\bar{n}_y\pi}{\bar{d}_y})^2+(\frac{\bar{n}_z\pi}{\bar{d}_z})^2\right]}\right]$$

and $\bar{E}_{102QBHD,\pm}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{0DT}(\bar{E})=\frac{\bar{g}_\nu}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{\max}}}\delta'(\bar{E}-\bar{E}_{102QBHD,\pm}) \tag{3.97}$$

The electron concentration can be expressed as

$$\bar{n}_{0D}=\frac{\bar{g}_\nu}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{605HD}) \tag{3.98}$$

where

$$\eta_{605HD}\equiv(\bar{k}_B\bar{T})^{-1}(\bar{E}_{F0DHD}-\bar{E}_{102QBHD,\pm})$$

and $\bar{E}_{F0DHD}$ is the Fermi energy in this case.

Using (1.31f) and (3.98) we can study the entropy in this case

The 0D DR in QDs of Zinc and Cadmium diphosphides in the absence of band-tails can be written as

$$\bar{E}_{72QB,\pm},\eta_g=\left[\beta_1+\frac{\beta_2\beta_{31}(\bar{n}_x,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right]\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]$$
$$\pm\Bigg\{\left[\beta_4\beta_{31}(\bar{n}_x,\bar{n}_y,\bar{n}_z)\left(\beta_5-\frac{\beta_2\beta_{31}(\bar{n}_x,\bar{n}_y,\bar{n}_z)}{8\beta_4}\right)\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\right]$$
$$+8\beta_4{}^2\left(1-\frac{\beta_{31}{}^2(\bar{n}_x,\bar{n}_y,\bar{n}_z)}{4}\right)-\beta_2\left(1-\frac{\beta_{31}{}^2(\bar{n}_x,\bar{n}_y,\bar{n}_z)}{4}\right)\left[\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2+\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2+\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2\right]\Bigg\}^{1/2} \tag{3.99}$$

where $\bar{E}_{QD72,\pm}$ is the quantized energy in this case.

The DOS function is given by

$$\bar{N}_{0DT}(\bar{E}) = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \delta'(\bar{E} - \bar{E}_{QD72,\pm}) \tag{3.100}$$

The electron concentration can be expressed as

$$\bar{n}_{0D} = \frac{\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{606HD}) \tag{3.101}$$

where

$$\eta_{606HD} \equiv (\bar{k}_B \bar{T})^{-1} (\bar{E}_{F0D} - \bar{E}_{QD72,\pm})$$

and $\bar{E}_{F0D}$ is the Fermi energy in this case.

Using (1.44) and (3.101) we can study the entropy in this case.

3.3 Results and discussion

Using the appropriate equation and the band constants from appendix 15, the normalized entropy in HD QBs of $CdGeAs_2$has been plotted as a function of film thickness for the generalized band model as shown by curve (a) where the curves (b), (c) and (d) are valid for three and two band models of Kane together with parabolic energy bands respectively. The case for $\delta = 0$ has been plotted in the same figure and is represented by curve (e) for the purpose of assessing the influence of crystal field splitting on the entropy in HD QBs of $CdGeAs_2$. The Figure 3.2 exhibits the variations of normalized entropy in HD QBs of $CdGeAs_2$ as a function of electron concentration for all the cases mentioned as above for Figure 3.1 In Figures 3.3, 3.5 and 3.7, the normalized entropy in HD QBs of InAs, GaAs and InSb has been plotted as a function of film thickness in accordance with the three and two band models of Kane together with parabolic energy bands as shown by curves (a), (b) and (c) in the respective figures. The Figures 3.4, 3.6 and 3.8 demonstrate the concentration dependence of the normalized entropy in HD QBs of InAs, GaAs and InSb for all the cases of Figure 3.3. The Figures 3.9, 3.10 and 3.12 illustrate the film thickness dependence of the normalized entropy in HD QBs of InAs, GaAs and InSb in accordance with the models of Stillman et al., Palik et al. at T=5K and T=15K as represented by curves (a), (b) and (c) respectively. The Figures 3.11 and 3.13 demonstrate the influence of carrier concentration on the normalized entropy in HD QBs of GaAs and InSb for all the cases of Figure 3.11. The Figure 3.14 exhibits the film thickness dependence of the normalized entropy for HD QBs of InSb and InAs in accordance with the model of Palik et al. at T=1K as represented by the curves (a) and (b) respectively. The Figure 3.15 illustrates the concentration dependence of normalized entropy for all the cases of Figure 3.14.

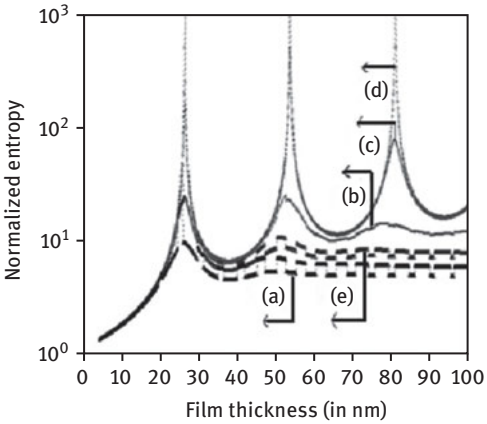

Figure 3.1: Plot of the normalized entropy in HDQBs of $CdGeAs_2$ as a function of film thickness has been shown in accordance with the (a) generalized band model ($\delta \neq 0$), (b) three and (c) two band models of Kane together with (d) parabolic energy bands. The special case for $\delta = 0$ (e) has also been shown to assess the influence of crystal field splitting.

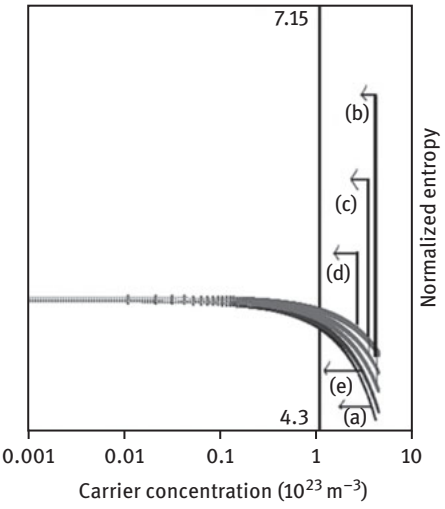

Figure 3.2: Plot of the normalized entropy in HDQBs of $CdGeAs_2$ as a function of carrier concentration for all cases of Figure 3.1.

The Figure 3.16 demonstrates the film thickness dependence of the normalized entropy for HD QBs of InSb and InAs in accordance with the model of Stillman et al. at T=2K as represented by the curves (a) and (b) respectively. The Figure 3.17 shows the concentration dependence of normalized entropy for all the cases of Figure 3.16. The Figure 3.18 depicts the film thickness dependence of the normalized entropy for

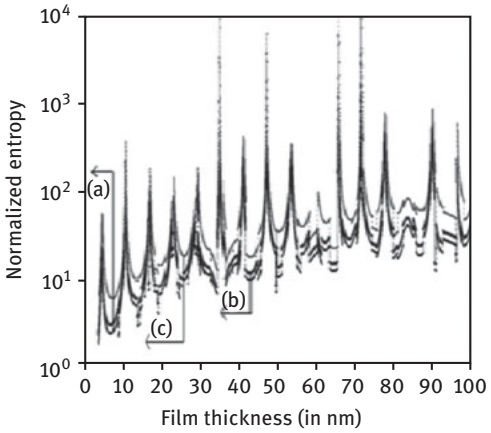

Figure 3.3: Plot of the normalized entropy in HDQBs of InAs as a function of film thickness in accordance with the (a) three and (b) two band models of Kane together with (c) parabolic energy bands.

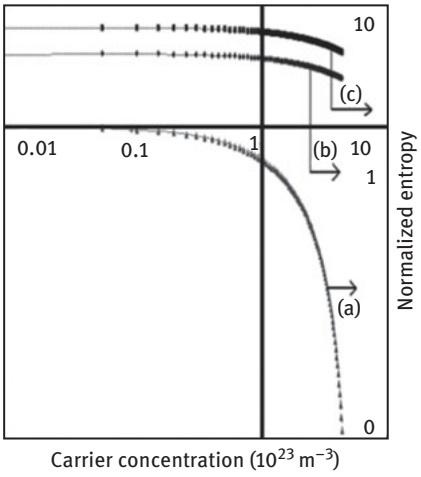

Figure 3.4: Plot of the normalized entropy in HDQBs of InAs as a function of carrier concentration for all the cases of Figure 3.3.

HDQBs of InSb and InAs in accordance with the model of Palik et al. as represented by the curves (a) and (b) in this context. The Figure 3.19 models the concentration dependence of normalized entropy for all the cases of Figure 3.11. The Figure 3.20 exhibits the variation of the normalized entropy with the film thickness in HDQBs of II–VI materials in accordance with Hopfield model, taking p-CdS as an example and considering both the cases $\bar{\lambda}_0 = 0$ and $\bar{\lambda}_0 \neq 0$) and GaP in accordance with the model of

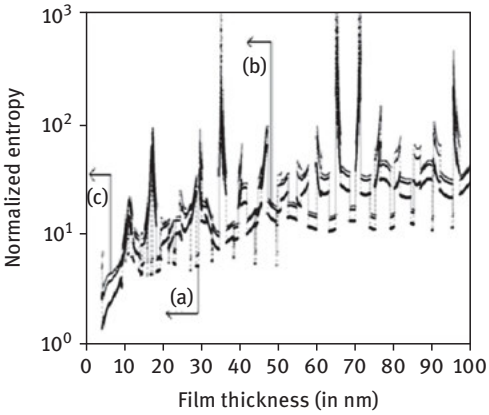

Figure 3.5: Plot of the normalized entropy from HDQBs of GaAs as a function of film thickness in accordance with the (a) three and (b) two band models of Kane together with (c) the parabolic energy bands.

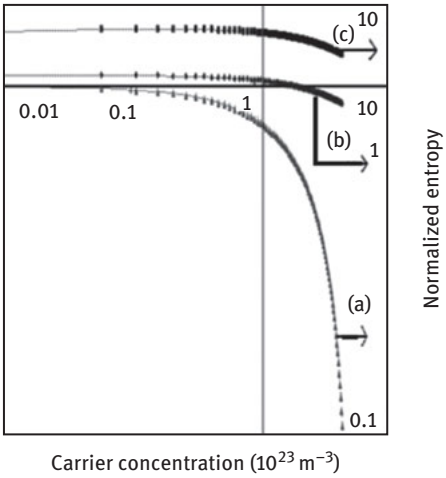

Figure 3.6: Plot of the normalized entropy in HDQBs of GaAs as a function of carrier concentration for all the cases of Figure 3.5.

Rees) as shown by curves (a), (b) and (c) respectively. The Figure 3.21 demonstrates the concentration variation of the normalized entropy for all cases of Figure 3.20. In Figure 3.22, the normalized entropy has been plotted as a function of film thickness for HDQBs of Germanium for both the models of Wang et al. and Cardona et al. as shown by curves (a) and (b) respectively. The Figure 3.23 exhibits the normalized entropyas a function of film thickness in HDQBs of Tellurium (by using the models of Bouat et al. at T=10K and T=20K and stressed Kane type materials (taking n-InSb as

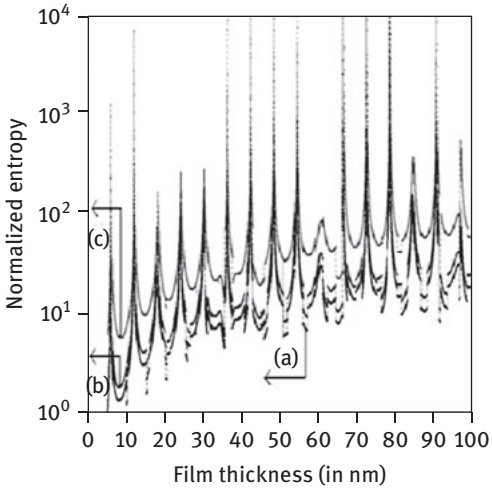

Figure 3.7: Plot of the normalized entropy in HDQBs of InSb as a function of film thickness for all the cases of Figure 3.3.

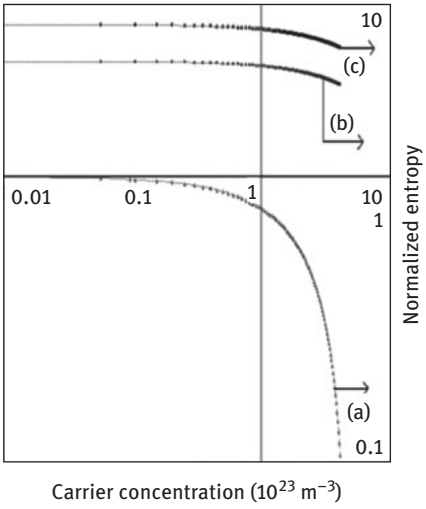

Figure 3.8: Plot of the normalized entropy in HDQBs of InSb as a function of carrier concentration for all the cases of Figure 3.4.

an example) in accordance with the models of Seiler et al. as shown by curves (a), (b) and (c) respectively. The Figure 3.24 shows the dependence of the normalized entropy on the carrier concentration for all the cases of Figure 3.23. In Figure 3.25, the normalized entropy has been plotted as a function of carrier concentration for HDQBs

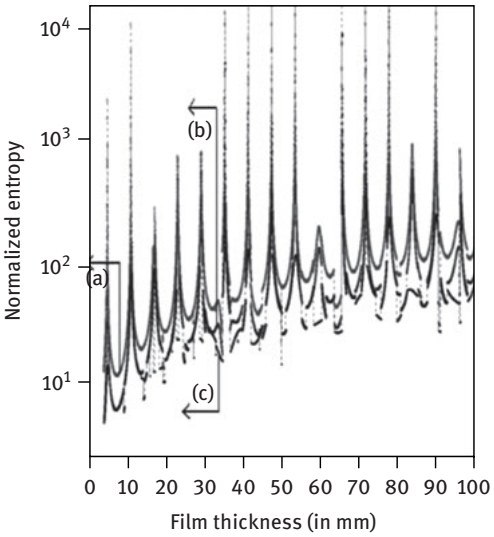

Figure 3.9: Plot of the normalized entropy in HDQBs of InAs as a function of film thickness in accordance with the models of (a) Stillman et al., (b) Newson et al. and (c) Rossler et al. respectively.

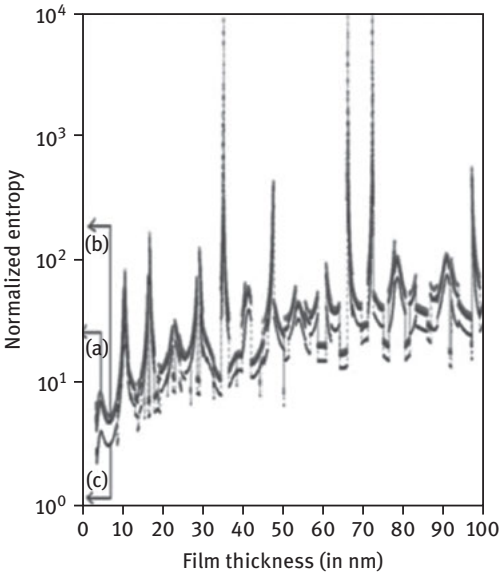

Figure 3.10: Plot of the normalized entropy in HDQBs of GaAs as a function of film thickness for all the cases of Figure 3.9.

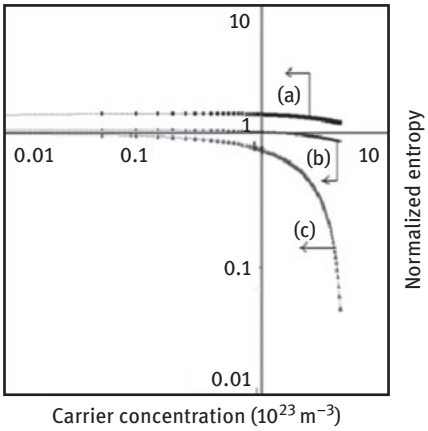

Figure 3.11: Plot of the normalized entropy in HDQBs of GaAs as a function of carrier concentration for all the cases of Figure 3.9.

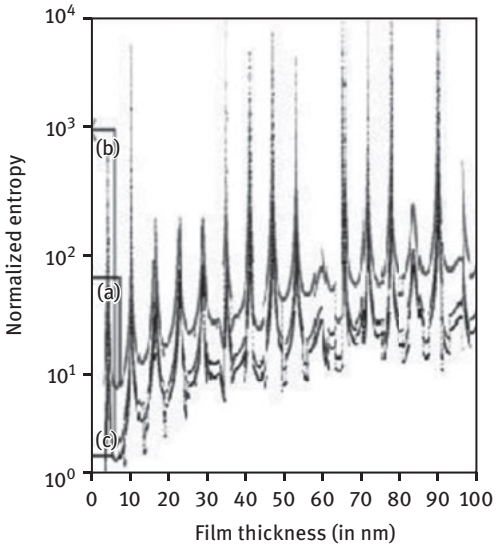

Figure 3.12: Plot of the normalized entropy in HDQBs of InSb as a function of film thickness for all the cases of Figure 3.9.

of Platinum Antimonide at T=5K, 10K and Lead Germanium Telluride at T=6K and 10K as shown by curves (a), (b), (c) and (d) respectively.

The Figure 3.26 depicts the plot of normalized entropy as a function of film thickness of GaSb at T=5K for (a), T=10K for (b) and T=15K for (c) respectively. The Figure 3.27 exhibits the carrier concentration dependence of the normalized entropy

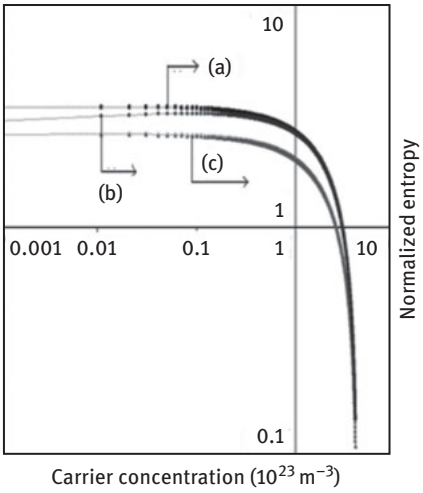

Figure 3.13: Plot of the normalized entropy in HDQBs of InSb as a function of carrier concentration for all the cases of Figure 3.9.

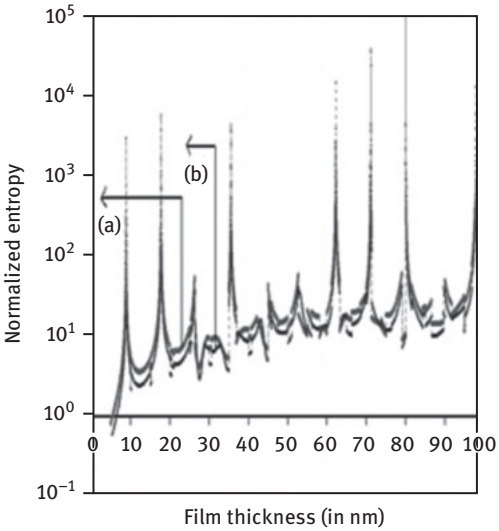

Figure 3.14: Plot of the normalized entropy in HDQBs of (a) InSb and (b) InAs as a function of film thickness in accordance with model of Agafonov et al.

for all the cases of Figure 3.26. The Figure 3.28 illustrates the variation of the normalized entropy with film thickness in HDQBs of PbSe at T=5K, 10K, 14K and 16K as shown by curves (a), (b), (c) and (d) respectively. The Figure 3.29 shows the dependence of

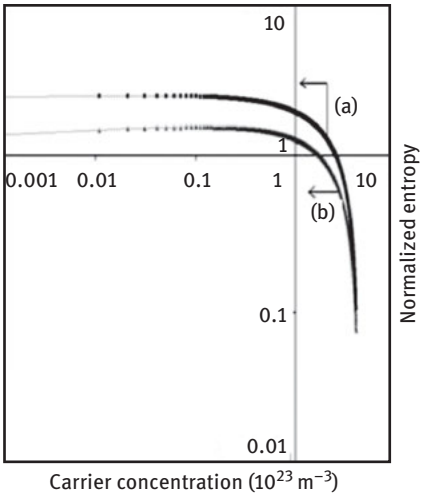

Figure 3.15: Plot of the normalized entropy in HDQBs of (a) InSb and (b) InAs as a function of carrier concentration for the case of Figure 1.14.

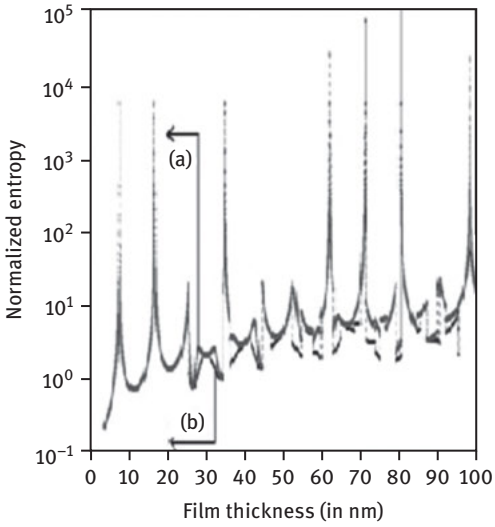

Figure 3.16: Plot of the normalized entropy in HDQBs of (a) InSb and (b) InAs as a function of film thickness in accordance with the model of Johnson et al.

normalized entropy on the carrier concentration in HDQBs of PbSe for all types of band models as stated in Figure 3.28. The Figure 3.30 shows the variation of entropy on film thickness for HDQBs of IV–VI materials (taking PbTe as an example) at T=5K, 10K and 15K together with Bismuth Telluride as shown by the curves (a), (b), (c) and (d)

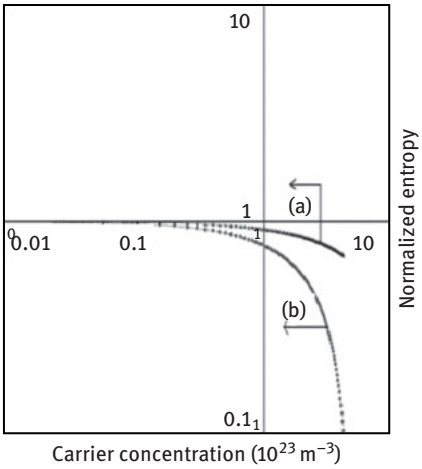

Figure 3.17: Plot of the normalized entropy in HD QBs of (a) InSb and (b) InAs as a function of carrier concentration for the case of Figure 3.16.

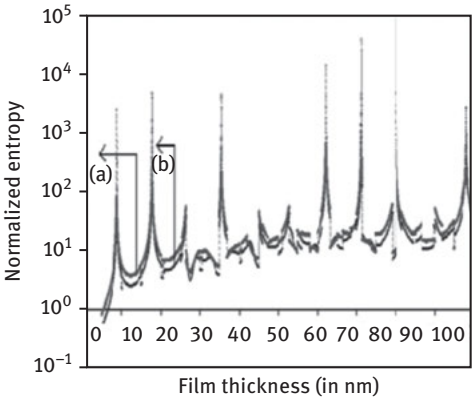

Figure 3.18: Plot of the normalized entropy in HD QBs of (a) InSb and (b) InAs as a function of film thickness in accordance with the model of Palik et al.

respectively. The Figure 3.31 models the variation of the entropy with the carrier concentration for HDQBs of IV–VI materials and Bismuth Telluride in accordance with the band models of Figure 3.30. The Figure 3.32 shows the plot of the normalized entropy as a function of film thickness in HDQBs of (a) II–V compound (CdSb), (b) zinc diphosphide, (c) cadmium diphosphide at T=4K and (d) T=8K as a function of film thickness respectively. For the purpose of simplified numerical computation, broadening has been neglected for obtaining all the plots. The inclusion of broadening will change the numerical magnitudes without altering the physics inside.

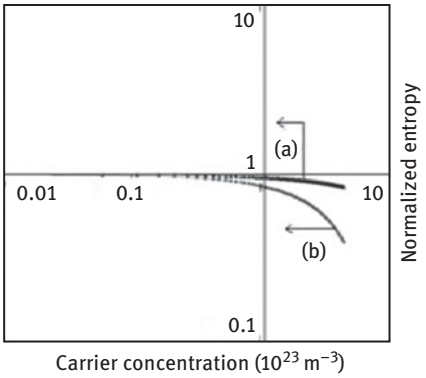

Figure 3.19: Plot of the normalized entropy in HD QBs of (a) InSb and (b) InAs as a function of carrier concentration for the case of Figure 3.18.

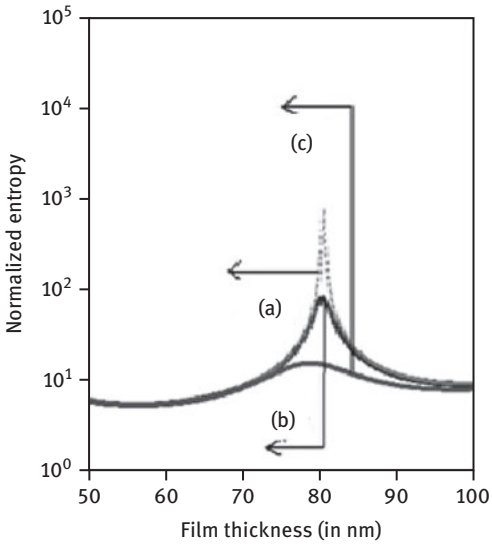

Figure 3.20: Plot of the normalized entropy in HD QBs of CdS with (a) $\bar{\lambda}_0 \neq 0$, (b) $\bar{\lambda}_0 = 0$ and (c) GaP as a function of film thickness in accordance with the models of Hopfield and Rees respectively.

The signature of 3D quantization is forthwith evident from the Figures 3.1, 3.3, 3.5, 3.7, 3.9, 3.10, 3.12, 3.14, 3.16, 3.18, 3.20, 3.22, 3.23, 3.26, 3.28, 3.30 and 3.32 for all materials as discussed having different band structures. It can be facilely discerned from the same that the normalized entropy oscillates with film thickness exhibiting spikes for various values of film thickness which are totally band structure dependent. The occurrence of peaks in the said figures originates from the totally quantized

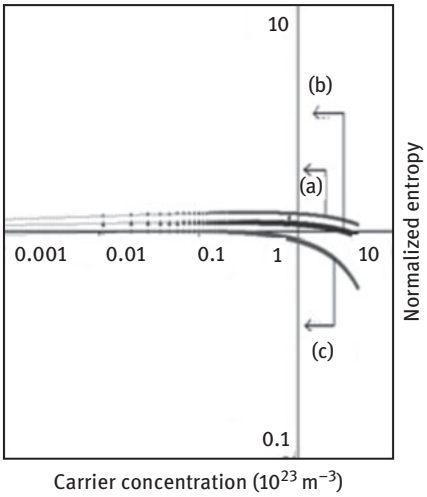

Figure 3.21: Plot of the normalized entropy in HD QBs of CdS with (a) $\bar{\lambda}_0 \neq 0$, (b) $\bar{\lambda}_0 = 0$ and (c) GaP as a function of carrier concentration for all the cases of Figure 3.20.

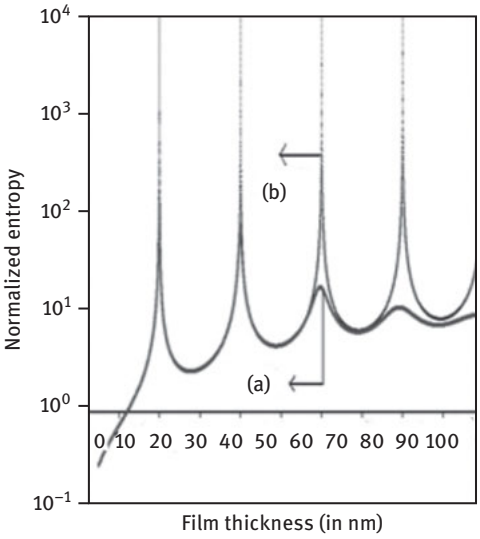

Figure 3.22: Plot of the normalized entropy in HD QBs of Germanium as a function of film thickness in accordance with the models of (a) Wang et al. and (b) Cardona et al. respectively.

energy levels of the carriers of the concerned dots. The entropy spectra are found bearing composite oscillations as function of the nano-thickness. These are generally due to selection rules in the quantum numbers along the three confined directions. The dependence of the normalized entropy on the carrier concentration is manifested

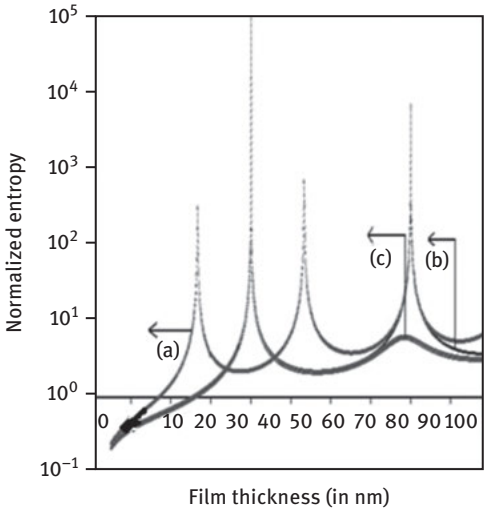

Figure 3.23: Plot of the normalized entropy in HD QBs of Tellurium and stressed Kane type material (n-InSb) as a function of film thickness in accordance with the models of (a) Bouat et al., (b) Ortenberg et al. and (c) Seiler et al. respectively.

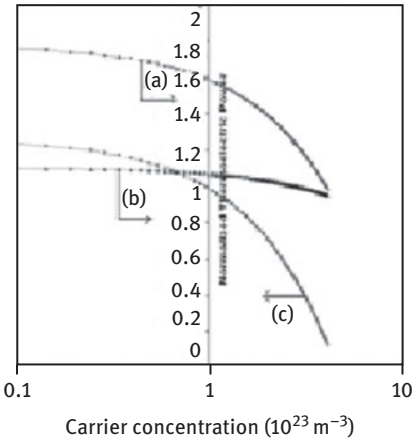

Figure 3.24: Plot of the normalized entropy in HD QBs of Tellurium and stressed Kane type material (n-InSb) as a function of carrier concentration for all the cases of Figure 3.23.

by the Figures 3.2, 3.4, 3.6, 3.8, 3.11, 3.13, 3.15, 3.17, 3.19, 3.21, 3.24, 3.25, 3.27, 3.29 and 3.31 for the different materials as considered here. It can be ascertained from the same figures that the entropy of all the corresponding materials decreases with increasing carrier concentration for relatively higher values of the carrier degeneracy. Although the entropy varies in various manners with all the variables in

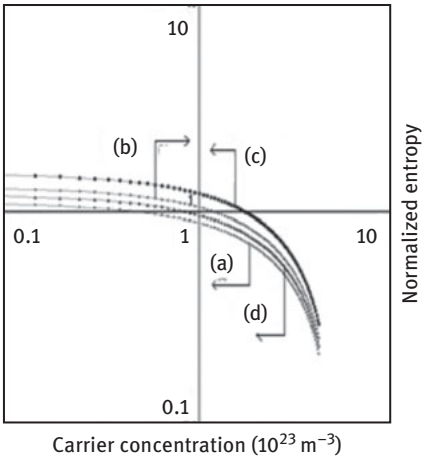

Figure 3.25: Plot of the normalized entropY in HD QBs of (a) Graphite, (b) Platinum antimonide, (c) zero gap (HgTe) and (d) $Pb_{1-x}Ge_xTe$ as a function of carrier concentration in accordance with the models of Ushio et al., Emtage, Ivanov-Omskii et al. and Vassilev respectively.

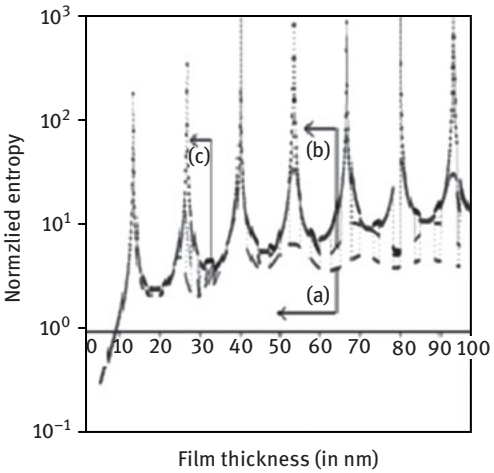

Figure 3.26: Plot of the normalized entropy in HD QBs of Gallium antimonide as a function of film thickness in accordance with the models of (a) Seiler et al., (b) Mathur et al. and (c) Zhang respectively.

all the limiting cases as evident from all the figures, the rate of variations in each case are totally band-structure dependent.

The quantum oscillations of the entropy in HD QBs exhibit different numerical magnitudes as compared to the same in UFs and QWs. It may be comprehended that the HD QBs lead to the discrete energy levels, somewhat like atomic energy levels,

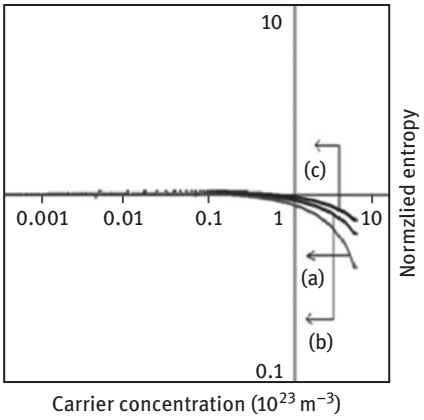

Figure 3.27: Plot of the normalized entropy in HD QBs of Gallium antimonide as a of normalized carrier concentration for all cases of Figure 3.26.

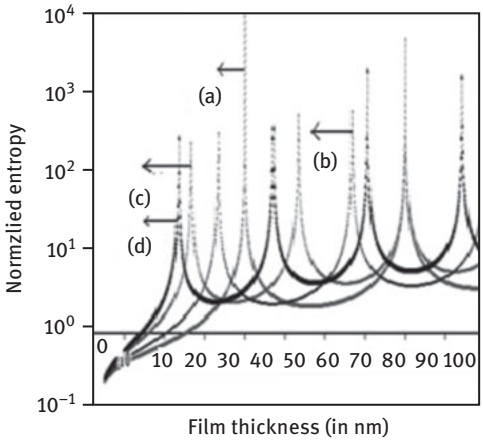

Figure 3.28: Plot of the normalized entropy in HD QBs of Bismuth as a function of film thickness in accordance with the models of (a) McClure et al, (b) Takaoka et al. (Hybrid model), (c) Cohen and (d) Lax et al. respectively.

which produce very large changes. This is in accordance to the inherent nature of the quantum confinement of the carrier gas as dealt with here. In HDQBs, there remain no free carrier states in between any two allowed sets of size-quantized levels unlike that found for UFs and QWs where the quantum confinements are 1D and 2D respectively. Consequently, the crossing of the Fermi level by the size-quantized levels in HD QBs would have much greater impact on the redistribution of the carriers among the allowed levels, as compared to that found for UFs and QWs respectively.

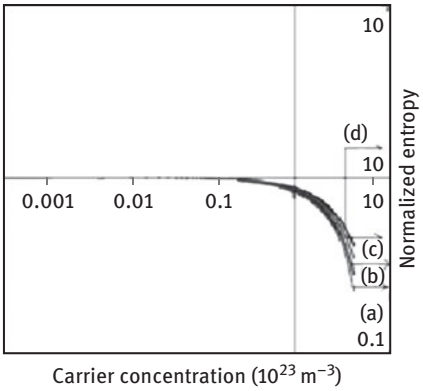

Figure 3.29: Plot of the normalized entropy in HD QBs of Bismuth as a function of carrier concentration for all the cases of Figure 3.28.

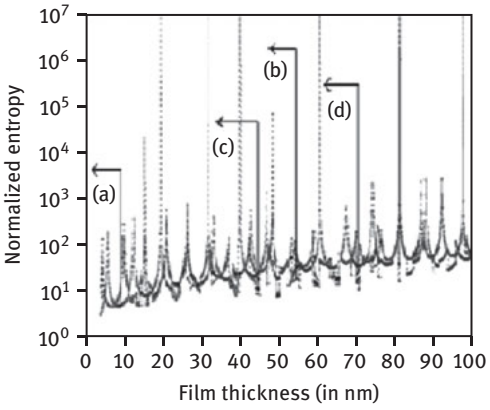

Figure 3.30: Plot of the normalized entropy in HD QBs of PbTe as a function of film thickness in accordance with the models of (a) Dimmock, (b) Bangert et al. and (c) Foley et al. The plot (d) refers to Bi_2Te_3 in accordance with the model of Stordeur et al.

The effect of spin splitting of the carriers in HD QBs of p-CdS on entropy can be numerically investigated from Figures 3.20 and 3.23. It appears that the absence of the spin splitting constant decreases the numerical value of the entropy in CdS for a particular range of film thickness. Itappears from Figure 3. 22 that the entropy in Germanium in accordance with the model of Wang et al. is comparatively low with that of the Cardona et al. model. The entropies in HDQBs of Te and stressed Kane type materials are depicted in Figures 3.23 and 3.24 with respect to film thickness and carrier concentration respectively. It appears that at extremely low and high film thicknesses, the entropy in HDQBs of Te dominates over that of the corresponding

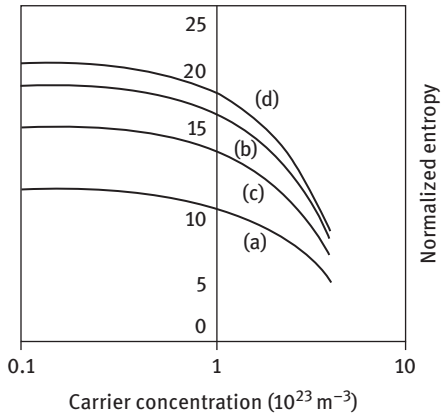

Figure 3.31: Plot of the normalized entropy in HD QBs of PbTe and Bi_2Te_3 as a function of carrier concentration for all the cases of Figure 3.30.

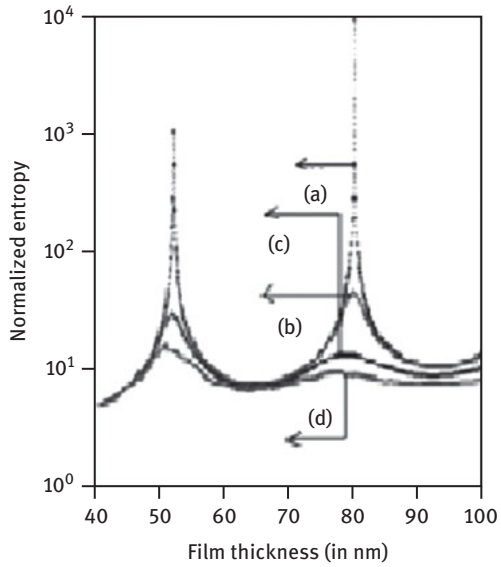

Figure 3.32: Plot of the normalized entropy in HD QBs of (a) II–V compound (CdSb), (b) zinc diphosphide, (c) cadmium diphosphide and (d) antimony as a function of film thickness in accordance with the models of Yamada, Chuiko and Ketterson respectively.

stressed InSb, although, at mid zone thickness, the entropy in stressed InSb exhibits a high peak together with the fact that the periods of oscillations of the entropy are comparatively higher in Te than that of stressed compounds.

In Figure 3.25, the entropy in HD QBs of Platinum antimonide and $Pb_{1-x}Ge_xTe$ materials have been plotted as a function of carrier concentration. From Figure 3.28,

it appears that the entropy in PbSe exhibits the high sharp peak in the mid thickness zone. From Figure 3.26, it is evident that the entropy in GaSb oscillates with film thickness exhibiting spikes. In Figures 3.30 and 3.31, the variation of the entropy in PbTe and Bi_2Te_3 against film thickness and carrier concentration has been demonstrated in accordance with the appropriate band models. In Figure 3.32, the variation of entropy in II–V compound, zinc and cadmium diphosphides as a function of film thickness has been shown in accordance with the appropriate band models. From Figure 3.30, it appears that the numerical values of entropy in HD QBs of PbTe and Bi_2Te_3 in accordance with all the band models are extremely higher than all other materials.

3.4 Open research problems

(R3.1) Investigate the entropy for QBs of the HDS in the presences of Gaussian, exponential, Kane, Halperian, Lax and Bonch-Burevich types of band tails for all systems whose unperturbed carrier energy spectra are defined in R1.1

(R3.2) Investigate the entropy for QBs of all the HD materials as considered in R4.1.under non uniform strain

(R3.3) Investigate the entropy in the presence of non uniform strain for QBs of HD negative refractive index, organic, magnetic and other advanced optical materials in the presence of an alternating electric field.

(R3.4) Investigate the entropy for the QBs of HD negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field.

(R3.5) Investigate the entropy for the multiple QBs of HD materials whose unperturbed carrier energy spectra are defined in R1.1.

(R3.6) Investigate the entropy for all the appropriate HD zero dimensional systems of this chapter in the presence of finite potential wells.

(R3.7) Investigate the entropy for all the appropriate HD zero dimensional systems of this chapter in the presence of parabolic potential wells.

(R3.8) Investigate the entropy for all the above appropriate problems in the presence of elliptical Hill and quantum square rings in the presence of strain.

(R3.9) Investigate the entropy for parabolic cylindrical HD zero dimensional systems in the presence of an arbitrarily oriented alternating electric field for all the HD materials whose unperturbed carrier energy spectra are defined in R1.1 in the presence of strain.

(R3.10) Investigate the entropy for HD zero dimensional systems of the negative refractive index and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field and non-uniform light waves and in the presence of strain.

(R3.11) Investigate the entropy for triangular HD zero dimensional systems of the negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field in the presence of strain.

(R3.12) Investigate the entropy for all the problems of (R4.1) in the presence of arbitrarily oriented magnetic field.

(R3.13) Investigate the entropy for all the problems of (R4.1)in the presence of alternating electric field.

(R3.14) Investigate the entropy for all the problems of (R4.1)in the presence of alternating magnetic field.

(R3.15) Investigate the entropy for all the problems of (R4.1)in the presence of crossed electric field and quantizing magnetic fields.

(R3.16) Investigate the entropy for all the problems of (R4.1)in the presence of crossed alternating electric field and alternating quantizing magnetic fields.

(R3.17) Investigate the entropy for HD QBs of the negative refractive index, organic and magnetic materials.

(R3.18) Investigate the entropy for HD QBs of the negative refractive index, organic and magnetic materials in the presence of alternating time dependent magnetic field.

(R3.19) Investigate the entropy for HD QBs of the negative refractive index, organic and magnetic materials in the presence of in the presence of crossed alternating electric field and alternating quantizing magnetic fields.

(R3.20) a) Investigate the entropy for HD QBs of the negative refractive index, organic, magnetic and other advanced optical materials in the presence of an arbitrarily oriented alternating electric field considering many body effects.
b) Investigate all the appropriate problems of this chapter for a Dirac electron.

(R3.21) Investigate all the appropriate problems of this chapter by including the many body, image force, broadening and hot carrier effects respectively.

(R3.22) Investigate all the appropriate problems of this chapter by removing all the mathematical approximations and establishing the respective appropriate uniqueness conditions.

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4 Entropy in heavily doped materials under magnetic quantization

If my only desire is to be desire-less then I will surely get the permanent visa to live in the wonderful world of SOLITUDE.

4.1 Introduction

It is well known that the band structure of materials can be dramatically changed by applying external fields. The effects of the quantizing magnetic field on the band structure of compound materials are more striking and can be observed easily in experiments [1–3]. Under magnetic quantization, the motion of the electron parallel to the magnetic field remains unaltered while the area of the wave vector space perpendicular to the direction of the magnetic field gets quantized in accordance with the Landau's rule of area quantization in the wave-vector space [3]. The energy levels of the carriers in a magnetic field (with the component of the wave-vector parallel to the direction of magnetic field be equated with zero) are termed as the Landau levels and the quantized energies are known as the Landau sub-bands. It is important to note that the same conclusion may be arrived either by solving the single-particle time independent Schrödinger differential equation in the presence of a quantizing magnetic field or by using the operator method. The quantizing magnetic field tends to remove the degeneracy and increases the band gap. A semiconductor, placed in a magnetic field B, can absorb radiative energy with the frequency $(\bar{\omega}_0 = (|\bar{e}|\bar{B}/\bar{m}_c))$. This phenomenon is known as cyclotron or diamagnetic resonance. The effect of energy quantization is experimentally noticeable when the separation between any two consecutive Landau levels is greater than $\bar{k}_B\bar{T}$. A number of interesting transport phenomena originate from the change in the basic band structure of the semiconductor in the presence of quantizing magnetic field. These have been widely been investigated and also served as diagnostic tools for characterizing the different materials having various band structures [4–7]. The discreteness in the Landau levels leads to a whole crop of magneto-oscillatory phenomena, important among which are (i) Shubnikov–de Haas oscillations in magneto-resistance; (ii) De Haas–van Alphen oscillations in magnetic susceptibility; (iii) magneto-phonon oscillations in thermoelectric power, etc.

In this chapter in Section 4.2.1, of the theoretical background, the entropy has been investigated in HD nonlinear optical materials in the presence of a quantizing magnetic field. Section 4.2.2 contains the results for HD III–V, ternary, and quaternary compounds in accordance with the three- and the two-band models of Kane. In the same section, the entropy in accordance with the models of Stillman

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et al. and Palik et al. has also been studied for the purpose of relative comparison. Section 4.2.3 contains the study of the entropy for HD II–VI materials under magnetic quantization. In Section 4.2.4, the entropy in HD IV–VI materials has been discussed in accordance with the models of Cohen, Lax, Dimmock, Bangert and Kastner, and Foley and Landenberg, respectively. In Section 4.2.5, the magneto-entropy for the stressed HDKane-type materials has been investigated. In Section 4.2.6, the entropy in HD Te has been studied under magnetic quantization. In Section 4.2.7, the magneto-entropy in n-GaP has been studied. In Section 4.2.8, the entropy in HD $PtSb_2$ has been explored under magnetic quantization. In section 4.2.9, the magneto-entropy in HD Bi_2Te_3 has been studied. In Section 4.2.10, the entropy in HD Ge has been studied under magnetic quantization in accordance with the models of Cardona et al. and Wang and Rossler, respectively. In Sections 4.2.11 and 4.2.12, the magneto-entropy in HD n-GaSb and II–V compounds has respectively been studied. In Sections 4.2.13 the magneto-entropy in HD $Pb_{1-x}Ge_xTe$ has been discussed. The Section 4.3 explores the result and discussions andSection 4.4 contains 11 open research problems.

4.2 Theoretical background

4.2.1 Entropy in HD nonlinear optical materials under magnetic quantization

The dispersion relation in non-linear optical materials can be written as

$$\gamma(\bar{E}) = \frac{\hbar^2 \bar{k}_s^2}{2\bar{m}_{\perp}^{*}} \bar{f}_3(\bar{E}) + \frac{\hbar^2 \bar{k}_z^2}{2\bar{m}_{||}^{*}} \bar{f}_4(\bar{E}) \pm \frac{\bar{e}\bar{B}\hbar\bar{E}_g}{6} \left[\frac{(\bar{E}_{g_0} + \Delta_{\perp})}{(\bar{E}_{g_0} + \frac{2}{3}\Delta_{\perp})}\right] \left[\bar{E} + \bar{E}_{g_0} + \delta + \frac{\Delta_{||}^2 - \Delta_{\perp}^2}{3\Delta_{||}}\right] \tag{4.1}$$

where,

$$\bar{f}_3(\bar{E}) = \frac{\bar{E}_g(\bar{E}_g + \Delta_{\perp})}{(\bar{E}_g + \frac{2}{3}\Delta_{\perp})} \left[(\bar{E} + \bar{E}_g)\left(\bar{E} + \bar{E}_g + \frac{2}{3}\Delta_{||}\right) + \delta\left(\bar{E} + \bar{E}_g + \frac{1}{3}\Delta_{||}\right) + \frac{1}{9}(\Delta_{||}^2 - \Delta_{\perp}^2)\right]$$

and

$$\bar{f}_4(E) = \frac{\bar{E}_g(\bar{E}_g + \Delta_{||})}{(\bar{E}_g + \frac{2}{3}\Delta_{||})} \left[(\bar{E} + \bar{E}_g)\left(\bar{E} + \bar{E}_g + \frac{2}{3}\Delta_{||}\right)\right]$$

The (4.1) can be expressed as

$$\frac{\hbar^2 \bar{k}_z^2}{2\bar{m}_{||}^{*}} + \left(\frac{\bar{b}_{||}\bar{c}_{\perp}}{\bar{b}_{\perp}\bar{c}_{||}}\right)\left(\frac{\hbar^2 \bar{k}_s^2}{2\bar{m}_{\perp}^{*}}\right) = \left\{\left[\frac{\bar{a}\bar{b}_{||}}{\bar{c}_{||}}\bar{E}^2 + \frac{(\bar{a}\bar{c}_{||} + \bar{b}_{||}c_{||} - a\bar{b}_{||})}{\bar{c}_{||}^{\,2}}\bar{E} + \frac{1}{\bar{c}_{||}}\left(1 - \frac{\bar{a}}{\bar{c}_{||}}\right)\left(1 - \frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\right.\right.$$

$$-\frac{1}{\bar{c}_{||}}\left(1-\frac{\bar{a}}{\bar{c}_{||}}\right)\left(1-\frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\frac{1}{(\bar{c}_{||}\bar{E}+1)}]+\frac{\bar{a}\bar{b}_{||}}{\bar{c}_{||}}\left[\delta E+\frac{2}{9}(\Delta_{||}^2-\Delta_{\perp}^2)\right]-\frac{2}{9}\frac{\bar{a}\bar{b}_{||}}{\bar{c}_{||}}\frac{(\Delta_{||}^2-\Delta_{\perp}^2)}{(\bar{c}_{||}E+1)}\Bigg\}$$
$$-\left(\frac{\hbar^2k_s^2}{2m_{\perp}^*}\right)\left\{\left(\frac{\bar{b}_{||}c_{\perp}}{b_{\perp}\bar{c}_{||}}\right)\left[\left(\frac{\delta}{2}+\frac{\Delta_{||}^2-\Delta_{\perp}^2}{6\Delta_{||}}\right)\frac{\bar{a}}{(\bar{a}\bar{E}+1)}+\left(\frac{\delta}{2}-\frac{\Delta_{||}^2-\Delta_{\perp}^2}{6\Delta_{||}}\right)\frac{\bar{c}_{||}}{(\bar{c}_{||}\bar{E}+1)}\right]\right\}$$
$$\pm\bar{e}_1\left[\frac{\rho_1}{\bar{E}+\bar{E}_g}+\frac{\rho_2}{\bar{E}+\bar{E}_g+\frac{2}{3}\Delta_{||}}\right] \tag{4.2}$$

where,

$$e_1=\left[\frac{\bar{e}\bar{B}\hbar(\bar{E}_{g_0}+\frac{2}{3}\Delta_{||})}{6(\bar{E}_{g_0}+\Delta_{||})}\frac{(\bar{E}_g+\Delta_{\perp})}{(\bar{E}_g+\frac{2}{3}\Delta_{\perp})}\right],\rho_1=\frac{(-\bar{E}_{g_0}+\bar{G}_1)}{(\frac{2}{3}\Delta_{||})},\bar{G}_1=\left[\bar{E}_{g_0}+\delta+\frac{\Delta_{||}^2-\Delta_{\perp}^2}{3\Delta_{||}}\right]$$

and

$$\rho_2=\frac{3}{2\Delta_{||}}\left[\frac{\Delta_{||}}{3}+\frac{\Delta_{\perp}^2}{3\Delta_{||}}-\delta\right]$$

Therefore, the dispersion relation of the conduction electrons in HD nonlinear optical materials in the presence of a quantizing magnetic field B can be written following the methods as developed in Chapter 1 as

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_{||}^*}=\bar{U}_{1,\pm}(\bar{E},\bar{n},\eta_g)+i\bar{U}_{2,\pm}(\bar{E},\bar{n},\eta_g) \tag{4.3a}$$

where

$$\bar{U}_{1,\pm}(\bar{E},\bar{n},\eta_g)=\left[\frac{-\bar{e}\bar{B}}{\bar{m}_{\perp}^*}\left(\bar{n}+\frac{1}{2}\right)\left(\frac{\bar{b}_{||}\bar{c}_{\perp}}{\bar{c}_{||}b_{\perp}}\right)+\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}\left[\left\{\left[\frac{a\bar{b}_{||}}{\bar{c}_{||}}\theta_0(\bar{E},\eta_g)\right.\right.\right.$$
$$+\frac{\bar{a}\ \bar{c}_{||}+\bar{b}_{||}\bar{c}_{||}-\bar{a}\bar{b}_{||}}{\bar{c}^2{}_{||}}\gamma_0(\bar{E},\eta_g)+\frac{1}{\bar{c}_{||}}\left(1-\frac{\bar{a}}{\bar{c}_{||}}\right)\left(1-\frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]$$
$$-\frac{1}{\bar{c}_{||}}(1-\bar{c}_{||})\left(1-\frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\bar{c}(\beta_1,\bar{E},\eta_g)+\frac{\bar{a}\bar{b}_{||}}{\bar{c}_{||}}\left[\delta\gamma_0(\bar{E},\eta_g)\right.$$
$$\left.\left.+\frac{2}{9}\left(\Delta_{||}^2-\Delta_{\perp}^2\right)\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]\right]-\frac{2}{9}\frac{\bar{a}\bar{b}_{||}}{\bar{c}_{||}}\left(\Delta_{||}^2-\Delta_{\perp}^2\right)\bar{c}\left(\beta_1,\bar{E},\eta_g\right)\right\}$$
$$-\frac{\hbar e\bar{B}}{\bar{m}_{\perp}^*}\left(\bar{n}+\frac{1}{2}\right)\left\{\left(\frac{\bar{b}_{||}\bar{c}_{\perp}}{\bar{c}_{||}\bar{b}_{\perp}}\right)\left[\left(\frac{\delta}{2}+\frac{\Delta_{||}^2-\Delta_{\perp}^2}{6\Delta_{||}}\right)\bar{a}\ \bar{c}(\beta_2,\bar{E},\eta_g)\right.\right.$$
$$\left.\left.+\left(\frac{\delta}{2}-\frac{\Delta_{||}^2-\Delta_{\perp}^2}{6\Delta_{||}}\right)\bar{c}_{||}\bar{c}\left(\beta_1,\bar{E},\eta_g\right)\right]\right\}\pm\frac{\rho_1\bar{e}_1}{\bar{E}_{g_0}}\bar{c}\left(\beta_2,\bar{E},\eta_g\right)\pm\frac{\rho_2\bar{e}_1}{(\bar{E}_{g_0}+\frac{2}{3}\Delta_{||})}\bar{c}\left(\beta_3,\bar{E},\eta_g\right)\Bigg],$$

$$\bar{U}_{2,\pm}(\bar{E},\bar{n},\eta_g)=\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}\left[\frac{1}{\bar{c}_{||}}\left(1-\frac{\bar{a}}{\bar{c}_{||}}\right)\left(1-\frac{\bar{b}_{||}}{\bar{c}_{||}}\right)\bar{D}(\beta_1,\bar{E},\eta_g)\right.$$

$$+\frac{2\bar{a}\bar{b}_{||}}{9\,\bar{c}_{||}}(\Delta_{||}^2-\Delta_{\perp}^2)\bar{D}(\beta_1,\bar{E},\eta_g)+\frac{\bar{}heB}{\bar{m}_{\perp}^*}\left(\bar{n}+\frac{1}{2}\right)\left\{\left(\frac{\bar{b}_{||}\bar{c}_{\perp}}{\bar{c}_{||}\bar{b}_{\perp}}\right)\left[\left(\frac{\delta}{2}+\frac{\Delta_{||}^2-\Delta_{\perp}^2}{6\Delta_{||}}\right)\bar{a}\bar{D}(\beta_2,\bar{E},\eta_g)\right.\right.$$

$$\left.\left.+\left(\frac{\delta}{2}-\frac{\Delta_{||}^2-\Delta_{\perp}^2}{6\Delta_{||}}\right)\bar{c}_{||}\bar{D}(\beta_1,\bar{E},\eta_g)\right]\right\}\mp\left[\frac{\rho_1 e_1}{\bar{E}_{g_0}}\bar{D}(\beta_2,\bar{E},\eta_g)\pm\frac{\rho_2 e_1}{(\bar{E}_{g_0}+\frac{2}{3}\Delta_{||}s)}\bar{D}(\beta_3,\bar{E},\eta_g)\right]\Bigg]$$

$$\beta_1=\bar{c}_{||},\beta_2=\frac{1_1}{\bar{E}_{g0}}=\bar{a},\beta_3=\frac{1}{(\bar{E}_{g0}+\frac{2}{3}\Delta_{||})},$$

$$\bar{C}(\beta_i,\bar{E},\eta_g)=\left[\frac{2}{\beta_i\eta_g\sqrt{\pi}}\right]\exp(-\bar{u}_i^2)\times\left[\sum_{p=1}^{\infty}\left\{\frac{\exp(\frac{-\bar{p}^2}{4})}{\bar{p}}\right\}\sinh(\bar{p}\bar{u}_i)\right],\bar{u}_i=\frac{1+\beta_i\bar{E}}{\beta_i\eta_g}$$

and

$$\bar{D}(\beta_i,\bar{E},\eta_g)=\left[\frac{\sqrt{\pi}}{\beta_i\eta_g}\exp(-\bar{u}_i^2)\right]$$

EEM at the Fermi level can be written from (4.3a) as

$$\bar{m}^*{}_{\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)=\bar{m}_{||}^*\overline{U'}_{1,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.3b}$$

where $\bar{E}_{FBHD}$ is the Fermi energy in this case.

Therefore, the double valued EEM in this case is a function of Fermi energy, magnetic field, quantum number and the scattering potential together with the fact that EEM exists in the band gap which is the general characteristics of HD materials.

The complex density-of-states function under magnetic quantization is given by

$$\bar{N}_B(\bar{E})=\bar{N}_{BR}(\bar{E})+i\bar{N}_{BI}(\bar{E})=\frac{e\bar{B}}{2\pi^2\hbar^2}\sqrt{2\bar{m}_{||}^*}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\frac{\overline{x'}}{2\sqrt{\bar{x}}}+\frac{i\,\overline{y'}}{2\sqrt{\bar{y}}}\right] \tag{4.4a}$$

where

$$\bar{x}=\frac{\sqrt{(\bar{U}_{1,\pm}(\bar{E},\bar{n},\eta_g))^2+(\bar{U}_{2,\pm}(\bar{E},\bar{n},\eta_g))^2}+(\bar{U}_{1,\pm}(\bar{E},\bar{n},\eta_g))}{2}$$

$$\bar{y}=\frac{\sqrt{(\bar{U}_{1,\pm}(\bar{E},\bar{n},\eta_g))^2+(\bar{U}_{2,\pm}(\bar{E},\bar{n},\eta_g))^2}-(\bar{U}_{1,\pm}(\bar{E},\bar{n},\eta_g))}{2}$$

and $\overline{x'}$and $\overline{y'}$ are the differentiations of $\bar{x}$ and $\bar{y}$ with respect to energy $\bar{E}$.

Therefore, from (4.4a), we can write

$$\bar{N}_{B\,\mathrm{Real}}(\bar{E}) = \frac{e\bar{B}}{4\pi^2\hbar^2}\sqrt{2\bar{m}_{||}^{*}}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{\overline{x'}}{\sqrt{\bar{x}}} \tag{4.4b}$$

and

$$\bar{N}_{B\,\mathrm{Imaginary}}(\bar{E}) = \frac{e\bar{B}}{4\pi^2\hbar^2}\sqrt{2\bar{m}_{||}^{*}}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{\overline{y'}}{\sqrt{\bar{y}}} \tag{4.4c}$$

The electron concentration is given by

$$\bar{n}_0 = \frac{g_v e B}{2\pi^2\hbar^2}\frac{\sqrt{2\bar{m}_{||}^{*}}}{\sqrt{2}}\sum_{\bar{n}=0}^{\bar{n}_{\max}} \left[\left[\sqrt{\bar{U}_{1,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)^2 + \left(\bar{U}_{2,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)\right)^2} + \left(\bar{U}_{1,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)\right)\right]^{1/2} \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\left[\sqrt{\left(\bar{U}_{1,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)\right)^2 + \left(\bar{U}_{2,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)\right)} + \left(\bar{U}_{1,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)\right)\right]^{1/2}\right] \tag{4.5}$$

Using (1.31f) and (4.5), we can study the entropy in this case.

4.2.2 Entropy in QWs of HD III–V materials under magnetic quantization

(a) The electron energy spectrum in III–V materials under magnetic quantization is given by

$$\frac{\bar{E}(\bar{E}+\bar{E}_{g0})(\bar{E}+\bar{E}_{g0}+\Delta)(\bar{E}_{g0}+\frac{2}{3}\Delta)}{\bar{E}_{g0}(\bar{E}_{g0}+\Delta)(\bar{E}+\bar{E}_{g0}+\frac{2}{3}\Delta)} = \left(\bar{n}+\frac{1}{2}\right)\hbar\bar{\omega}_0 + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c} \pm \frac{e\bar{B}\hbar\Delta}{6\bar{m}_c(\bar{E}+\bar{E}_{g0}+\frac{2}{3}\Delta)} \tag{4.6}$$

The (4.6) can be written as

$$\left[\frac{\bar{a}\bar{b}}{\bar{c}}\bar{E}^2 + \left(\frac{\bar{a}\ \bar{c}+\bar{b}\bar{c}-\bar{a}\bar{b}}{\bar{c}^2}\right)\bar{E} + \frac{1}{\bar{c}}\left(1-\frac{\bar{a}}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right) - \frac{1}{\bar{c}}\left(1-\frac{\bar{a}}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)\frac{1}{(1+\bar{c}\bar{E})}\right]$$
$$= \left(\bar{n}+\frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c} + \frac{e\bar{B}\hbar\Delta}{6\bar{m}_c(1+\bar{c}\bar{E})(\bar{E}_{g0}+\frac{2}{3}\Delta)}$$

where, $\bar{a} = \frac{1}{\bar{E}_{g0}}$, $\bar{b} = \frac{1}{\bar{E}_{g0}+\Delta}$ and $\bar{c} = \frac{1}{\bar{E}_{g0}+\frac{2}{3}\Delta}$

Therefore

$$\frac{\bar{a}\bar{b}}{\bar{c}}\bar{I}(5)+\left(\frac{\bar{a}\bar{b}+\bar{b}\bar{c}-\bar{a}\bar{b}}{\bar{c}^2}\right)\bar{I}(4)+\left[\frac{1}{\bar{c}}\left(1-\frac{\bar{a}}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)-\left(\bar{n}+\frac{1}{2}\right)\hbar\bar{\omega}_0\right]$$

$$\bar{I}(1)-\bar{g}_{\pm}\left[\bar{G}(\bar{C},\bar{E},\eta_g)-i\bar{H}(\bar{C},\bar{E},\eta_g)\right]=\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c}\bar{I}(1) \tag{4.7}$$

where,

$$\bar{g}_{\pm}=\left[\frac{1}{\bar{c}}\left(1-\frac{\bar{a}}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)\pm\frac{e\bar{B}\hbar\Delta}{6\bar{m}_c(\bar{E}_{g_0}+\frac{2}{3}\Delta)}\right],$$

$$\bar{G}(\bar{C},\bar{E},\eta_g)=\left[\frac{2}{\bar{C}\eta_g\sqrt{\pi}}\right]\exp(-\bar{u}^2)\times\left[\sum_{p=1}^{\infty}\left\{\frac{\exp(\frac{-\bar{p}^2}{4})}{\bar{p}}\right\}\sinh(\bar{p}\ \bar{u})\right],\bar{u}=\frac{1+\bar{c}\bar{E}}{\bar{C}\eta_g},$$

$$\bar{H}(\bar{C},\bar{E},\eta_g)=\left[\frac{\sqrt{\pi}}{\bar{C}\eta_g}\exp(-\bar{u}^2)\right]$$

Therefore

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c}=\left[\frac{\bar{a}\bar{b}}{\bar{c}}\right]\theta_0(\bar{E},\eta_g)\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}+\left(\frac{\bar{a}\bar{c}+\bar{b}\bar{c}-\bar{a}\bar{b}}{\bar{c}^2}\right)\gamma_0(\bar{E},\eta_g)\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}$$
$$+\left[\frac{1}{\bar{c}}\left(1-\frac{\bar{a}}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)-\left(\bar{n}+\frac{1}{2}\right)\hbar\bar{\omega}_0\right]-\bar{g}_{\pm}\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}\left[\bar{G}(\bar{C},\bar{E},\eta_g)-i\bar{H}(\bar{C},\bar{E},\eta_g)\right] \tag{4.8}$$

Therefore, the dispersion relation is given by

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c}=\bar{U}_{3,\pm}(\bar{E},\bar{n},\eta_g)+i\bar{U}_{4,\pm}(\bar{E},\eta_g) \tag{4.9a}$$

where

$$\bar{U}_{3,\pm}(\bar{E},\bar{n},\eta_g)=\left[\frac{\bar{a}\bar{b}}{\bar{c}}\theta_0(\bar{E},\eta_g)\times\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}+\left(\frac{\bar{a}\bar{c}+\bar{b}\bar{c}-\bar{a}\bar{b}}{\bar{c}^2}\right)\gamma_0(\bar{E},\eta_g)\times\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}\right.$$
$$\left.+\frac{1}{\bar{c}}\left(1-\frac{\bar{a}}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)-\left(\bar{n}+\frac{1}{2}\right)\hbar\omega_0+\bar{g}_{\pm}\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}\bar{G}(\bar{C},\bar{E},\eta_g)\right]$$

and

$$\bar{U}_{4,\pm}(\bar{E},\eta_g)=\bar{g}_{\pm}\left[\frac{1+Erf(\bar{E}/\eta_g)}{2}\right]^{-1}\bar{H}(\bar{C},\bar{E},\eta_g)$$

The complex Landau energy $\bar{E}_{nHD1}$ in this case can be obtained by substituding $\bar{k}_z = 0$ and $\bar{E} = \bar{E}_{nHD}$ in (4.9a)

EEM at the Fermi level can be written from (4.9a) as

$$\bar{m}^*_{\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \bar{m}^*_{||}\overline{U'}_{3,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.9b}$$

Thus, EEM is a function of Fermi energy, Landau quantum number and scattering potential together with the fact it is double valued due to spin.

The complex density of states function under magnetic quantization is given by

$$\bar{N}_B(\bar{E}) = \bar{N}_{B\,Real}(\bar{E}) + i\bar{N}_{B\,Imaginary}(\bar{E}) = \frac{e\bar{B}}{2\pi^2\hbar^2}\sqrt{2\bar{m}_c^*}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\frac{\overline{x'}}{2\sqrt{\bar{x}}} + \frac{i\,\overline{y'}}{2\sqrt{\bar{y}}}\right] \tag{4.10a}$$

where

$$\bar{x} = \frac{\sqrt{(\bar{U}_{3,\pm}(\bar{E}, \bar{n}, \eta_g))^2 + (\bar{U}_{4,\pm}(\bar{E}, \bar{n}, \eta_g))^2} + (\bar{U}_{3,\pm}(\bar{E}, \bar{n}, \eta_g))}{2}$$

$$\bar{y} = \frac{\sqrt{(\bar{U}_{3,\pm}(\bar{E}, \bar{n}, \eta_g))^2 + (\bar{U}_{4,\pm}(\bar{E}, \bar{n}, \eta_g))^2} - (\bar{U}_{3,\pm}(\bar{E}, \bar{n}, \eta_g))}{2}$$

and $\overline{x'}_1$ and $\overline{y'}_1$ are the differentiations of $\bar{x}$ and $\bar{y}$ with respect to energy $\bar{E}$.

From (4.10a), we can write

$$\bar{N}_{B\,Real}(\bar{E}) = \frac{e\bar{B}}{4\pi^2\hbar^2}\sqrt{2\bar{m}_c^*}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{\overline{x'}_1}{\sqrt{\bar{x}_1}} \tag{4.10b}$$

and

$$\bar{N}_{B\,Imaginary}(\bar{E}) = \frac{e\bar{B}}{4\pi^2\hbar^2}\sqrt{2\bar{m}_c^*}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{\overline{y'}_1}{\sqrt{\bar{y}_1}} \tag{4.10c}$$

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi^2\hbar^2}\sqrt{\bar{m}_c^*}\sum_{\bar{n}=0}^{\bar{n}_{\max}} \left[\left[\sqrt{\bar{U}_{3,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g)^2 + (\bar{U}_{4,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^2} + (\bar{U}_{3,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g))\right]^{1/2} \sum_{\bar{r}=1}^{\bar{r}=\bar{s}} \bar{L}(\bar{r})[\sqrt{(\bar{U}_{3,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^2 + (\bar{U}_{4,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g))} + (\bar{U}_{3,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g))]^{1/2}\right] \tag{4.11}$$

Using (1.31f) and (4.11) we can study the entropy in this case.

(b) Two band model of Kane

The magneto-dispersion law in this case is given by

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c} = \gamma_3\left(\bar{E},\eta_g\right) - \left(\bar{n}+\frac{1}{2}\right)\hbar\bar{\omega}_0 \mp \frac{1}{2}\bar{g}^*\mu_0\bar{B} \tag{4.12a}$$

where $\bar{g}^*$is the magnitude of the effective $\bar{g}$ factor at the edge of the conduction band and $\mu_0$is the Bohr magnetron.

EEM at the Fermi level can be written from (4.12a) as

$$\bar{m}^*(\bar{E}_{FBHD},\eta_g) = \bar{m}_c\gamma'_2(\bar{E}_{FBHD},\eta_g) \tag{4.12b}$$

Thus EEM is independent of quantum number.

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\sqrt{\bar{m}_c^*}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{5,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})[(\bar{U}_{5,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right] \tag{4.13}$$

where

$$\bar{U}_{5,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) = \gamma_2(\bar{E}_{FBHD},\eta_g) - \left(\bar{n}+\frac{1}{2}\right)\hbar\omega_0 \mp \frac{1}{2}\bar{g}^*\mu_0\bar{B}$$

Using (1.31f) and (4.13a), we can study the entropy in this case.

(c) Parabolic Energy Bands

The magneto-dispersion law in this case is given by

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c} = \gamma_3(\bar{E},\eta_g) - \left(\bar{n}+\frac{1}{2}\right)\hbar\omega_0 \mp \frac{1}{2}\bar{g}^*\mu_0\bar{B} \tag{4.14a}$$

EEM at the Fermi level can be written from (4.14a) as

$$\bar{m}^*(\bar{E}_{FBHD},\eta_g) = \bar{m}_c^*\gamma'_3(\bar{E}_{FBHD},\eta_g) \tag{4.14b}$$

Thus, EEM in heavily doped (HD) parabolic energy bands is a function of Fermi energy and scattering potential, whereas in the absence of bandtails the same mass is a constant quantity invariant of any variables.

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\sqrt{\bar{m}_c^*}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{6,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})[(\bar{U}_{6,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right] \tag{4.15}$$

where

$$\bar{U}_{6,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g)=\gamma_3(\bar{E}_{FBHD},\eta_g)-\left(n+\frac{1}{2}\right)\hbar\omega_0\mp\frac{1}{2}\bar{g}^{*}\mu_0\bar{B}$$

Using (1.31f) and (4.15), we can find the entropy in this case.

(d) The model of Stillman et al.

The (1.107) under the condition of band tailing assumes the form

$$\bar{k}^2=\left[\frac{[\bar{t}_{11}-\sqrt{(\bar{t}_{11})^2-4\bar{t}_{12}\gamma_3(\bar{E},\eta_g)}]}{2\bar{t}_{12}}\right] \tag{4.16}$$

Therefore, the magneto-dispersion law is given by

$$\bar{k}_z^2=\bar{U}_7(\bar{E},\bar{n},\eta_g) \tag{4.17a}$$

where

$$\bar{U}_7(\bar{E},\bar{n},\eta_g)=\left[\frac{[\bar{t}_{11}-\sqrt{(\bar{t}_{11})^2-4\bar{t}_{12}\gamma_3(\bar{E},\eta_g)}]}{2\bar{t}_{12}}-\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]$$

The EEM at the Fermi Level can be written from (4.17a) as

$$\bar{m}^{*}(\bar{E}_{FBHD},\eta_g)=\frac{\hbar^2}{2}\overline{U'}_7(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.17b}$$

The electron concentration is given by

$$\bar{n}_0=\frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\sqrt{\bar{m}_c^{*}}\sum_{\bar{n}=0}^{\bar{n}\max}\left[(\bar{U}_7(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}+\sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})[(\bar{U}_7(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right] \tag{4.18}$$

Using (1.31f) and (4.18), we can study the entropy in this case.

(e) The model of Palik et al

To the fourth order in effective mass theory and taking into account the interactions of the conduction, light hole, heavy-hole and split-off hole bands, the electron energy spectrum in III–V materials in the presence of a quantizing magnetic field $\vec{B}$ can be written as

$$\bar{E} = \bar{J}_{31} + \left(\bar{n} + \frac{1}{2}\right)\hbar\omega_0 + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c^*} \pm \frac{1}{4}\left(\frac{\bar{m}_c^*}{m_0}\right)\hbar\omega_0\bar{g}_0^* \pm \bar{k}_{30}\bar{\alpha}\left(\bar{n} + \frac{1}{2}\right)(\hbar\bar{\omega}_0)^2 \pm \bar{k}_{31}\bar{\alpha}\hbar\omega_0\left(\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c^*}\right) + \bar{k}_{32}\bar{\alpha}\left[\hbar\omega_0(\bar{n} + \frac{1}{2}) + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c^*}\right]^2 \tag{4.19}$$

where,

$$\bar{J}_{31} = -\frac{1}{2}\alpha\hbar\omega_0\left[(1-\bar{y}_{11})/(2+\bar{x}_{11})^2\right], \bar{J}_{32},$$

$$\bar{J}_{32} = \left\{\left[\frac{1}{3}(1-\bar{x}_{11})^2 - (2+\bar{x}_{11}^2\right)](2+\bar{x}_{11}).\bar{y}_{11} + \frac{1}{2}(1-\bar{x}_{11}^2)(1+\bar{x}_{11})(1+\bar{y}_{11})\right\},$$

$$\bar{g}_0^* = 2\left\{1 - \left[\frac{(1-\bar{x}_{11})}{(2+\bar{x}_{11})}\right]\left[\frac{(1-\bar{y}_{11})}{\bar{y}_{11}}\right]\right\},$$

$$\bar{k}_{30} = (1-\bar{y}_{11})(1-\bar{x}_{11})\left\{\left[(2+\frac{3}{2}\bar{x}_{11}+\bar{x}_{11}^2).\frac{(1-\bar{y}_{11})}{(2+\bar{x}_{11})^2}\right] - \frac{2}{3}\bar{y}_{11}\right\}$$

$$\bar{k}_{31} = (1-\bar{y}_{11})\left[\frac{(1-\bar{x}_{11})}{(2+\bar{x}_{11})}\right].\left\{\left[(2+\frac{3}{2}\bar{x}_{11}+\bar{x}_{11}^2).\frac{(1-\bar{y}_{11})}{(2+\bar{x}_{11})^2}\right] - \frac{2}{3}(1-\bar{x}_{11})\bar{y}_{11}\right\},$$

$$\bar{k}_{32} = -\left[\left(1+\frac{1}{2}\bar{x}_{11}^2\right)\Big/\left(1+\frac{1}{2}\bar{x}_{11}\right)\right](1-\bar{y}_{11})^2\bar{x}_{11} = \left[1+\left(\frac{\Delta}{\bar{E}_{g0}}\right)\right]^{-1} \text{ and } \bar{y}_{11} = \frac{\bar{m}_c^*}{m_0}$$

Under the condition of heavy doping, the (A.20) assumes the form

$$\bar{J}_{34}\bar{k}_z^4 + \bar{J}_{35,\pm}(\bar{n})k_z^2 + \bar{J}_{36,\pm}(\bar{n}) - \gamma_3(\bar{E},\eta_g) = 0 \tag{4.20}$$

where

$$\bar{J}_{34} = \bar{\alpha}\bar{k}_{32}\left(\frac{\hbar^2}{2\bar{m}_c^*}\right)^2, \bar{J}_{35,\pm}(\bar{n}) = \left[\frac{\hbar^2}{2\bar{m}_c^*} \pm \alpha\bar{k}_{31}\hbar\omega_0.\frac{\hbar^2}{2\bar{m}_c^*} + \alpha\bar{k}_{32}\hbar\omega_0.\frac{\hbar^2}{2\bar{m}_c^*}(\bar{n}+\frac{1}{2})\right],$$

$$\bar{J}_{36,\pm}(\bar{n}) = \left[\bar{J}_{31} \pm \frac{1}{4}\left(\frac{\bar{m}_c^*}{m_0}\right)\hbar\omega_0\bar{g}_0^* \pm \bar{k}_{30}\alpha(\hbar\omega_0)^2\left(\bar{n}+\frac{1}{2}\right) + \bar{k}_{32}\alpha\left[(\hbar\omega_0)(\bar{n}+\frac{1}{2})\right]^2\right]$$

The (4.20) can be written as

$$\bar{k}_z^2 = \bar{A}_{35,\pm}(\bar{E},\bar{n},\eta_g) \tag{4.21a}$$

where,

$$\bar{A}_{35,\pm}(\bar{E},\bar{n},\eta_g) = (2\bar{J}_{34})^{-1}\left[-\bar{J}_{35,\pm}(\bar{n}) + \sqrt{(\bar{J}_{35,\pm}(\bar{n}))^2 - 4\bar{J}_{34}\left[\bar{J}_{36,\pm}(\bar{n}) - \gamma_3(\bar{E},\eta_g)\right]}\right]$$

EEM at the Fermi level can be written from (A.22a) as

$$\bar{m}^*{}_{\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) = \frac{\hbar^2}{2}\bar{A}'_{35,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.21b}$$

Thus, EEM is a function of Fermi energy, Landau quantum number and the scattering potential.

The electron concentration is given by

$$\bar{n}_0 = \frac{e\bar{B}\bar{g}_v}{2\pi^2\hbar^2}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\bar{Y}_{34HD}(\bar{E}_{FBHD},\bar{n},\eta_g) + \bar{Z}_{34HD}(\bar{E}_{FBHD},\bar{n},\eta_g)\right] \tag{4.22}$$

where

$$\bar{Y}_{34HD}(\bar{E}_{FBHD},\bar{n},\eta_g) = \left[\sqrt{\bar{A}_{35HD,+}(\bar{E}_{FBHD},\bar{n},\eta_g)} + \sqrt{\bar{A}_{35HD,+}(\bar{E}_{FBHD},\bar{n},\eta_g)}\right]$$

and

$$\bar{Z}_{34HD}(\bar{E}_{FBHD},\bar{n},\eta_g) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}_B(\bar{r})[\bar{Y}_{34HD}(\bar{E}_{FBHD},\bar{n},\eta_g)]$$

Using (1.31f) and (4.22), we can study the entropy in this case.

4.2.3 Entropy in HD II–VI materials under magnetic quantization

The magneto dispersion relation of the carriers in heavily doped II–VI materials are given by

$$\gamma_3(\bar{E},\eta_g) = \bar{a}'_0\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) + \bar{b}'_0\bar{k}_z^2 \pm \lambda'_0\left[\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2} \tag{4.23}$$

The (4.23) can be written as

$$\bar{k}_z^2 = \bar{U}_{8\pm}(\bar{E},\bar{n},\eta_g) \tag{4.24a}$$

where

$$\bar{U}_{8\pm}(\bar{E},\bar{n},\eta_g) = (\overline{b'}_0)^{-1}\left[\gamma_3(\bar{E},\eta_g) - \frac{2e\bar{B}\,\bar{a}'_0}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \mp \bar{\lambda}_0\left[\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2}\right]$$

EEM at the Fermi level can be written from (4.24a) as

$$\bar{m}_c^*(\bar{E}_{FBHD}, \eta_g) = \frac{\hbar^2}{2}\bar{U}'_{8\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.24b}$$

The electron concentration is given by

$$\bar{n}_0 = \frac{e\bar{B}\bar{g}_v}{\pi^2\hbar^2}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\bar{Y}_{35HD}(\bar{E}_{FBHD}, \bar{n}, \eta_g) + \bar{Z}_{35HD}(\bar{E}_{FBHD}, \bar{n}, \eta_g)\right] \tag{4.25}$$

where

$$\bar{Y}_{35HD}(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \left[\sqrt{\bar{U}_{8+}(\bar{E}_{FBHD}, \bar{n}, \eta_g)} + \sqrt{\bar{U}_{8-}(\bar{E}_{FBHD}, \bar{n}, \eta_g)}\right]$$

and

$$\bar{Z}_{34HD}(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}_B(\bar{r})[\bar{Y}_{35HD}(\bar{E}_{FBHD}, \bar{n}, \eta_g)]$$

Using (1.31f) and (4.25), we can study the entropy in this case.

4.2.4 Entropy in HD IV–VI materials under magnetic quantization

The electron energy spectrum in IV–VI materials are defined by the models of Cohen, Lax, Dimmock and Bangert and Kastner, respectively. The magneto entropy in HD IV–VI materials is discussed in accordance with the said model for the purpose of relative comparison.

(a) Cohen Model

In accordance with the Cohen model, the dispersion law of the carriers in IV–VI materials is given by

$$\bar{E}(1+\alpha\bar{E}) = \frac{\bar{p}_x^2}{2\bar{m}_1} + \frac{\bar{p}_z^2}{2\bar{m}_3} - \frac{\alpha\bar{E}\bar{p}_y^2}{2\bar{m}'_2} + \frac{\bar{p}_y^2(1+\alpha\bar{E})}{2\bar{m}_2} + \frac{\alpha\bar{p}_y^4}{4\bar{m}_2\bar{m}'_2} \tag{4.26}$$

where, $\bar{p}_i = \hbar\bar{k}_i,\ i = \bar{x},\ \bar{y},\ \bar{z},\ \bar{m}_1,\ \bar{m}_2\ and\ \bar{m}_3$ are the effective carrier masses at the band-edge along $\bar{x}$, $\bar{y}$ and $\bar{z}$ directions respectively and $\bar{m}'_2$ is the effective-mass tensor component at the top of the valence band (for electrons) or at the bottom of the conduction band (for holes).

The magneto electron energy spectrum in IV–VI materials in the presence of quantizing magnetic field $\bar{B}$ along $\bar{z}$-direction can be written as

$$\bar{E}(1+\alpha\bar{E}) = \left(\bar{n}+\frac{1}{2}\right)\hbar\omega(\bar{E}) \pm \frac{1}{2}\bar{g}^*\mu_0\bar{B} + \frac{3}{8}\alpha\left(\bar{n}^2+\bar{n}+\frac{1}{2}\right)\hbar^2\omega^2(\bar{E}) + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_3} \tag{4.27a}$$

where,

$$\omega(\bar{E}) \equiv \frac{|e|\bar{B}}{\sqrt{\bar{m}_1\bar{m}_2}}\left[1+\alpha\bar{E}\left(1-\frac{\bar{m}_2}{\bar{m}'_2}\right)\right]^{1/2}$$

Therefore, the magneto dispersion law in HD IV–VI materials can be expressed as

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_3} = \bar{U}_{16,\pm}(\bar{E},\bar{n},\eta_g) \tag{4.27b}$$

where,

$$\bar{U}_{16,\pm}(\bar{E},\bar{n},\eta_g) = \left[\gamma_2(\bar{E},\eta_g) - \left(\bar{n}+\frac{1}{2}\right)\frac{\hbar e\bar{B}}{\sqrt{\bar{m}_1\bar{m}_2}} \mp \frac{1}{2}\bar{g}^*\mu_0\bar{B} - \frac{3\alpha}{8}\left(\bar{n}^2+\bar{n}+\frac{1}{2}\right)\left(\frac{\hbar e\bar{B}}{\sqrt{\bar{m}_1\bar{m}_2}}\right)^2 - \gamma_3(\bar{E},\eta_g)\left[\frac{\alpha}{2}\left(\bar{n}+\frac{1}{2}\right)\frac{\hbar e\bar{B}}{\sqrt{\bar{m}_1\bar{m}_2}}\left(1-\frac{\bar{m}_2}{\bar{m}'_2}\right) + \frac{3\alpha^2}{8}\left(\bar{n}^2+\bar{n}+\frac{1}{2}\right)\left(\frac{\hbar e\bar{B}}{\sqrt{\bar{m}_1\bar{m}_2}}\right)^2\left(1-\frac{\bar{m}_2}{\bar{m}'_2}\right)\right]\right]$$

EEM at the Fermi level can be written from (4.27b) as

$$\bar{m}^*_{\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) = \bar{m}_3\overline{U'}_{16,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.27c}$$

Thus, EEM is a function of Fermi energy, Landau quantum number and the scattering potential.

The carrier statistics in this case can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\sqrt{\bar{m}_3}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\left(\bar{U}_{16+}(\bar{E}_{FBHD},\bar{n},\eta_g)\right)^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}_B(\bar{r})\left(\bar{U}_{16+}(\bar{E}_{FBHD},\bar{n},\eta_g)\right)^{1/2}\right] \tag{4.28}$$

Using (1.31f) and (4.28), we can study the entropy in this case.

(b) Lax Model

In accordance with this model, the magneto dispersion relation assumes the form

$$\bar{E}(1+\alpha\bar{E}) = \left(\bar{n}+\frac{1}{2}\right)\hbar\bar{\omega}_{03}(\bar{E}) + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_3} \pm \frac{1}{2}\mu_0\bar{g}^*\bar{B} \tag{4.29}$$

where

$$\omega_{03}(\bar{E}) \equiv \frac{e\bar{B}}{\sqrt{\bar{m}_1\bar{m}_2}}$$

The magneto-dispersion relation in HD IV–VI materials, can be written following (A.30) as

$$\gamma_2(\bar{E},\eta_g)=\left(\bar{n}+\frac{1}{2}\right)+\hbar\omega_{03}(E)+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_3}\pm\frac{1}{2}\bar{g}^*\mu_0\bar{B} \tag{4.30}$$

(4.30) can be written as

$$\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_3}=\bar{U}_{17,\pm}(\bar{E},\bar{n},\eta_g) \tag{4.31a}$$

where

$$\bar{U}_{17,\pm}(\bar{E},\bar{n},\eta_g)=\gamma_2(\bar{E},\eta_g)-\left(\bar{n}+\frac{1}{2}\right)\hbar\omega_{03}(\bar{E})\pm\frac{1}{2}\bar{g}^*\mu_0\bar{B}$$

EEM at the Fermi level can be written from (4.31a) as

$$\bar{m}^*(\bar{E}_{FBHD},\eta_g)=\bar{m}_3\overline{U'}_{17,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.31b}$$

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\sqrt{\bar{m}_3}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{17+}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}+\sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}_B(\bar{r})(\bar{U}_{17+}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right] \tag{4.32}$$

Using (1.31f) and (4.32), we can study the entropy in this case.

(c) Dimmock Model

The dispersion relation under magnetic quantization in HD IV–VI materials can be expressed in accordance with Dimmock model as

$$\begin{aligned}
&\gamma_2(\bar{E},\eta_g)+\alpha\gamma_3(\bar{E},\eta_g)\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}_t^+}-\frac{1}{\bar{m}_t^-}\right)+\alpha\gamma_3(\bar{E},\eta_g)\bar{x}\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}_l^+}-\frac{1}{\bar{m}_l^-}\right)\\
&=\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_t^*}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_l^*}+\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_t^-}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_l^-}+\alpha\left[\frac{\hbar^4\bar{k}_s^4}{4\bar{m}_t^-\bar{m}_t^+}+\frac{\hbar^2\bar{k}_s^2\bar{k}_z^2}{4\bar{m}_l^-\bar{m}_l^+}+\frac{\hbar^2\bar{k}_z^2\bar{k}_s^2}{4\bar{m}_t^+\bar{m}_t^-}+\frac{\hbar^4\bar{k}_z^4}{4\bar{m}_l^-\bar{m}_l^+}\right]\\
&=\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}_t^+}-\frac{1}{\bar{m}_t^-}\right)+\bar{x}\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}_l^*}-\frac{1}{\bar{m}_l^-}\right)\\
&+\alpha\left[\frac{\hbar^4}{4\bar{m}_t^-\bar{m}_t^+}\left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)^2+\bar{x}\left[\frac{\hbar^4 e\bar{B}}{2\bar{m}_l^+\bar{m}_t^-\hbar}+\frac{\hbar^4 e\bar{B}}{2\bar{m}_t^+\bar{m}_l^-\hbar}\right]\left(\bar{n}+\frac{1}{2}\right)+\frac{\hbar^4}{4\bar{m}_l^-\bar{m}_l^+}\bar{x}^2\right]
\end{aligned} \tag{4.33}$$

where $\bar{x}=\bar{k}_z^2$

Therefore, the magneto dispersion relation in HD IV–VI materials, whose unperturbed carriers obey the Dimmock Model can be expressed as

$$\bar{k}_z^2 = \bar{U}_{170}(\bar{E}, \bar{n}, \eta_g) \tag{4.34}$$

where

$$\bar{U}_{170}(\bar{E}, \bar{n}, \eta_g) = [2\bar{p}_9]^{-1}[-\bar{q}_9(\bar{E}, \bar{n}, \eta_g) + [\bar{q}_9^2(\bar{E}, \bar{n}, \eta_g) + 4\bar{p}_9\bar{R}_9(\bar{E}, \bar{n}, \eta_g)]^{1/2}], \tag{4.35}$$

$$\bar{p}_9 = \frac{\alpha\hbar^4}{4\bar{m}_l^- \bar{m}_l^+}, \bar{q}_9(\bar{E}, \bar{n}, \eta_g) = \left[\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}_l^*} + \frac{1}{\bar{m}_l^-}\right) + \frac{\alpha\hbar^3 e\bar{B}}{2}\left(\bar{n} + \frac{1}{2}\right)\left(\frac{1}{\bar{m}_t^- \bar{m}_l^+} + \frac{1}{\bar{m}_l^- \bar{m}_t^+}\right) - \bar{\alpha}\gamma_3(\bar{E}, \eta_g)\left(\frac{1}{\bar{m}_l^+} + \frac{1}{\bar{m}_l^-}\right)\right]$$

and

$$\bar{R}_9(\bar{E}, \bar{n}, \eta_g) = \gamma_3(\bar{E}, \eta_g) + \alpha e\bar{B}\gamma_3(\bar{E}, \eta_g)\left(\bar{n} + \frac{1}{2}\right)\hbar\left(\frac{1}{\bar{m}_l^+} + \frac{1}{\bar{m}_l^-}\right) - \frac{\alpha\hbar^2}{\bar{m}_t^- \bar{m}_t^+}\left[e\bar{B}\left(\bar{n} + \frac{1}{2}\right)^2\right] \tag{4.36a}$$

EEM at the Fermi level can be written from (4.34) as

$$\bar{m}^*(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \frac{\hbar^2}{2}\bar{U}'_{17}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.36b}$$

Thus, EEM is a function of Fermi energy, Landau quantum number and the scattering potential.

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{17}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{17}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2}\right] \tag{4.37}$$

Using (1.31f) and (4.37), we can study the entropy in this case.

(d) Model of Bangert and Kastner

In accordance with this model [8], the carrier energy spectrum in HD IV–VI materials can be written following (3.68) as

$$\frac{\bar{k}_s^2}{\rho_{11}^2(\bar{E}, \eta_g)} + \frac{\bar{k}_y^2}{\rho_{12}^2(\bar{E}, \eta_g)} = 1 \tag{4.38}$$

where

$$\rho_{11}(\bar{E}, \eta_g) = \frac{1}{\sqrt{\bar{S}_1(\bar{E}, \eta_g)}}, \rho_{12}(\bar{E}, \eta_g) = \frac{1}{\sqrt{\bar{S}_2(\bar{E}, \eta_g)}},$$

$$\bar{S}_1(\bar{E},\eta_g)=\left[2\gamma_0(\bar{E},\eta_g)\right]^{=1}\left[\frac{(\bar{R})^2}{\bar{E}_g}\left\{\bar{c}_1(\bar{\alpha}_1\bar{E},\bar{E}_g)-i\bar{D}_1(\bar{\alpha}_1\bar{E},\bar{E}_g)\right\}\frac{(\bar{S})^2}{\Delta'_c}\left\{\bar{c}_2(\bar{\alpha}_2\bar{E},\bar{E}_g)\right.\right.$$
$$\left.\left.-i\bar{D}_2(\bar{\alpha}_2\bar{E},\bar{E}_g)\right\}+\frac{(\bar{Q})^2}{\Delta''_c}\left\{\bar{c}_3(\bar{\alpha}_3\bar{E},\bar{E}_g)-i\bar{D}_3(\alpha_3\bar{E},\bar{E}_g)\right\}\right]$$

and

$$\bar{S}_2(\bar{E},\eta_g)+\left[2\gamma_0(\bar{E},\eta_g)\right]^{-1}\left[\frac{(2\bar{A})^2}{\bar{E}_g}\left\{\bar{c}_1(\alpha_1\bar{E},\bar{E}_g)-i\bar{D}_1(\bar{\alpha}_1\bar{E},\bar{E}_g)\right\}\right.$$
$$\left.+\frac{(\bar{S}+\bar{Q})^2}{\Delta''_c}\left\{\bar{c}_3(\bar{\alpha}_3\bar{E},\bar{E}_g)-i\bar{D}_3(\bar{\alpha}_3\bar{E},\bar{E}_g)\right\}\right]$$

Since $\bar{S}_1(\bar{E},\eta_g)$ and $\bar{S}_2(\bar{E},\eta_g)$ are complex, the energy spectrum is also complex in the presence of Gaussian band tails.

Therefore, the magneto dispersion law in the presence of a quantizing magnetic field B which makes an angle θ with k_z axis can be written as

$$\bar{k}_z^2=\bar{U}_{18}(\bar{E},\bar{n},\eta_g) \tag{4.39a}$$

where

$$\bar{U}_{18}(\bar{E},\bar{n},\eta_g)=\left[\rho_{11}^2(\bar{E},\eta_g)\sin^2\theta+\rho_{12}^2(\bar{E},\eta_g)\cos^2\theta\right]-$$
$$\left[\frac{2e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\left[(\rho_{11}^2(\bar{E},\eta_g)\rho_{12}^2(\bar{E},\eta_g))\right)^{-1}\{\rho_{11}^2(\bar{E},\eta_g)\sin^2\theta+\rho_{12}^2(\bar{E},\eta_g)\cos^2\theta\}^{3/2}\right]\right]$$

EEM at the Fermi level can be written from (A.39a) as

$$\bar{m}_c^*(\bar{E}_{FBHD},\bar{n},\eta_g)=\frac{\hbar^2}{2}\ \textit{Real part of}[\bar{U}_{18}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.39b}$$

Thus, EEM is a function of Fermi energy, Landau quantum number and the scattering potential and the orientation of the applied quantizing magnetic field. The electron concentration can be written as

$$\bar{n}_0=\frac{e\bar{g}_v\bar{B}}{\pi^2\hbar^2}\text{Real Part of}\left[\sum_{\bar{n}=0}^{\bar{n}\max}\left[(\bar{U}_{18}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}+\sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{18}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right]\right] \tag{4.40}$$

Using (1.31f) and (4.40), we can study the entropy in this case.

(e) Model of Foley and Langenberg

The dispersion relation of the conduction electrons of IV–VI materials in accordance with Foley et al. can be written as [9]

$$\bar{E}+\frac{\bar{E}_g}{2}=\bar{E}_0(\bar{k})+\left[[\bar{E}_+(\bar{k})+\frac{\bar{E}_g}{2}]^2+\bar{P}_\perp^2\bar{k}_s^2+\bar{P}_\parallel^2\bar{k}_z^2\right]^{1/2} \tag{4.41}$$

where $\bar{E}_+(\bar{k})=\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^+}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_\parallel^+}, \bar{E}_-(\bar{k})=\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^-}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_\parallel^-}$ represents the contribution from the interaction of the conduction and the valence band edge states with the more distant bands and the free electrons term, $\frac{1}{\bar{m}_\perp^\pm}=\frac{1}{2}[\frac{1}{\bar{m}_{tc}}\pm\frac{1}{\bar{m}_{tv}}], \frac{1}{\bar{m}_\parallel^\pm}=\frac{1}{2}[\frac{1}{\bar{m}_{lc}}\pm\frac{1}{\bar{m}_{lv}}]$

Following the methods as given in chapter 1, the dispersion relation in HD IV–VI materials in the present case is given by

$$\left[\left[\gamma_3(\bar{E},\eta_g)+\frac{\bar{E}_{g_0}}{2}\right]-\left[\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^-}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_\parallel^-}\right]\right]^2=\left[\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^-}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_\parallel^-}\right]+\frac{\bar{E}_{g_0}^2}{4}$$
$$+\bar{E}_{g_0}\left[\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_\perp^-}+\frac{\hbar^2\bar{k}_z^2}{2\bar{m}_\parallel^-}\right]+\bar{P}_\parallel^2\bar{k}_z^2+\bar{P}_\perp^2\bar{k}_s^2 \tag{4.42}$$

Therefore, the magneto-dispersion relation in HD IV–VI materials can be written as

$$\gamma_3^2(\bar{E},\eta_g)+\frac{\bar{E}_{g_0}^2}{4}+\bar{E}_{g_0}\gamma_3(\bar{E},\eta_g)+\left[\frac{\hbar e\bar{B}}{\bar{m}_\perp^-}(\bar{n}+\frac{1}{2})+\frac{\hbar^2\bar{x}}{2\bar{m}_\parallel^-}\right]^2-2\Big[\gamma_3(\bar{E},\eta_g)$$
$$+\frac{\bar{E}_{g_0}}{2}\Big]\left[\frac{\hbar e\bar{B}(\bar{n}+\frac{1}{2})}{\bar{m}_\perp^-}+\frac{\hbar^2\bar{x}}{2\bar{m}_\parallel^-}\right]=\left[\frac{\hbar e\bar{B}(\bar{n}+\frac{1}{2})}{\bar{m}_\perp^+}+\frac{\hbar^2\bar{x}}{2\bar{m}_\parallel^+}\right]$$
$$+\left[\frac{\hbar e\bar{B}}{\bar{m}_\perp^+}\left(\bar{n}+\frac{1}{2}\right)+\frac{\hbar^2\bar{x}}{2\bar{m}_\parallel^+}\right]^2+\bar{P}_\parallel^2\bar{x}+\bar{P}_\perp^2\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \tag{4.43}$$

where $\bar{k}_z^2=\bar{x}$ Therefore, the magneto dispersion relation in IV–VI HD materials, where unperturbed carriers follow the model of Foley et al. can be expressed as

$$\bar{k}_z^2=\bar{U}_{19}(\bar{E},\bar{n},\eta_g) \tag{4.44a}$$

Where

$$\bar{U}_{19}(\bar{E},\bar{n},\eta_g)=[2\bar{p}_{91}]^{-1}\left[-\bar{q}_{91}(\bar{E},\bar{n},\eta_g)+\left\{\bar{q}_{91}^2(\bar{E},\bar{n},\eta_g)+4\bar{p}_{91}\bar{R}_{91}(\bar{E},\bar{n},\eta_g)\right\}^{1/2}\right]$$

$$\bar{p}_{91}=\frac{\hbar^4}{4}\left[\frac{1}{(\bar{m}_\parallel^2)^2}-\frac{1}{(\bar{m}_\parallel^-)^2}\right]$$

$$\bar{q}_{91}(\bar{E},\bar{n},\eta_g)=\left[\frac{\hbar^2 e\bar{B}}{\bar{m}_{\perp}^{-}\bar{m}_{||}^{+}}\left(\bar{n}+\frac{1}{2}\right)+\bar{P}_{||}^{2}+\frac{\hbar^2\bar{E}_{g0}}{2\bar{m}_{||}^{+}}-\frac{\hbar^2 e\bar{B}\left(\bar{n}+\frac{1}{2}\right)}{\bar{m}_{\perp}^{-}\bar{m}_{||}^{-}}+\frac{\hbar^2}{\bar{m}_{||}^{-}}\left(\gamma_3(\bar{E},\eta_g)+\frac{\bar{E}_{g0}}{2}\right)\right]$$

$$\bar{R}_{91}(\bar{E},\eta_g,\bar{n})=\left[\gamma_3^2(\bar{E},\eta_g)+\bar{E}_{g0}\gamma_3(\bar{E},\eta_g)-\frac{2\hbar e\bar{B}}{\bar{m}_{\perp}^{-}}\left(\gamma_3(\bar{E},\eta_g)+\frac{\bar{E}_{g0}}{2}\right)\left(\bar{n}+\frac{1}{2}\right)\right.$$
$$\left.-\bar{E}_{g0}\frac{\hbar e\bar{B}}{m_{\perp}^{+}}\left(\bar{n}+\frac{1}{2}\right)-\bar{P}_{\perp}^{2}.\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]$$

EEM at the Fermi level can be written from (A.44a) as

$$\bar{m}^{*}(\bar{E}_{FBHD},\bar{n},\eta_g)=\frac{\hbar^2}{2}\overline{U'}_{19}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.44b}$$

Thus, as noted already in this case also EEM is a function of Fermi energy, Landau quantum number and the scattering potential.

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{19}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}+\sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{19}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right]\right] \tag{4.45}$$

Using (1.31f) and (4.45), we can study the entropy in this case.

4.2.5 Entropy in HD stressed Kane-type materials under magnetic quantization

The dispersion relation of the conduction electrons in HDKane-type materials can be written following (1.206) of Chapter 1 as

$$\frac{\bar{k}_x^2}{\bar{a}_{||}^2(\bar{E},\eta_g)}+\frac{\bar{k}_y^2}{\bar{b}_{||}^2(\bar{E},\eta_g)}+\frac{\bar{k}_z^2}{\bar{c}_{||}^2(\bar{E},\eta_g)}=1 \tag{4.46}$$

where

$$\bar{a}_{||}(\bar{E},\eta_g)=\frac{1}{\sqrt{\bar{P}_{||}(\bar{E},\eta_g)}},\bar{b}_{||}(\bar{E},\eta_g)=\frac{1}{\sqrt{\bar{Q}_{||}(\bar{E},\eta_g)}}$$

and

$$\bar{c}_{||}(\bar{E},\eta_g)=\frac{1}{\sqrt{\bar{S}_{||}(\bar{E},\eta_g)}}$$

The electron energy spectrum in HDKane-type materials in the presence of an arbitrarily oriented quantizing magnetic field B which makes an angle $\bar{\alpha}_1,\bar{\beta}_1$ and $\bar{\gamma}_1$ with k_x,k_y and k_z axes respectively, can be written as

$$(\overline{k'}_z)^2 = \bar{U}_{41}(\bar{E}, \bar{n}, \eta_g) \tag{4.47a}$$

Where

$$\bar{U}_{41}(\bar{E}, \bar{n}, \eta_g) = \bar{I}_2(\bar{E}, \eta_g)[1 - \bar{I}_3(\bar{E}, \bar{n}, \eta_g)]$$

$$\bar{I}_2(\bar{E}, \eta_g) = [[\bar{a}_{11}(\bar{E}, \eta_g)]^2 \cos^2\alpha_1 + [\bar{b}_{11}(\bar{E}, \eta_g)]^2 \cos^2\beta_1 + [\bar{c}_{11}(\bar{E}, \eta_g)]^2 \cos^2\gamma_1]$$

and

$$\bar{I}_3(\bar{E}, \bar{n}, \eta_g) = \frac{2e\bar{B}}{\hbar}(\bar{n} + \frac{1}{2})[\bar{a}_{11}(\bar{E}, \eta_g)\bar{b}_{11}(\bar{E}, \eta_g)\bar{c}_{11}(\bar{E}, \eta_g)]^{-1}[\bar{I}_2(\bar{E}, \eta_g)]^{1/2}$$

EEM at the Fermi level can be written from (4.47a) as

$$\bar{m}^*(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \frac{\hbar^2}{2}\overline{U'}_{41}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.47b}$$

From (4.47b) we observe that EEM is a function of Fermi energy, Landau quantum number, the scattering potential and the orientation of the applied quantizing magnetic field.

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}\max}\left[(\bar{U}_{41}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{41}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2}\right]\right] \tag{4.48}$$

Using (1.31f) and (4.48), we can study the entropy in this case.

4.2.6 Entropy in HD Te under magnetic quantization

The magneto dispersion relation of the conduction electrons in HD Te can be expressed as

$$\bar{k}_z^2 = \bar{U}_{42\pm}(\bar{E}, \bar{n}, \eta_g) \tag{4.49a}$$

where

$$\bar{U}_{42,\pm}(\bar{E},\bar{n},\eta_g) = (2\psi_1^2)^{-1}\left[\left\{2\gamma_3(\bar{E},\eta_g)\psi_1 + \psi_3^2 - 4\psi_1\psi_2\frac{e\bar{B}}{\bar{h}}(\bar{n}+\frac{1}{2})\right\} - \left\{\psi_3^4 + 4\psi_1\psi_3^2\gamma_3(\bar{E},\eta_g)\right\} + \frac{8e\bar{B}}{\bar{h}}(\bar{n}+\frac{1}{2})(\psi_1^2\psi_4^2 - \psi_1\psi_2\psi_3)\right\}^{-1/2}\right]$$

EEM at the Fermi level can be written from (4.49a) as

$$\bar{m}_{\pm}^{*}(\bar{E}_{FBHD},\bar{n},\eta_g)=\frac{\hbar^2}{2}\overline{U'}_{42\pm}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.49b}$$

Thus from (4.49b), we note that EEM is a function of three variables namely Fermi energy, Landau quantum number and the scattering potential.

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{42,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}+\sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{42,\pm}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right]\right] \tag{4.49c}$$

Using (1.31f) and (4.49c), we can study the entropy in this case.

4.2.7 Entropy in HD Gallium Phosphide under magnetic quantization

The magneto-dispersion relation in HD GaP can be written following (1.248) of chapter 1 as

$$\bar{k}_z^2=\bar{U}_{43}(\bar{E},\bar{n},\eta_g) \tag{4.50a}$$

where

$$\bar{U}_{43}(\bar{E},\bar{n},\eta_g)=(2\bar{b}^2)^{-1}\left[\left\{2\gamma_3(\bar{E},\eta_g)\bar{b}+\bar{c}-2\bar{D}\bar{b}-4\bar{a}\bar{b}\frac{e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\right\}\right.$$
$$+\left\{[\bar{c}^2+4\bar{b}\bar{c}\gamma_3(\bar{E},\eta_g)+4\bar{D}^2b^2-4\bar{c}\bar{D}\bar{b}]-\frac{8e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\right.$$
$$\left.\left.(2\bar{a}\bar{b}^2\bar{D}+4\gamma_3(\bar{E},\eta_g)\bar{b}^2\bar{a}+\bar{a}\bar{b}\bar{c}-2\bar{b}^2\bar{a}\gamma_3(\bar{E},\eta_g)-\bar{b}^2\bar{c})\right\}^{-1/2}\right]$$

$$\bar{a}=\frac{\hbar^2}{2\bar{m}_{\perp}^{*}}+\bar{b},\ \bar{b}=\frac{\hbar^2}{2\bar{m}_{||}^{*}},\ \bar{c}=\left(\frac{\hbar^2\bar{k}_0}{\bar{m}_{||}^{*}}\right)^2,\ \bar{D}=|V_G|$$

EEM at the Fermi level can be expressed from (4.50a) as

$$\bar{m}^{*}(\bar{E}_{FBHD},\bar{n},\eta_g)=\frac{\hbar^2}{2}\bar{U}'_{43}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.50b}$$

Thus, from (4.50b) it appears that EEM is the function of Fermi energy, Landau quantum number and the scattering potential.

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{43}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}+\sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{43}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right]\right] \tag{4.50c}$$

Using (1.31f) and (4.50c), we can study the entropy in this case.

4.2.8 Entropy in HD platinum antimonide under magnetic quantization

The magneto dispersion relation in HD $PtSb_2$ can be written as

$$\bar{k}_z^2 = \bar{U}_{44}(\bar{E}, \bar{n}, \eta_g) \tag{4.51a}$$

where

$$\bar{U}_{44}(\bar{E}, \bar{n}, \eta_g) = \frac{1}{2\bar{T}_{41}}[\bar{T}_{71}(\bar{E}, \bar{n}, \eta_g) + \sqrt{\bar{T}_{71}^2(\bar{E}, \bar{n}, \eta_g) + 4\bar{T}_{41}\bar{T}_{71}(\bar{E}, \bar{n}, \eta_g)}],$$

$$\bar{T}_{71}(\bar{E}, \bar{n}, \eta_g) = \left[\bar{T}_{51}(\bar{E}, \eta_g) - \bar{T}_{31}\frac{2eB}{\hbar}(\bar{n} + \frac{1}{2})\right]$$

and

$$\bar{T}_{72}(\bar{E}, \bar{n}, \eta_g) = \left[\bar{T}_{61}(\bar{E}, \eta_g) + \frac{2eB}{\hbar}(\bar{n} + \frac{1}{2})\bar{T}_{21}(\bar{E}, \eta_g)\right]$$

EEM at the Fermi level can be written from (4.51a) as

$$\bar{m}^*(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \frac{\hbar^2}{2}\overline{U'}_{44}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.51b}$$

Thus, from the above equation we infer that EEM is a function of Landau quantum number, the Fermi energy and the scattering potential.

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{45}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{45}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2}\right]\right] \tag{4.52}$$

Using (1.31f) and (4.52), we can study the entropy in this case.

4.2.9 Entropy in HD Bismuth Telluride under magnetic quantization

The magneto-dispersion relation in HD Bi_2Te_3 can be written as

$$\bar{k}_x^2 = \bar{U}_{45}(\bar{E}, \eta_g, \bar{n}) \tag{4.53a}$$

where

$$\bar{U}_{45}(\bar{E}, \eta_g, \bar{n}) = \frac{\gamma_2(\bar{E}, \eta_g) - (\bar{n} + \frac{1}{2})\frac{e\hbar\bar{B}}{M_{31}}}{\omega_1}$$

and

$$\bar{M}_{31} = \frac{\bar{m}_0}{\left(\bar{\alpha}_{22}\bar{\alpha}_{33} - \frac{(\bar{\alpha}_{23})^2}{4}\right)^{1/2}}$$

EEM at the Fermi evel can be written from (4.53a) as

$$\bar{m}^*(\bar{E}_{FBHD}, \eta_g) = \frac{\hbar^2}{2}\overline{U'}_{45}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.53b}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{44}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{44}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2}\right]\right] \tag{4.54}$$

Using (1.31f) and (4.54), we can study the entropy in this case.

4.2.10 Entropy in HD Germanium under magnetic quantization

(a) Model of Cardona et al.

The magneto-dispersion relation in HD Ge can be written following (1.300) as

$$\bar{k}_x^2 = \bar{U}_{46}(\bar{E}, \eta_g, \bar{n}) \tag{4.55a}$$

where

$$\bar{U}_{46}(\bar{E}, \bar{n}, \eta_g) = \frac{2\bar{m}_{||}^*}{\hbar^2}\left[\gamma_3(\bar{E}, \eta_g) + \frac{\bar{E}_{g_0}}{2} - \left[\frac{\bar{E}_{g_0}^2}{4} + \frac{\bar{E}_{g_0}\hbar^2}{\bar{m}_{\perp}^*}\frac{2e\bar{B}}{\hbar}(\bar{n} + \frac{1}{2})\right]\right]^{1/2}$$

EEM at the Fermi level can be written from (4.55a) as

$$\bar{m}^*(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \frac{\hbar^2}{2}\overline{U'}_{46}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.55b}$$

From (4.55b) it appears that EEM is a function of Fermi energy and Landau quantum number due to band non-parabolicity.

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{46}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{46}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2}\right]\right] \tag{4.56}$$

Using (1.31f) and (4.56), we can study the entropy in this case.

(b) Model of Wang and Ressler

The magneto-dispersion relation in HD Gecan be written following (1.321) as

$$\bar{k}_x^2 = \bar{U}_{47}(\bar{E}, \eta_g, \bar{n}) \tag{4.57a}$$

where

$$\bar{U}_{47}(\bar{E}, \bar{n}, \eta_g) = \left(\frac{\bar{m}_{||}^*}{\hbar^2 \bar{\alpha}_6}\right)\left[1 - \alpha_5\left(\bar{n} + \frac{1}{2}\right)\hbar\omega_\perp - \left\{\theta_7(\bar{n}) - 4\alpha_6\gamma_3(\bar{E}, \eta_g)\right\}^{1/2}\right], \omega_\perp = \frac{e\bar{B}}{\bar{m}_\perp^*}$$

and

$$\theta_7(\bar{n}) = \left[1 + (\alpha_5)^2\left\{(\bar{n} + \frac{1}{2})\hbar\omega_\perp\right\}^2 - 2\alpha_5\left(\bar{n} + \frac{1}{2}\right)\hbar\omega_\perp + 4\alpha_6\left(\bar{n} + \frac{1}{2}\right)\hbar\omega_\perp - 4\alpha_6\alpha_4\left\{(\bar{n} + \frac{1}{2})\hbar\omega_\perp\right\}^2\right]$$

EEM at the Fermi level can be written from (4.57a) as

$$\bar{m}^*(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \frac{\hbar^2}{2}\overline{U'}_{47}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.57b}$$

From (4.57b) we note that the mass is a function of Fermi energy and quantum number due to band non-parabolicity.

The electron concentration under the condition of extreme degeneracy can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{47}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{47}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2}\right]\right] \tag{4.58}$$

Using (1.31f) and (4.58), we can study the entropy in this case.

4.2.11 Entropy in HD Gallium antimonide under magnetic quantization

The magneto-dispersion relation in HD GaSbcan be written following (1.338) as

$$\bar{k}_x^2 = \bar{U}_{48}(\bar{E}, \eta_g, \bar{n}) \tag{4.59a}$$

where

$$\bar{U}_{47}(\bar{E}, \bar{n}, \eta_g) = \left[-\frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right) + (2\alpha_9^2)^{-1}\left[\left\{2\alpha_9\gamma_3^2(\bar{E}, \eta_g) + \alpha_9\bar{E}'_{g_0} + \frac{\alpha_{10}(\bar{E}'_{g_0})^2}{4}\right\}\right.\right.$$

$$\left(\frac{\bar{m}_{||}^{*}}{\hbar^2\bar{\alpha}_6}\right)\left[1-\alpha_5\left(\bar{n}+\frac{1}{2}\right)\hbar\omega_{\perp}-\{\theta_7(\bar{n})-4\alpha_6\gamma_3(\bar{E},\eta_g)\}^{1/2}\right],\omega_{\perp}=\frac{e\bar{B}}{\bar{m}_{\perp}^{*}}$$

$$-\left\{\alpha_9^2(\bar{E}'_{g_0})^2+\frac{\alpha_{10}^2(\bar{E}'_{g_0})^4}{16}+\alpha_9\alpha_{10}\gamma_3(\bar{E},\eta_g)(\bar{E}'_{g_0})^2+\frac{\alpha_9\alpha_{10}(\bar{E}'_{g_0})^3}{2}\right\}^{1/2}\Bigg]\Bigg]$$

$$\alpha_9=\frac{\hbar^2}{2\bar{m}_0}\text{ and }\alpha_{10}=\frac{2\hbar^2}{\bar{E}'_{g_0}}\left(\frac{1}{\bar{m}_c}-\frac{1}{\bar{m}_0}\right)$$

EEM at the Fermi level can be written from (4.59a) as

$$\bar{m}^{*}(\bar{E}_{FBHD},\eta_g)=\frac{\hbar^2}{2}\overline{U'}_{48}(\bar{E}_{FBHD},\bar{n},\eta_g) \tag{4.59b}$$

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}\max}\left[(\bar{U}_{48}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}+\sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{48}(\bar{E}_{FBHD},\bar{n},\eta_g))^{1/2}\right]\right] \tag{4.60}$$

Using (1.31f) and (4.60), we can study the entropy in this case.

4.2.12 The entropy in HD II–V materials under magnetic quantization

The dispersion relation of the holes are given by [10]

$$\bar{\mathrm{E}}=\theta_1\bar{\mathrm{k}}_{\mathrm{x}}^2+\theta_2\bar{\mathrm{k}}_{\mathrm{y}}^2+\theta_3\bar{\mathrm{k}}_{\mathrm{z}}^2+\delta_4\bar{\mathrm{k}}_{\mathrm{x}}\bar{\mathrm{m}}\left[\{\theta_5\bar{\mathrm{k}}_{\mathrm{x}}^2+\theta_6\bar{\mathrm{k}}_{\mathrm{y}}^2+\theta_7\bar{\mathrm{k}}_{\mathrm{z}}^2+\delta_5\bar{\mathrm{k}}_{\mathrm{x}}\}^2+\mathrm{G}_3^2\bar{\mathrm{k}}_{\mathrm{y}}^2+\Delta_3^2\right]^{1/2}\pm\Delta_3 \tag{4.61}$$

where, $\bar{\mathrm{k}}_{\mathrm{x}}$, $\bar{\mathrm{k}}_{\mathrm{y}}$ and $\bar{\mathrm{k}}_{\mathrm{z}}$ are expressed in the units of

$$\theta_1=\frac{1}{2}(\bar{\mathrm{a}}_1+\bar{\mathrm{b}}_1),\theta_2=\frac{1}{2}(\bar{\mathrm{a}}_2+\bar{\mathrm{b}}_2),\theta_3=\frac{1}{2}(\bar{\mathrm{a}}_3+\bar{\mathrm{b}}_3),\delta_4=\frac{1}{2}(x\bar{\mathrm{A}}+\bar{\mathrm{B}}),$$

$$\theta_5=\frac{1}{2}(\bar{\mathrm{a}}_1-\bar{\mathrm{b}}_1),\theta_6=\frac{1}{2}(\bar{\mathrm{a}}_2-x\bar{\mathrm{b}}_2),\theta_7=\frac{1}{2}(\bar{\mathrm{a}}_3-\bar{\mathrm{b}}_3),\delta_5=\frac{1}{2}(\bar{\mathrm{A}}-\bar{\mathrm{B}}),$$

$\bar{\mathrm{a}}_{\mathrm{i}}(\mathrm{i}=1,2,3,4),\bar{\mathrm{b}}_{\mathrm{i}},\bar{\mathrm{A}},\bar{\mathrm{B}},\bar{\mathrm{G}}_3$ and Δ_3 are system constants

The hole energy spectrum in HD II–V materials can be expressed following the method of Chapter 1 as

$$y_3(\bar{E},n_g)=\theta_1\bar{k}_x^2+\theta_2\bar{k}_y^2+\theta_3\bar{k}_z^2+\delta_4\bar{k}_x\pm\left[\left\{\theta_5\bar{k}_x^2+\theta_6\bar{k}_y^2+\theta_7\bar{k}_z^2+\delta_5\bar{k}_x\right\}^2+\bar{G}_3^2\bar{k}_y^2+\Delta_3^2\right]^{\frac{1}{2}}\pm\Delta_3 \tag{4.62}$$

the magneto dispersion law in HD II–V materials assumes the form

$$\bar{k}_y^2 = \bar{U}_{49,\pm}(\bar{E}, \eta_g, \bar{n}) \tag{4.63a}$$

where,

$$\bar{U}_{49,\pm}(\bar{E}, \bar{n}, \eta_g) = -[\bar{I}_{35}\gamma_3(\bar{E}, \eta_g) + \bar{I}_{36,\pm}(\bar{n}) \pm [\gamma_3^2(\bar{E}, \eta_g) + \gamma_3(\bar{E}, \eta_g)\bar{I}_{38,\pm}(\bar{n}) + \bar{I}_{39,\pm}(\bar{n})]^{1/2}]$$

$$\bar{I}_{35} = \frac{\theta_2}{(\theta_2^2 - \theta_5^2)}, \bar{I}_{36,\pm}(\bar{n}) = \frac{\bar{I}_{33,\pm}(n)}{2(\theta_2^2 - \theta_5^2)}, \bar{I}_{38,\pm}(\bar{n}) = (4\theta_5^2)^{-1}[4\theta_2\bar{I}_{33,\pm}(\bar{n}) + 8\theta_2^2\bar{I}_{31,\pm}(\bar{n}) - \theta_5^2\bar{I}_{31,\pm}(\bar{n})],$$

$$\bar{I}_{39,\pm} = (4\theta_5^2)^{-1}[\bar{I}^2{}_{33,\pm}(\bar{n}) + 4\theta_2^3\bar{I}_{34,\pm}(\bar{n}) - 4\theta_5^3\bar{I}_{34,\pm}(\bar{n})], \bar{I}_{33,\pm}(\bar{n}) = [\bar{G}_3^2 + 2\theta_5\bar{I}_{32}(\bar{n}) - 2\theta_2\bar{I}_{31,\pm}(\bar{n})],$$

$$\bar{I}_{34,\pm}(\bar{n}) = [\bar{I}_{32,\pm}^2(\bar{n}) + \Delta_3^2 - \bar{I}_{31,\pm}(\bar{n})],$$

$$\bar{I}_{31,\pm}(\bar{n}) = \left[(\bar{n} + \frac{1}{2})\hbar\bar{\omega}_{31} - \frac{\delta_4^2}{4\theta_1} \pm \Delta_3\right], \bar{I}_{32}(\bar{n}) = \left[(\bar{n} + \frac{1}{2})\hbar\bar{\omega}_{32} - \frac{\delta_5^2}{4\theta_5}\right],$$

$$\bar{\omega}_{31} = \frac{\bar{e}\bar{B}}{\sqrt{\bar{M}_{31}\bar{M}_{32}}}, \bar{\omega}_{32} = \frac{\bar{e}\bar{B}}{\sqrt{\bar{M}_{33}\bar{M}_{34}}}, \bar{M}_{31} = \frac{\hbar^2}{2\theta_1}, \bar{M}_{32} = \frac{\hbar^2}{2\theta_3}, \bar{M}_{33} = \frac{\hbar^2}{2\theta_5}$$

and

$$\bar{M}_{34} = \frac{\hbar^2}{2\theta_7}.$$

EEM at the Fermi level can be written from (4.63a) as

$$\bar{m}_{\pm}^{*}(\bar{E}_{FBHD}, \bar{n}, \eta_g) = \frac{\hbar^2}{2}\overline{U'}_{49,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.63b}$$

From (4.63b) we note that EEM is a function of Fermi energy, Landau quantum number and the scattering potential.

The electron concentration under extreme degeneracy can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar^2}\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{U}_{49,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}}\bar{L}(\bar{r})(\bar{U}_{49,\pm}(\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2}\right]\right] \tag{4.64}$$

Using (1.31f) and (4.64), we can study the entropy in this case.

4.2.13 Entropy in HD lead germanium telluride under magnetic quantization

The dispersion relation of the carriers in n-type $Pb_{1-x}Ga_xTe$ with x=0.01 can be written following Vassilev [11] as

$$[\bar{E} - 0.606\bar{k}_s^2 - 0.0722\bar{k}_z^2][\bar{E} + \bar{E}_{g_0} + 0.411\bar{k}_s^2 + 0.0377\bar{k}_z^2] = 0.23\bar{k}_s^2 + 0.02\bar{k}_z^2 \pm [0.06\bar{E}_{g_0} + 0.061\bar{k}_s^2 + 0.0066\bar{k}_z^2]k_s \tag{4.65}$$

where $\bar{E}_{g_0} = (0.21eV)$is the energy gap for the transition point, the zero of the energy $\bar{E}$ is at the edge of the conduction band of the Γpoint of the Brillouin zone and is measured positively upwards, $\bar{k}_x$, $\bar{k}_y$ and $\bar{k}_z$ are in the units of $10^9\bar{m}^{-1}$.

The magneto-dispersion law in HD $Pb_{1-x}Ge_xTe$ can be expressed following the methods as given in Chapter 1 as

$$\left[\frac{2\theta_0(\bar{E},\eta_g)}{1+Erf(\bar{E}/\eta_g)}\right] + \gamma_3(\bar{E},\eta_g)\left[\overline{E_{g_0}} - 0.345x - 0.390\frac{e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\right] = \frac{0.46e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2}) + 0.02\bar{x} \pm [0.06\bar{E}_{g_0} + 0.122\frac{e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2}) + 0.0066\bar{x}](\frac{2e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2}))^{1/2} + \left[\bar{E}_{g_0} + \frac{0.822e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2}) + 0.377\bar{x}\right]\left[\frac{1.212e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2}) + 0.722\bar{x}\right] \tag{4.66}$$

The (4.66) assumes the form

$$\bar{k}_z^2 = \bar{U}_{50,\pm}(\bar{E},\eta_g,\bar{n}) \tag{4.67a}$$

Where

$$\bar{U}_{50,\pm}(\bar{E},\bar{n},\eta_g) = (2\bar{p}_{10})^{-1}\left[-\bar{q}_{10}(\bar{E},\bar{n},\eta_g) + \left\{\bar{q}_{10}^2(\bar{E},\bar{n},\eta_g) + 4\bar{p}_{10}\bar{R}_{10,\pm}(\bar{E},\bar{n},\eta_g)\right\}^{1/2}\right]$$

$$\bar{p}_{10}(0.377\times0.722), \bar{q}_{10}(\bar{E},\bar{n},\eta_g) = \left[0.02 + 0.345\gamma_3(\bar{E},\eta_g) \pm 0.0066(\tfrac{2\bar{B}}{\hbar}(\bar{n}+\tfrac{1}{2}))^{1/2} + 0.377\times\tfrac{1.212e\bar{B}}{\hbar}(\bar{n}+\tfrac{1}{2}) + 0.722\left[\bar{E}_{g_0} + 0.822\tfrac{e\bar{B}}{\hbar}(\bar{n}+\tfrac{1}{2})\right]\right]$$

and

$$\bar{R}_{10,\mp}(\bar{E},\bar{n},\eta_g) = \left[\frac{2\theta_0(\bar{E},\eta_g)}{1+Erf(\bar{E}/\eta_g)} + \gamma_3(E,\eta_g)\left[\bar{E}_{g_0} - 0.390\frac{e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]\right] \mp (0.06\bar{E}_{g_0} + 0.122\frac{\bar{e}\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\left(\frac{2e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\right)^{1/2}$$

$$- \left(\bar{E}_{g_0} + 0.822 \frac{\bar{e}\bar{B}}{\hbar} (\bar{n} + \frac{1}{2}) \right) \frac{1.212 e\bar{B}}{\hbar} (\bar{n} + \frac{1}{2}) - \frac{0.46 e\bar{B}}{\hbar} (\bar{n} + \frac{1}{2}) \Bigg]$$

EEM at the Fermi level can be written from (4.67a) as

$$\bar{m}^{*}_{\mp} (\bar{E}_{FBHD}, \eta_g) = \frac{\hbar^2}{2} \bar{U}'_{50, \mp} (\bar{E}_{FBHD}, \bar{n}, \eta_g) \tag{4.67b}$$

Thus, from (4.67b) we note that EEM is a function of the Fermi energy, Landau quantum number and the scattering potential.

The electron concentration under extreme degeneracy can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2 \hbar^2} \left[\sum_{\bar{n}=0}^{\bar{n}_{\max}} \left[(\bar{U}_{50, \pm} (\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} + \sum_{\bar{r}=1}^{\bar{r}=\bar{s}} \bar{L}(\bar{r}) (\bar{U}_{50, \pm} (\bar{E}_{FBHD}, \bar{n}, \eta_g))^{1/2} \right] \right] \tag{4.68}$$

Using (1.31f) and (4.68), we can study the entropy in this case.

4.3 Results and discussion

Using the appropriate equations and the energy band constants as given in Appendix 15, in Figure 4.1 the normalized entropy has been plotted as a function of inverse magnetic field for HD Cd_3As_2 as shown in plot (a) of Figure 4.1 where the plot (b) represents the case for $\delta = 0$ and has been drawn to assess the influence of crystal field splitting on the entropy in HD Cd_3As_2. The plot (c) and (d) in the same Figure refer to the three and two band models of Kane; whereas the plot (e) exhibits the parabolic energy bands. Figure 4.2 exhibits the plot of the normalized entropy as a function of impurity concentration for HD Cd_3As_2 for all cases of Figure 4.1. The plot (a) of Figure 4.3 shows the variation of the normalized entropy in HD Cd_3As_2 as a function of orientation of the quantizing magnetic field for $\delta \neq 0$ and the plot (b) refers for $\delta = 0$. Figures 4.4 to 4.6 represent the variation of entropy as functions of inverse quantizing magnetic field, impurity concentration and angular orientation of the quantizing magnetic field for HD $CdGeAs_2$ for the respective cases of Figures 4.1 to 4.3. It should be noted that under varying magnetic field, the concentration has been set to the value of $10^{24} \bar{m}^{-3}$, while, under varying electron concentration, the magnetic field is fixed to 2 tesla. It appears from Figures 4.1 and 4.4 that the entropy oscillates with $1/B$. It is well known that density-of-states in materials under magnetic quantization exhibits oscillatory dependence with inverse quantizing magnetic field, which is being reflected in this case. In fact, all electronic properties of electronic materials in the presence of quantizing magnetic field exhibit periodic variation with inverse quantizing magnetic field. The origin of oscillations of the entropy is the same as

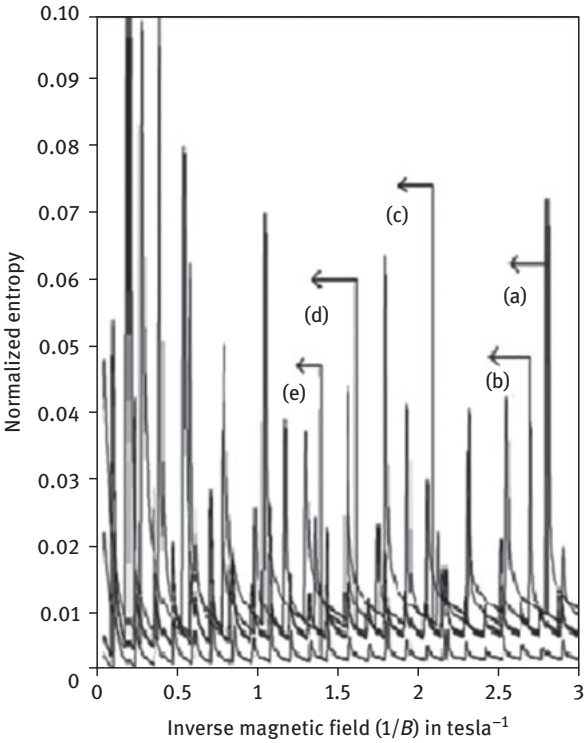

Figure 4.1: Plot of the normalized entropy as function of inverse magnetic field for HD Cd_3As_2 in accordance with the (a) generalized band model ($\delta \neq 0$), (b) $\delta = 0$, (c) three- and (d) two-band models of Kane together with parabolic energy bands (e).

that of the Shubnikov de Haas oscillations. The influence of crystal field splitting, on the entropy can easily be conjectured by comparing the appropriate plots of Figures 4.1 and 4.4. Besides, the differences among three and two band models of Kane together with parabolic energy bands for entropy of HD Cd_3As_2, and HD $CdGeAs_2$ can easily be assessed by comparing the appropriate plots of Figures 4.1 and 4.3. From Figures 4.2 and 4.5, it appears that entropy oscillates with impurity concentration in HD

Cd_3As_2 and HD $CdGeAs_2$ with different numerical values exhibiting the signature of the SdH effect. Although the rates of variations are different, the influence of spectra constants on all types of band models follows the same trend as observed in Figures 4.2 and 4.5, respectively. From Figures 4.3 and 4.6, it appears that the entropy shows sinusoidal dependence with increasing θ and the variation is periodically repeated which appears from these figures. For three- and two-band models of Kane together with parabolic energy bands, the entropy becomes θ invariant and for this reason these plots are not shown in Figures 4.3 and 4.6 respectively. The

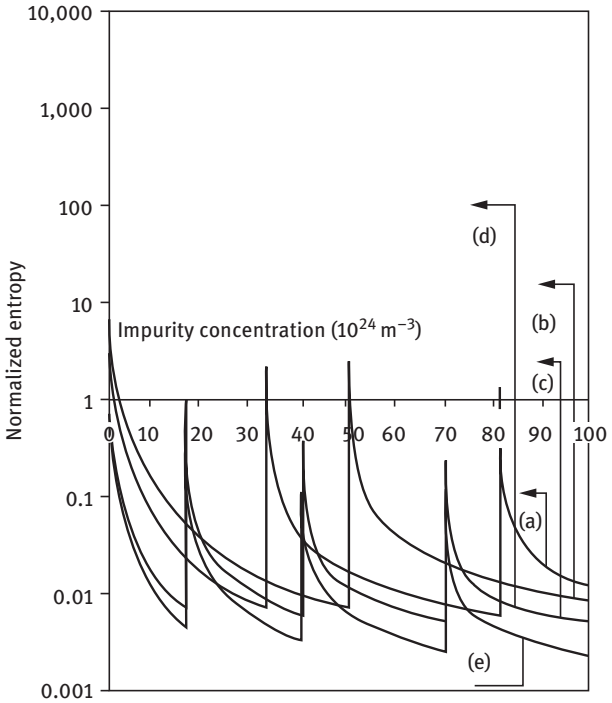

Figure 4.2: Plot of the normalized entropy as function of impurity concentration for HD Cd_3As_2 for all the cases of Figure 4.1.

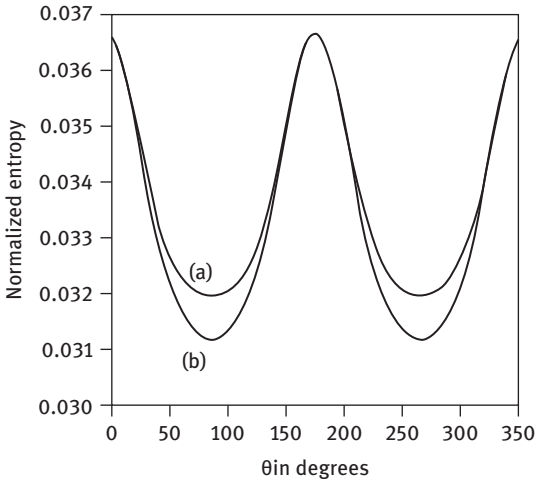

Figure 4.3: Plot of the normalized entropy as function of angular orientation of the quantizing magnetic field for HD Cd_3As_2 for (a) $\delta \neq 0$ and (b) $\delta = 0$.

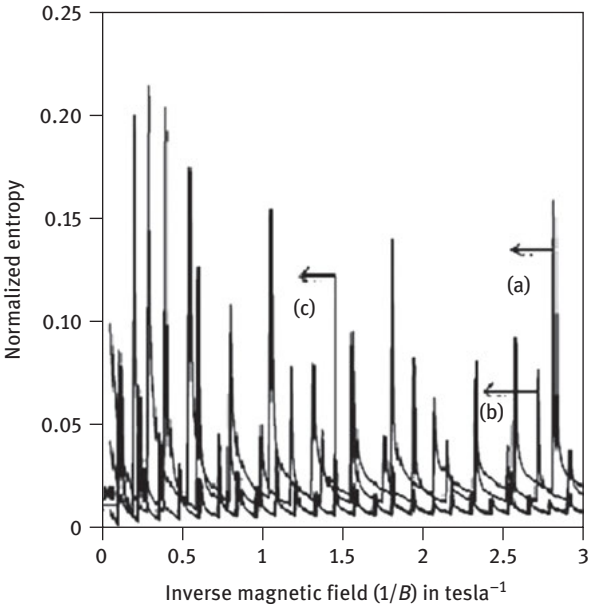

Figure 4.4: Plot of the normalized entropy as a function of inverse magnetic field for HD $CdGeAs_2$ in accordance with the generalized band model (a) $\delta \neq 0$, (b) $\delta = 0$ (c) three- and (d) two-band models of Kane.

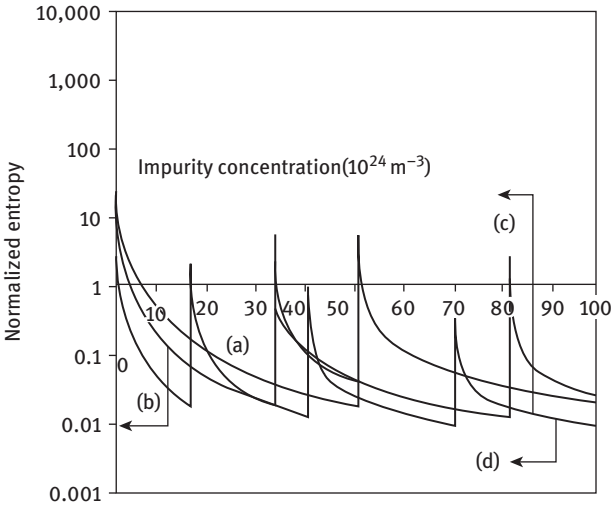

Figure 4.5: Plot of the normalized entropy as a function of impurity concentration for HD $CdGeAs_2$ for all the cases of Figure 4.4.

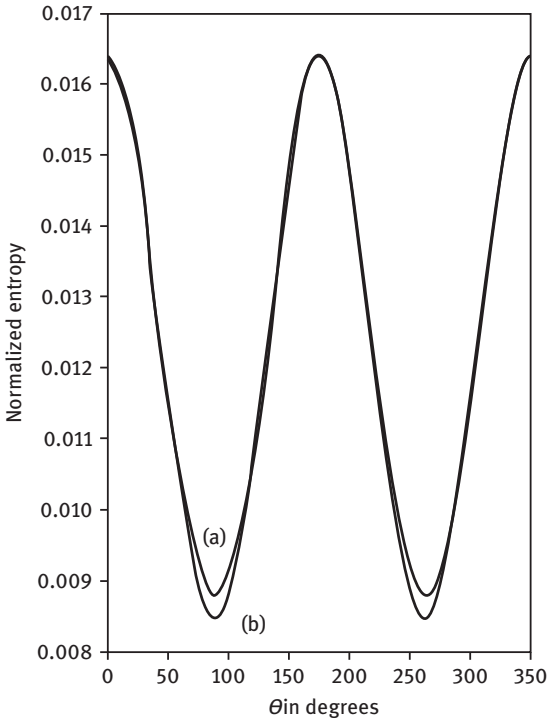

Figure 4.6: Plot of the normalized entropy as a function of angular orientation of the quantizing magnetic field for HD $CdGeAs_2$ for (a) $\delta \neq 0$ and (b) $\delta = 0$.

normalized entropy for InAs and InSb as a function of *1/B* has been plotted in Figures 4.7 and 4.9 for three and two-band models of Kane together with parabolic energy bands, respectively. The normalized entropy as a function of impurity concentration for three and two band models of Kane for HD InAs and InSb has been plotted in Figures 4.8 and 4.10, respectively. It appears from the numerical values that the influence of the three band model of Kane in the energy spectrum of III-V, ternary and quaternary compounds are difficult to distinguish from that of the two band model of Kane. The normalized entropy has been plotted as a function of *1/B* for HD p-CdS in Figure 4.11 where the plots (a) and (b) are valid for $\bar{\lambda}_0 = 0$ and $\bar{\lambda}_0 \neq 0$ respectively. Figure 4.12 exhibits the plot of the same as a function of impurity concentration for all cases of Figure 4.11. The influence of the term $\bar{\lambda}_0$which represents the splitting of the two-spin states by the spin orbit coupling and the crystalline field is apparent from Figures 4.11 and 4.12.

The normalized entropy in HD PbTe accordance the models of Cohen, Lax, Dimmock, Bangert and Kastner and Foley and Langenberg have been plotted in Figures 4.13 and 4.14, respectively, as functions of inverse quantizing magnetic

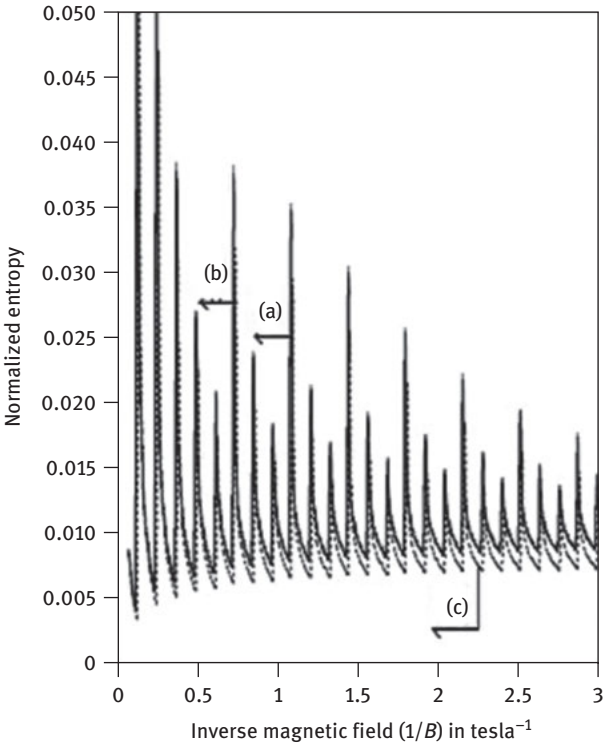

Figure 4.7: Plot of the normalized entropy as a function of inverse magnetic field for HD InAs in accordance with the (a) three and (b) two-band models of Kane together with (c) the parabolic energy bands.

field and impurity concentration, respectively. Figures 4.15 and 4.16 exhibit the plots of normalized entropy in this case as functions of inverse quantizing magnetic field and impurity concentration for HD PbSnTe. Figures 4.17 and 4.18 demonstrate the same for stressed HD InSb and it appears that the influence of stress leads to the enhancement of the entropy in this case. The influence of spin splitting has not been considered in obtaining the oscillatory plots since the peaks in all figures would increase in number with decrease in amplitude if spin splitting term is included in the respective numerical computations without introducing new physics. The effect of collision broadening has not been taken into account in this simplified analysis although the effects of collisions are usually small at low temperatures, the sharpness of the amplitude of the oscillatory plots would somewhat be reduced by collision broadening. Nevertheless, the present analysis would remain valid qualitatively since the effects of collision broadening can usually be taken into account by an effective increase in temperature. Although in a more rigorous statement

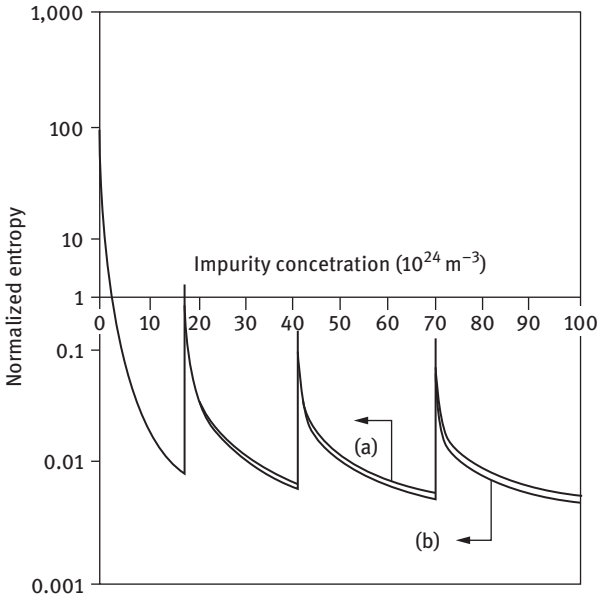

Figure 4.8: Plot of the normalized entropy as a function of impurity concentration for HD InAs in accordance with the (a) three and (b) two-band energy models of Kane.

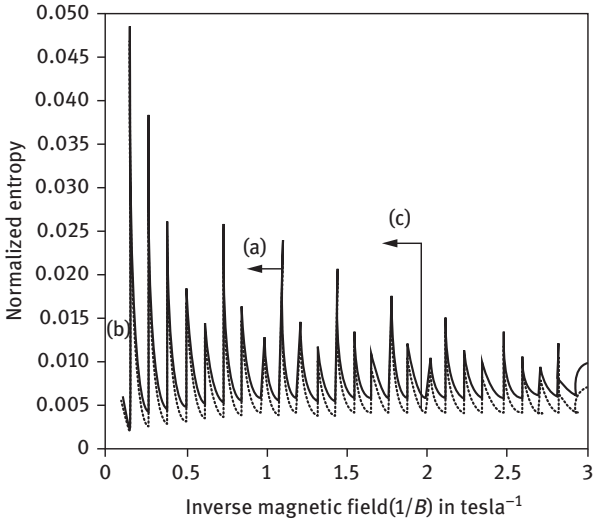

Figure 4.9: Plot of the normalized entropy as a function of inverse magnetic field for HD InSb in accordance with the (a) three- and (b) two-band models of Kane together with (c) the parabolic energy bands.

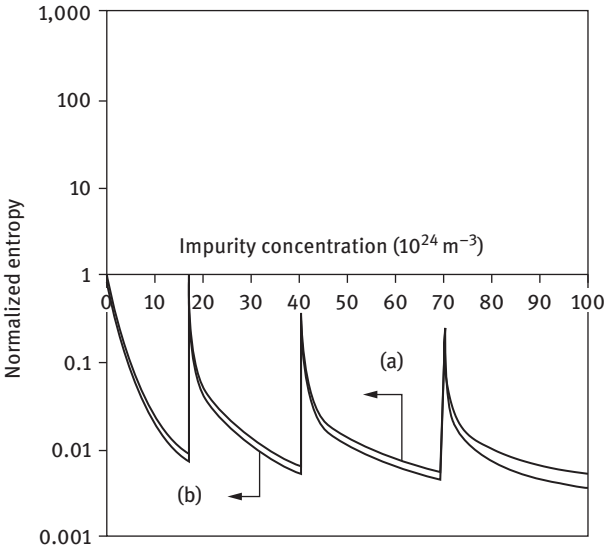

Figure 4.10: Plot of the normalized entropy as a function of impurity concentration for HD InSb in accordance with the (a) three and (b) two-band models of Kane.

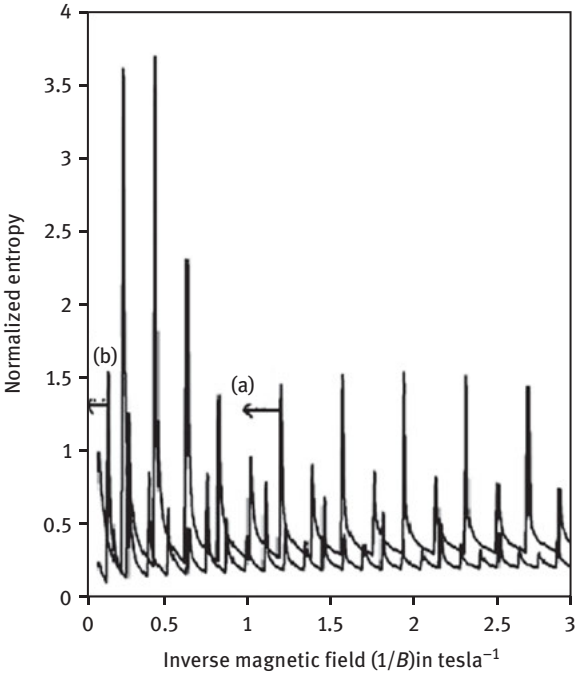

Figure 4.11: Plot of the normalized entropy as a function of inverse magnetic field in HD p-CdS for (a) $\bar{\lambda}_0 = 0$ and (b) $\bar{\lambda}_0 \neq 0$.

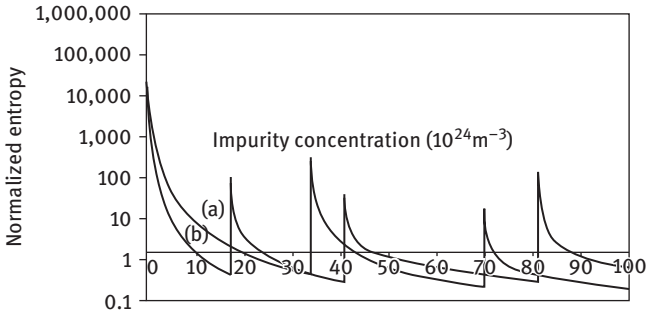

Figure 4.12: Plot of the normalized entropy as a function of impurity concentration field in HD p-CdS for (a) $\bar{\lambda}_0 = 0$ and (b) $\bar{\lambda}_0 \neq 0$.

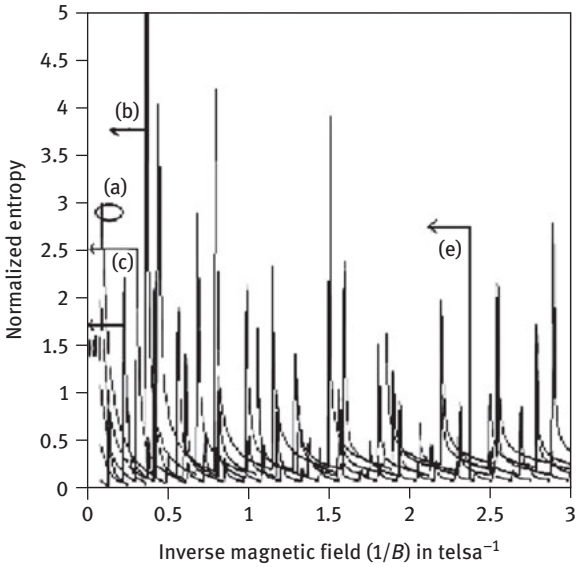

Figure 4.13: Plot of the normalized entropy as a function of inverse magnetic field for HD PbTe in accordance with the models of (a) Cohen, (b) Lax, (c) Dimmock, (d) Bangert and Kastner and (e) Foley and Langenberg, respectively.

the effect of electron–electron interaction should be considered along with the self-consistent procedure, the simplified analysis as presented in this chapter exhibits the basic qualitative features of the entropy in the present case for degenerate materials having various band structures under the magnetic quantization with reasonable accuracy.

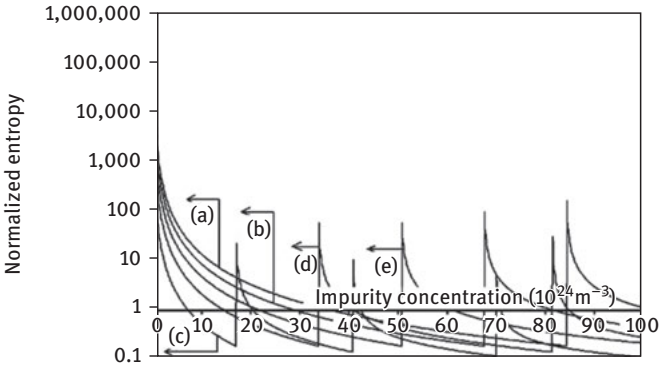

Figure 4.14: Plot of the normalized entropy as a function of impurity concentration for HD PbTe for all the cases of Figure 4.13.

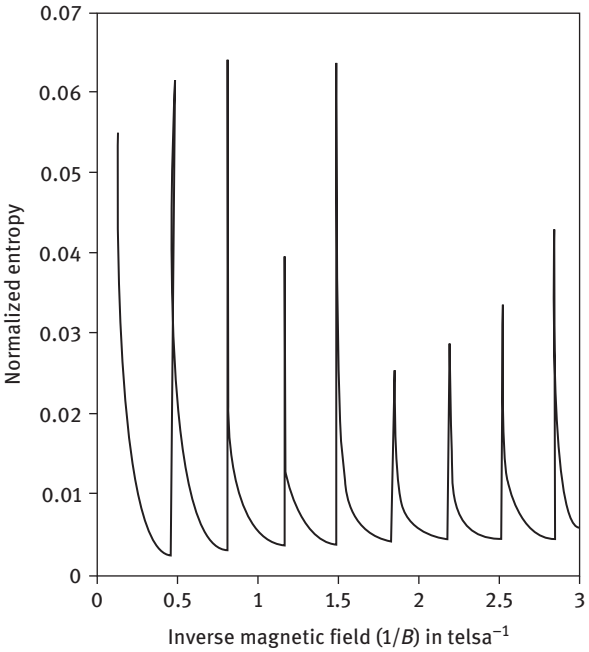

Figure 4.15: Plot of the normalized entropy as a function of inverse magnetic field for HD PbSnTe.

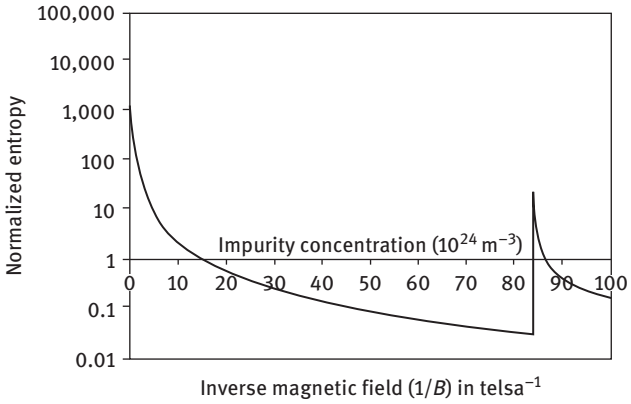

Figure 4.16: Plot of the normalized entropy as a function of impurity concentration field for HD PbSnTe.

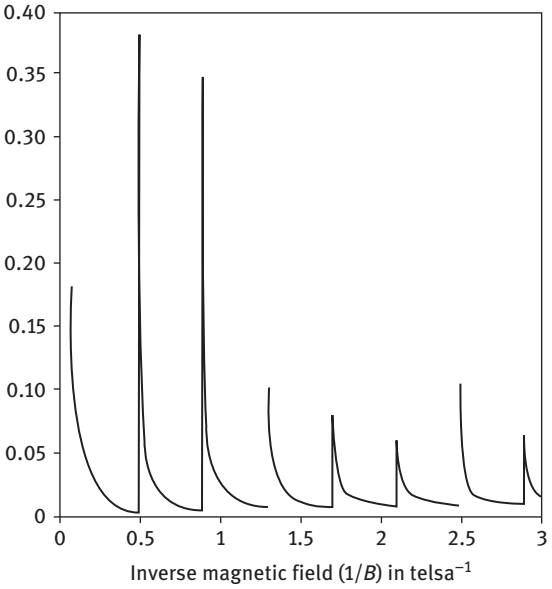

Figure 4.17: Plot of the normalized entropy as a function of inverse magnetic field for stressed HD InSb.

4.4 Open research problems

(R 4.1) Investigate the entropy both in the presence and the absence of an arbitrarily oriented quantizing magnetic field by considering all types of scattering mechanisms including broadening and the electron spin (applicable

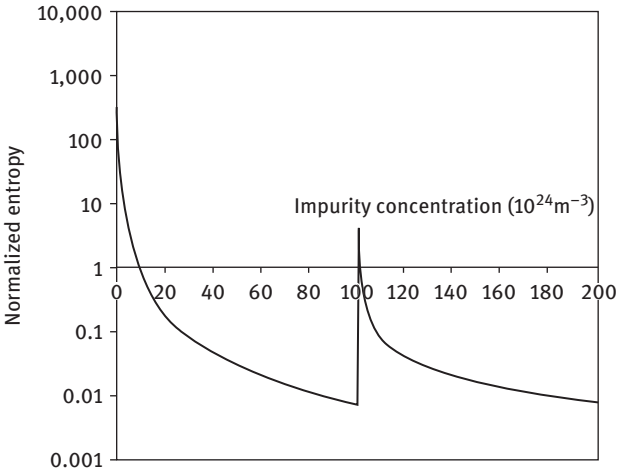

Figure 4.18: Plot of the normalized entropy as a function of impurity concentration field for stressed HD InSb.

under magnetic quantization) for all the bulk materials whose unperturbed carrier energy spectra are defined in Chapter 1.

(R 4.2) Investigate the entropy considering all types of scattering mechanisms in the presence of quantizing magnetic field under an arbitrarily oriented (a) non-uniform electric field and (b) alternating electric field respectively for all the materials whose unperturbed carrier energy spectra are defined in Chapter 1 by including spin and broadening, respectively.

(R 4.3) Investigate the entropy by considering all types of scattering mechanisms under an arbitrarily oriented alternating quantizing magnetic field by including broadening and the electron spin for all the materials whose unperturbed carrier energy spectra as defined in Chapter 1.

(R 4.4) Investigate the entropy by considering all types of scattering mechanisms under an arbitrarily oriented alternating quantizing magnetic field and crossed alternating electric field by including broadening and the electron spin for all the materials whose unperturbed carrier energy spectra as defined in Chapter 1.

(R 4.5) Investigate the entropy by considering all types of scattering mechanisms under an arbitrarily oriented alternating quantizing magnetic field and crossed alternating nonuniform electric field by including broadening and the electron spin whose for all the materials unperturbed carrier energy spectra as defined in Chapter 1.

(R 4.6) Investigate the entropy in the presence and absence of an arbitrarily oriented quantizing magnetic field by considering all types of scattering mechanisms under exponential, Kane, Halperin, Lax, and Bonch–Bruevich band

tails [4] for all the materials whose unperturbed carrier energy spectra as defined in Chapter 1 by including spin and broadening (applicable under magnetic quantization).

(R 4.7) Investigate the entropy in the presence ofan arbitrarily oriented quantizing magnetic field by considering all types of scattering mechanisms for all the materials as defined in (R5.6) under an arbitrarily oriented (a) nonuniform electric field and (b) alternating electric field, respectively, whose unperturbed carrier energy spectra as defined in Chapter 1.

(R 4.8) Investigate the entropy by considering all types of scattering mechanisms for all the materials as described in (R5.6) under an arbitrarily oriented alternating quantizing magnetic field by including broadening and the electron spin whose unperturbed carrier energy spectra as defined in Chapter 1.

(R 4.9) Investigate the entropy by considering all types of scattering mechanisms as discussed in (R5.6) under an arbitrarily oriented alternating quantizing magnetic field and crossed alternating electric field by including broadening and the electron spin for all the materials whose unperturbed carrier energy spectra as defined in Chapter 1.

(R 4.10) Investigate all the appropriate problems of this chapter after proper modifications introducing new theoretical formalisms for functional, negative refractive index, macro molecular, organic and magnetic materials.

(R 4.11) Investigate all the appropriate problems of this chapter for HD p-InSb, p-CuCl and stressed materials having diamond structure valence bands whose dispersion relations of the carriers in bulk materials are given by Cunningham [6], Yekimov et al. [7], and Roman et al. [8], respectively. (replace the green part by (r1.14 to r1.17)

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5 The entropy in heavily doped nanomaterials under magneto-size quantization

I must pray as if everything depends on God but i must work as if everything depends on me.

5.1 Introduction

In Section 5.2.1, of the theoretical background, the entropy has been investigated in ultra-thin films (UFs) of HD nonlinear optical materials in the presence of a quantizing magnetic [1–15] (Place the references at the indicated place).

field.Section 5.2.2 contains the results for UFs of HD III–V, ternary, and quaternary compounds in accordance with the three- and the two-band models of Kane. In the same section, the entropy in accordance with the models of Stillman etal. and Palik etal. have also been studied for the purpose of relative comparison. Section 5.2.3 contains the study of the entropy for UFs of HD II–VI materials under magnetic quantization. In Section 5.2.4, the entropy in UFs of HD IV–VI materials has been discussed in accordance with the models of Cohen, Lax, Dimmock, Bangert and Kastner, and Foley and Landenberg, respectively. In Section 5.2.5, the magnetoentropy for the stressed UFs of HDKane-type materials has been investigated. In Section 5.2.6, the entropy in UFs of HD Te has been studied under magnetic quantization. In Section 5.2.7, the magnetoentropy in UFs of HD n-GaP has been studied. In Section 5.2.8, the entropy in ultra-thin film of HD $PtSb_2$ has been explored under magnetic quantization. In Section 5.2.9, the magnetoentropy in UFs of HD Bi_2Te_3 has been studied. In Section 5.2.10, the entropy in UFs of HD Ge has been studied under magnetic quantization in accordance with the models of Cardona etal. and Wang and Rossler, respectively. In Sections 5.2.11 and 5.2.12, the magnetoentropy in UFs of HD n-GaSb and II–V compounds have respectively been studied. In Section 5.2.13, the magnetoentropy in UFs of HD $Pb_{1-x}Ge_xTe$ has been discussed.Section 5.3 explores the result and discussion and it contains 12 open research problems for this chapter.

5.2 Theoretical background

5.2.1 Electron energy spectrum in HD nonlinear optical materials under magneto-size quantization

The entropy of the conduction electrons in UFs of HD nonlinear optical materials in the presence of a quantizing magnetic field B can be written following (4.3a) as

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$$\frac{\hbar^2\left(\frac{\bar{n}_z\pi}{d_z}\right)^2}{2\bar{m}^*_{||}} = \bar{U}_{1,\pm}(e_{81},\bar{n},\eta_g) + \bar{U}_{2,\pm}(e_{81},\bar{n},\eta_g) \tag{5.1}$$

where e_{81} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-e_{81}) \tag{5.2}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\mathrm{Re}\,al\ Part\ of\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{5,1}) \tag{5.3}$$

where $\eta_{5,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5}-e_{81})$, $\bar{E}_{F5}$ is the Fermi energy in this case and $\bar{F}_j(\eta)$ is the one parameter Fermi-Dirac integral of order j as defined in (1.85).

Thus, using (5.3) and (1.31f), we can study the entropy in this case.

5.2.2 Entropy in QWs of HD III–V materials under magneto-size quantization

(a) Three-band model of Kane

In accordance with three-band model of Kane, DR in the present case can be written as

$$\frac{\hbar^2\left(\frac{\bar{n}_z\pi}{d_z}\right)^2}{2\bar{m}^*_{||}} = \bar{U}_{3,\pm}(e_{82},\bar{n},\eta_g) + \bar{U}_{4,\pm}(e_{82},\bar{n},\eta_g) \tag{5.4}$$

where e_{82} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-e_{82}) \tag{5.5}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\mathrm{Re}\,al\ Part\ of\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{6,1}) \tag{5.6}$$

where

$$\eta_{6,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5}-e_{82}),$$

Thus, using (5.6) and (1.31f), we can study the entropy in this case.

(b) Two band model of Kane

The electron energy spectrum in this case is given by

$$\frac{\hbar^2\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2}{2\bar{m}_c} = \gamma_2(e_{83}, \bar{n}, \eta_g) - \left(\bar{n} + \frac{1}{2}\right)\hbar\omega_0 \mp \frac{1}{2}\bar{g}^*\mu_0\bar{B} \tag{5.7}$$

where e_{83} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E} - e_{83}) \tag{5.8}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{7,1}) \tag{5.9}$$

where

$$\eta_{7,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{83}),$$

Thus, using (5.9) and (1.31f), we can study the entropy in this case.

(c) Parabolic Energy Bands

The electron energy spectrum in this case is given by

$$\frac{\hbar^2\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2}{2\bar{m}_c} = \gamma_3(e_{84}, \eta_g) - \left(\bar{n} + \frac{1}{2}\right)\hbar\omega_0 \mp \frac{1}{2}\bar{g}^*\mu_0\bar{B} \tag{5.10}$$

where e_{84} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E} - \bar{e}_{84}) \tag{5.11}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{8,1}) \tag{5.12}$$

where

$$\eta_{8,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{84}),$$

Thus, using (5.12) and (1.31f), we can study the entropy in this case.

(d) The model of Stillman et al.

The DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_7(e_{85}, \bar{n}, \eta_g) \tag{5.13}$$

where e_{85} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{85}) \tag{5.14}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{9,1}) \tag{5.15}$$

where

$$\eta_{9,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{85}),$$

Thus, using (5.15) and (1.31f), we can study the entropy in this case.

(e) The model of Palik et al.

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = A_{35,\pm}(e_{86}, \bar{n}, \eta_g) \tag{5.16}$$

where e_{86} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{86}) \tag{5.17}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{10,1}) \tag{5.18}$$

where

$$\eta_{10,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{86}),$$

Thus, using (5.18) and (1.31f), we can study the entropy in this case.

5.2.3 Entropy in HD II–VI materials under magneto-size quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{8,\pm}(e_{87}, \bar{n}, \eta_g) \tag{5.19}$$

where e_{87} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-e_{87}) \tag{5.20}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{11,1}) \tag{5.21}$$

where

$$\eta_{11,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5}-e_{87}),$$

Thus, using (5.21) and (1.31f), we can study the entropy in this case.

5.2.4 Entropy in HD IV–VI materials under magneto size-quantization

The electron energy spectrum in IV–VI materials is defined by the models of Cohen, Lax, Dimmock and Bangert, and Kastner, respectively. The magnetoentropy in HD IV–VI materials is discussed in accordance with the said model for the purpose of relative comparison.

(a) Cohen Model

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{16,\pm}(e_{88}, \bar{n}, \eta_g) \tag{5.22}$$

where e_{88} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-e_{88}) \tag{5.23}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{12,1}) \tag{5.24}$$

where

$$\eta_{12,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{88}),$$

Thus, using (5.24) and (1.31f), we can study the entropy in this case.

(b) Lax Model

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{17,\pm}(e_{89}, \bar{n}, \eta_g) \tag{5.25}$$

where e_{89} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{89}) \tag{5.26}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{13,1}) \tag{5.27}$$

where

$$\eta_{13,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{89}),$$

Thus, using (5.27) and (1.31f), we can study the entropy in this case.

(c) Dimmock Model

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{170}(e_{90}, \bar{n}, \eta_g) \tag{5.28}$$

where e_{90} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{90}) \tag{5.29}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{14,1}) \tag{5.30}$$

where

$$\eta_{14,1} = (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F5} - e_{90}),$$

Thus, using (5.30) and (1.31f), we can study the entropy in this case.

(d) Model of Bangert and Kastner

DR in the present case can be written as

$$\left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2 = \bar{U}_{18}(e_{91}, \bar{n}, \eta_g)\Big|_{e=0} \tag{5.31}$$

where e_{91} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{91}) \tag{5.32}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \mathrm{Re}\, al\ Part\ of \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{15,1}) \tag{5.33}$$

where

$$\eta_{15,1} = (\bar{k}_B \bar{T})^{-1}(\bar{E}_{F5} - e_{91}),$$

Thus, using (5.33) and (1.31f), we can study the entropy in this case.

(e) Model of Foley and Langenberg

DR in the present case can be written as

$$\left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2 = \bar{U}_{19}(e_{92}, \bar{n}, \eta_g) \tag{5.34}$$

where e_{92} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{92}) \tag{5.35}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{16,1}) \tag{5.36}$$

where

$$\eta_{16,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{92}),$$

Thus, using (5.36) and (1.31f), we can study the entropy in this case.

5.2.5 Entropy in HD stressed Kane type materials under magneto-size quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{41}(e_{93}, \bar{n}, \eta_g)\Big|_{e=0} \tag{5.37}$$

where e_{93} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{93}) \tag{5.38}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\mathrm{Re}\,al\ Part\ of \sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{17,1}) \tag{5.39}$$

where

$$\eta_{17,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{93}),$$

Thus, using (5.39) and (1.31f), we can study the entropy in this case.

5.2.6 Entropy in HD Te under magneto size-quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{42} \pm (e_{94}, \bar{n}, \eta_g) \tag{5.40}$$

where e_{94} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{94}) \tag{5.41}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{18,1}) \tag{5.42}$$

where

$$\eta_{18,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{94}),$$

Thus, using (542) and (1.31f), we can study the entropy in this case.

5.2.7 Entropy in HD gallium phosphide under magneto size quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{43}(e_{94}, \bar{n}, \eta_g) \tag{5.43}$$

where e_{94} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{94}) \tag{5.44}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{19,1}) \tag{5.45}$$

where

$$\eta_{19,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - \bar{e}_{94})$$

Thus, using (5.45) and (1.31f), we can study the entropy in this case.

5.2.8 Entropy in HD platinum antimonide under magneto size quantization

The DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{44}(e_{95}, \bar{n}, \eta_g) \tag{5.46}$$

where e_{95} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{95}) \tag{5.47}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{20,1}) \tag{5.48}$$

where

$$\eta_{20,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{95})$$

Thus, using (5.48) and (1.31f), we can study the entropy in this case.

5.2.9 Entropy in HD bismuth telluride under magneto size quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{45}(e_{96}, \bar{n}, \eta_g) \tag{5.49}$$

where e_{96} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{96}) \tag{5.50}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{21,1}) \tag{5.51}$$

where

$$\eta_{21,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{96})$$

Thus, using (5.51) and (1.31f), we can study the entropy in this case.

5.2.10 Entropy in HD germanium under magneto size quantization

(a) Model of Cardona et al.

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{46}(e_{97}, \bar{n}, \eta_g) \tag{5.52}$$

where e_{97} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-e_{97}) \tag{5.53}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{22,1}) \tag{5.54}$$

where

$$\eta_{22,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5}-e_{97})$$

Thus, using (5.54) and (1.31f), we can study the entropy in this case.

(b) Model of Wang and Ressler

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{47}(e_{98}, \bar{n}, \eta_g) \tag{5.55}$$

where e_{98} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-e_{98}) \tag{5.56}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{n=0}^{n_{\max}}\sum_{n_t=1}^{n_{z\max}}\bar{F}_{-1}(\eta_{23,1}) \tag{5.57}$$

where

$$\eta_{23,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5}-\bar{e}_{98})$$

Thus, using (5.57) and (1.31f), we can study the entropy in this case.

5.2.11 Entropy in HD gallium antimonide under magneto-size quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{48}(e_{99}, \bar{n}, \eta_g) \tag{5.58}$$

where e_{99} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{99}) \tag{5.59}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{24,1}) \tag{5.60}$$

where

$$\eta_{24,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{99})$$

Thus, using (5.60) and (1.31f), we can study the entropy in this case.

5.2.12 Entropy in HD II–V materials under magneto size quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{49\pm}(e_{100}, \bar{n}, \eta_g) \tag{5.61}$$

where e_{100} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{100}) \tag{5.62}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{25,1}) \tag{5.63}$$

where

$$\eta_{25,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{100})$$

Thus, using (5.63) and (1.31f), we can study the entropy in this case.

5.2.13 Entropy in HD lead germanium telluride under magneto size quantization

DR in the present case can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{U}_{50\pm}(e_{101}, \bar{n}, \eta_g) \tag{5.64}$$

where e_{101} is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{Bn_z} = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \delta'(\bar{E} - e_{101}) \tag{5.65}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \bar{F}_{-1}(\eta_{26,1}) \tag{5.66}$$

where

$\eta_{26,1} = (\bar{k}_B\bar{T})^{-1}(\bar{E}_{F5} - e_{101})$ Thus, using (5.66) and (1.31f), we can study the entropy in this case.

5.3 Results and discussion

Using the appropriate equations, in Figure 5.1, the normalized entropy in ultrathin films of tetragonal materials (taking HD Cd_3As_2 as an example) as a function of inverse magnetic field have been plotted in curve (a) where as the curve (b) of the same figure represents the same variation for HD $CdGeAs_2$ (an example of non-linear optical material)in accordance with the generalized band model ($\delta \neq 0$). The curve (c) is valid for III-V materials (taking InSb as an example).

The three-band energy model of Kane for InSb is valid for such highly non-parabolic material. The influence of energy band constants for the three

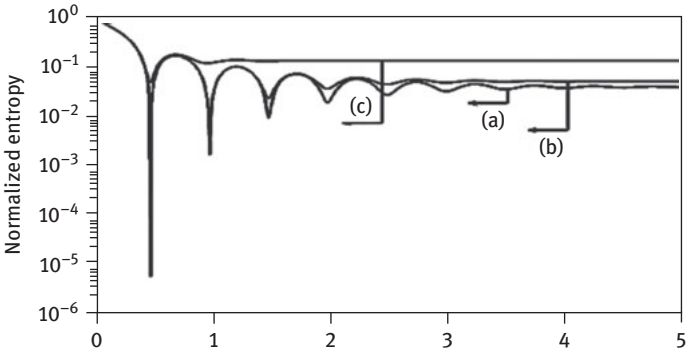

Figure 5.1: Plot of the normalized entropy as a function of inverse magnetic field for HD UFs of (a) Cd_3As_2 and (b) $CdGeAs_2$ in accordance with the generalized band model ($\delta \neq 0$). The plot (c) refers to n-InSb in accordance with the three band model of Kane ($n_0 = 10^{15} m^{-2}$ and $d_z = 10nm$).

aforementioned compounds can be estimated from the said curves. For all figure of this chapter lattice temperature has been taken as $\bar{T} = 10K$ and consequently for the purpose of simplified numerical computation we have considered only the first sub-band occupancy in connection with the quantization due to the Born–Von Karman boundary condition for various Landau levels due to the quantizing magnetic field. It appears that the thermoelectric power exhibits a periodic oscillation with increase in the magnetic field, which has also been discussed in Chapter 5.

In Figure 5.2, we have plotted the normalized entropy as a function of film thickness under constant magnetic field for all the cases of Figure 5.1. The entropy appears to exhibit composite oscillations because of the ad-mixture of size quantized levels with the Landau sub-bands. The nature of the variation of the entropy from a stair case to the highly zigzag can be explained as the combined influence of the magnetic quantization with the size quantization. As the thickness starts lowering, the influence of the field decreases due to which the stair case variation is retrieved.

The entropy as function of carrier concentration for said materials for both magnetic ($\bar{n} = 0$) and size ($\bar{n}_z = 1$) quantum limits has been plotted in Figure 5.3 from which we can conclude that the entropy decreases with carrier concentration for relatively large values where as for the relatively low values of the carrier degeneracy, the magneto thermo power shows the converging tendency. It appears from Figures 5.1 to 5.3 that HD InSb exhibits largest numerical entropy as compared to HD Cd_3As_2 and HD $CdGeAs_2$ for UFs under magnetic quantization. In Figures 5.4 to 5.6, we have plotted the entropy for ultrathin films of HD II-VI and stressed III-V materials as functions of inverse magnetic field, thickness and carrier concentration respectively. The film thickness for Figures 5.4 and 5.6 are kept to 10nm, while $\bar{B} = 2$ tesla for Figures 5.5 and 5.6 respectively.

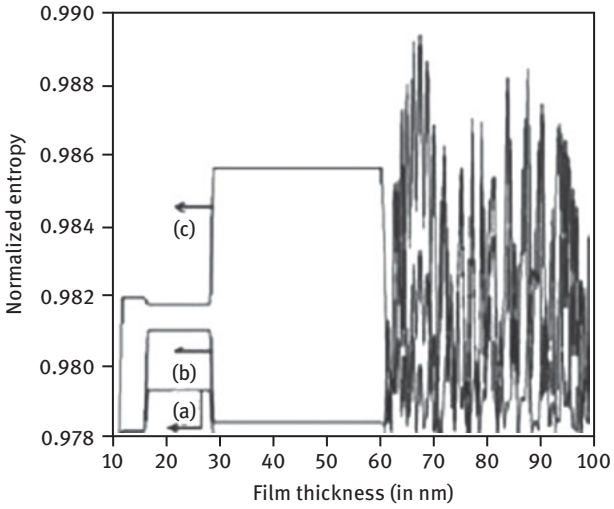

Figure 5.2: Plot of the normalized entropy as a function of film thickness for HD UFs of (a) Cd_3As_2 and (b) $CdGeAs_2$ in accordance with the generalized band model ($\delta \neq 0$). The plot (c) refers to n-InSb in accordance with the three-band model of Kane.

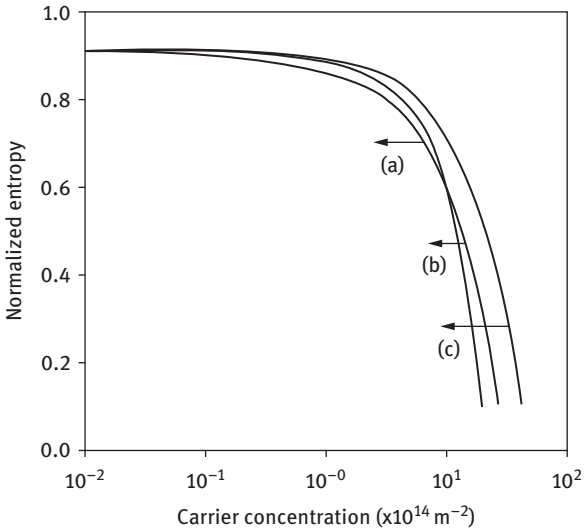

Figure 5.3: Plot of the normalized entropy as a function of carrier concentration for HD UFs of (a) Cd_3As_2 and (b) $CdGeAs_2$ in accordance with the generalized band model ($\delta \neq 0$). The plot (c) refers to n-InSb in accordance with the three-band model of Kane.

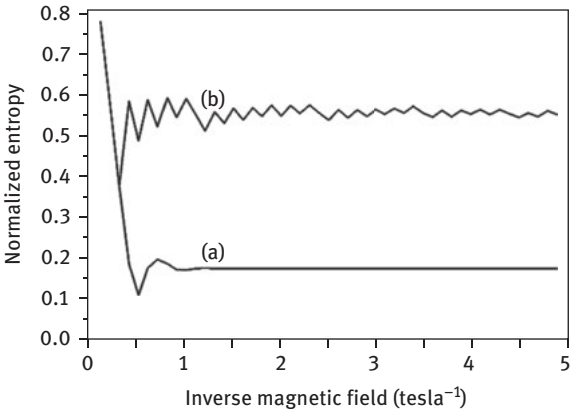

Figure 5.4: Plot of the normalized entropy as a function of inverse magnetic field for HD UFs of (a) HD CdS ($\bar{\lambda}_0 \neq 0$) and (b) stressed HD InSb.

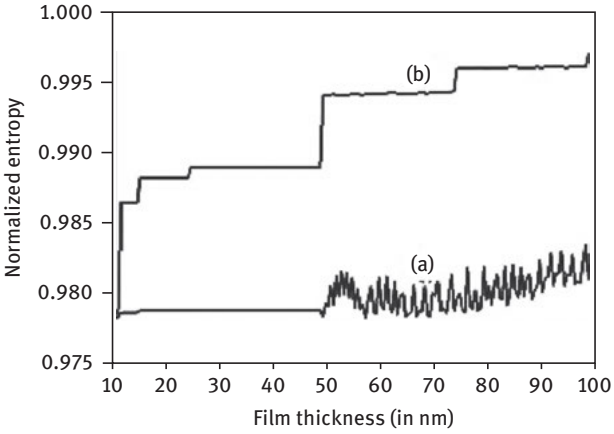

Figure 5.5: Plot of the normalized entropy as a function film thickness for HD UFs of (a) HDCdS ($\bar{\lambda}_0 \neq 0$) and (b) stressed HD InSb.

It appears form the Figures 5.4 to 5.6 that the normalized entropy for UFs of stressed HD InSb exhibits higher numerical values as compared to the corresponding UFs of HD CdS. Figure 5.7 exhibits the plots of the normalized entropy as function of inverse magnetic field for UFs of HD PbSe in accordance with the models of (a) Lax and (b) Cohen, respectively. Besides the plot (c) in the same figure is valid for HD IV–VI materials (using HD PbTe as an example) whose carrier dispersion laws follow the Cohen model. The Figures 5.8 and 5.9 demonstrate the said variations as a function of film thickness and carrier concentration respectively. It

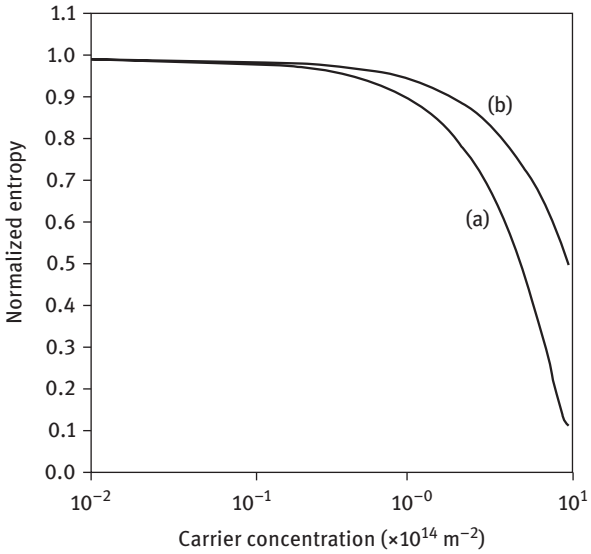

Figure 5.6: Plot of the normalized entropy as a function of carrier concentration for HD UFs of (a) HD CdS ($\bar{\lambda}_0 \neq 0$) and (b) stressed HD InSb.

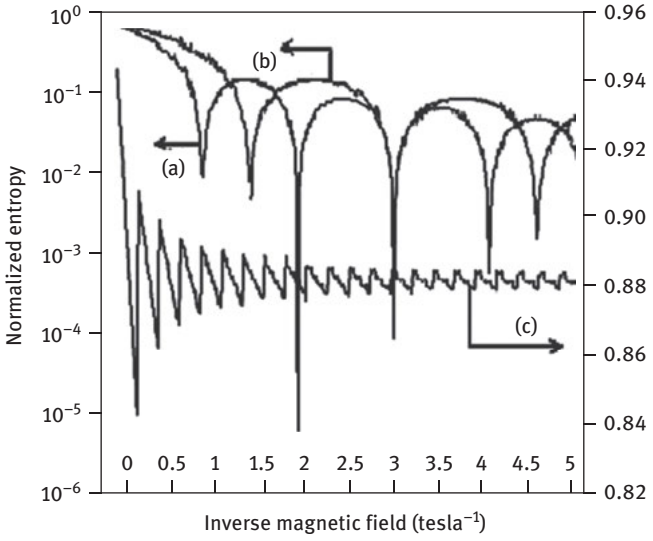

Figure 5.7: Plot of the normalized entropy as a function of inverse magnetic field for UFs of HD PbSe in accordance with the (a) Lax and (b) Cohen models. The plot (c) refers to HD PbTe following Cohen model.

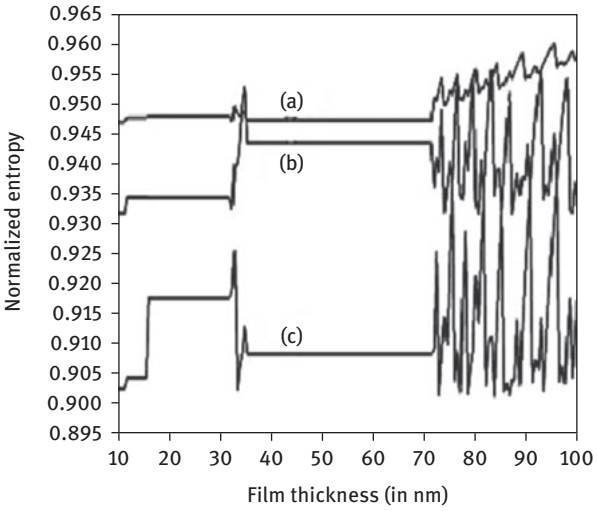

Figure 5.8: Plot of the normalized entropy as a function of film thickness for UFs of HD PbSe in accordance with the (a) Lax and (b) Cohen models. The plot (c) refers to HD DHDPbTe following Cohen model.

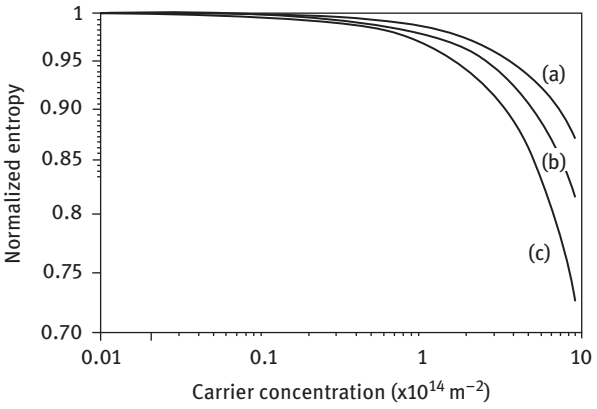

Figure 5.9: Plot of the normalized entropy as a function of carrier concentration for UFs of HD PbSe in accordance with the (a) Lax and (b) Cohen models. The plot (c) refers to HD PbTe following Cohen model.

appears that the HD PbSe exhibits higher entropy than that of HD PbTe. For the purpose of simplicity the spin effects has been neglected in the computations. The inclusion of spin increases the number of oscillatory spikes by two with the decrement in amplitudes. The use of the data in the figures as presented in this chapter can also be used to compare the entropy for other types of materials.

5.4 Open research problems

(R5.1) Investigate the entropy in the presence of arbitrarily oriented quantizing magnetic field in the presence of electron spin and broadening by considering all types of scattering mechanisms for UFs by considering the presence of finite, parabolic and circular potential wells applied separately for all the HD materials whose unperturbed carrier energy spectra are defined in Chapter 1.

(R5.2) Investigate (R5.1) in the presence of an additional arbitrarily oriented (a) non-uniform electric field and (b) alternating electric field respectively for all the HD materials whose unperturbed carrier energy spectra are defined in this Chapter 1 by considering all types of scattering mechanisms.

(R5.3) Investigate the entropy in the presence of arbitrarily oriented alternating quantizing magnetic field in the presence of electron spin and broadening by considering all types of scattering mechanisms for HD UFs by incorporating the presence of finite, parabolic and circular potential wells applied separately for all the HD materials whose unperturbed carrier energy spectra are defined in Chapter 1.

(R5.4) Investigate the entropy under an arbitrarily-oriented alternating quantizing magnetic field and crossed alternating electric field by including broadening and the electron spin for HD UFs of all the materials whose unperturbed carrier energy spectra are defined in Chapter 1 by considering all types of scattering mechanisms.

(R5.5) Investigate the entropy under an arbitrarily-oriented alternating quantizing magnetic field and crossed alternating nonuniform electric field by including broadening and the electron spin whose for HD UFs of all the materials unperturbed carrier energy spectra are defined in Chapter 1 by considering all types of scattering mechanisms.

(R5.6) Investigate the entropy in the presence of a quantizing magnetic field under exponential, Kane, Halperin, Lax, and Bonch-Bruevich band tails [1] for HD UFs of all the materials whose unperturbed carrier energy spectra are defined in Chapter 1 by considering all types of scattering mechanisms.

(R5.7) Investigate the entropy in the presence of quantizing magnetic field for HD UFs of all the materials as defined in (R5.6) under an arbitrarily oriented (a) non-uniform electric field and (b) alternating electric field, respectively, by considering all types of scattering mechanisms.

(R5.8) Investigate the entropy for the HD UFs of all the materials as described in (R5.6) under an arbitrarily-oriented alternating quantizing magnetic field by including broadening and the electron spin by considering all types of scattering mechanisms.

(R5.9) Investigate the entropy for HD UFs of all the materials as discussed in (R5.6) under an arbitrarily-oriented alternating quantizing magnetic field

and crossed alternating electric field by including broadening and the electron spin by considering all types of scattering mechanisms.

(R5.10) Investigate all the appropriate problems after proper modifications introducing new theoretical formalisms for all types of HD UFs of all the materials as discussed in (R5.6) for functional, negative refractive index, macro molecular, organic, and magnetic materials by considering all types of scattering mechanisms in the presence of strain.

(R5.11) Investigate all the appropriate problems of this chapter for all types of HD UFs for p-InSb, p-CuCl and materials having diamond structure valence bands whose dispersion relations of the carriers in bulk materials are given by Cunningham [2], Yekimov et al. [3], and Roman et al. [4], respectively by considering all types of scattering mechanisms in the presence of strain.

(R5.12) Investigate the influence of deep traps and surface states separately for all the appropriate problems of all the chapters after proper modifications by considering all types of scattering mechanisms.

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Part II: **Entropy in heavily doped quantum confined superlattices**

Every accomplishment starts with the decision to try.

6 Entropy in quantum wires of heavily doped superlattices

The great aim of education is not knowledge but tremendous action in the positive direction.

6.1 Introduction

In recent years, modern fabrication techniques have generated altogether a new dimension in the arena of quantum effect devices through the experimental realization of an important artificial structure known as semiconductor superlattice (SL) by growing two similar but different semiconducting compounds in alternate layers with finite thicknesses [1]. The materials forming the alternate layers have the same kind of band structure but different energy gaps. The concept of SL was developed for the first time by Keldysh [2] and was successfully fabricated by Esaki and Tsu [2]. SLs are being extensively used in thermal sensors [3], quantum cascade lasers [4], photodetectors [5], light emitting diodes [6], multiplication [7], frequency multiplication [8], photocathodes [9], thin film transistor [10], solar cells [11], infrared imaging [12], thermal imaging [13], infrared sensing [14], and also in other microelectronic devices.

The most extensively studied III-V SL is the one consisting of alternate layers of GaAs and $Ga_{1-x}Al_xAs$ owing to the relative easiness of fabrication. The GaAs and $Ga_{1-\ x}Al_xAs$ layers form the quantum wells and the potential barriers, respectively. The III–V SLs are attractive for the realization of high-speed electronic and optoelectronic devices [15]. In addition to SLs with usual structure, other types of SLs such as II–VI [16], IV–VI [17], and HgTe/CdTe [18], SLs have also been investigated in the literature. The IV–VI SLs exhibit quite different properties as compared to the III–V SL due to the specific band structure of the constituent materials [19]. The epitaxial growth of II-VI SL is a relatively recent development and the primary motivation for studying the mentioned SLs made of materials with the large band gap is in their potential for optoelectronic operation in the blue [19]. HgTe/CdTe SLs have raised a great deal of attention since 1979, when as a promising new materials for long wavelength infrared detectors and other electro-optical applications [20]. Interest in Hg-based SLs has been further increased as new properties with potential device applications were revealed [20, 21]. These features arise from the unique zero band-gap material HgTe [22] and the direct band-gap semiconductor CdTe, which can be described by the three-band mode of Kane [23]. The combination of the aforementioned materials with specified dispersion relation makes HgTe/CdTe SL very attractive, especially because of the tailoring of the material properties for various applications by varying the energy band constants of the SLs.

We note that all the aforementioned SLs have been proposed with the assumption that the interfaces between the layers are sharply defined, of zero thickness, that is,

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devoid of any interface effects. The SL potential distribution may be then considered as a one-dimensional array of rectangular potential wells. The aforementioned advanced experimental techniques may produce SLs with physical interfaces between the two materials crystallographically abrupt; adjoining their interface will change at least on an atomic scale. As the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the electrons [24]. The influence of finite thickness of the interfaces on the electron dispersion law is very important, since the electron energy spectrum governs the electron transport in SLs. In addition to it, for effective mass SLs, the electronic subbands appear continually in real space [25].

In this chapter, the entropy in III–V, II–VI, IV–VI, HgTe/CdTe, and strained-layer quantum wire heavily doped SLs (QWHDSLs) with graded interfaces has been studied in Sections 6.2.1 to 6.2.5. From Sections 6.2.6 to 6.2.10, the entropy in III–V, II–VI, IV–VI, HgTe/CdTe, and strained-layer quantum wire HD effective mass SLs,respectively, has been presented. Section 6.3 contains the Results and Discussion pertinent to this chapter. Section 6.4 presents single open research problem.

6.2 Theoretical background

6.2.1 Entropy in III–V quantum wire HD SLs with graded interfaces

The electron dispersion law in bulk specimens of the HD constituent materials of III–V SLs whose undoped energy band structures are defined by three-band model of Kane can be expressed as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}^*_{cj}} = \bar{T}_{1j}(\bar{E},\Delta_j,\bar{E}_{gj},\eta_{gj}) + i\bar{T}_{2j}(\bar{E},\Delta_j,\bar{E}_{gj},\eta_{gj}) \tag{6.1}$$

where

$$\bar{j} = 1,2,\ \bar{T}_{1j}(\bar{E},\Delta_j,\bar{E}_{gj},\eta_{gj}) = (2/(1-Erf(\bar{E}/\eta_{gj}))[(\bar{a}_j\bar{b}_j/\bar{c}_j).\theta_0(\bar{E}/\eta_{gj}) + [(\bar{a}_j\bar{c}_j + \bar{b}_j\bar{c}_{j_j} - \bar{a}_j\bar{b}_j)/\bar{c}^2{}_j$$

$$\gamma_0(\bar{E}/\eta_{gj}) + [1/\bar{c}_j)(1-(\bar{a}_j/\bar{c}_j))(1-(\bar{b}_j/\bar{c}_j))\frac{1}{2}[1+Erf(\bar{E}/\eta_{gj})] - (1/\bar{c}_j)(1-(\bar{a}_j/\bar{c}_j))$$

$$(1-(\bar{b}_j/\bar{c}_j))(2/(\bar{c}_j\eta_{gj}\sqrt{\pi})\exp(-\bar{u}_j^2)\left[\sum_{\bar{p}=1}^{\infty}(\exp(-\bar{p}^2/4)/\bar{p})\sinh(\bar{p}\bar{u}_j)\right],$$

$$\bar{b}_j \equiv (\bar{E}_{gj}+\Delta_j)^{-1}, \bar{c}_j \equiv \left(\bar{E}_{gj}+\frac{2}{3}\Delta_j\right)^{-1}, \bar{u}_j \equiv \frac{1+\bar{c}_j\bar{E}}{\bar{c}_j\eta_{gj}}$$

and

$$\bar{T}_{2j}(\bar{E},\Delta_j,\bar{E}_{gj},\eta_{gj}) \equiv \left(\frac{2}{1+Erf(\bar{E}/\eta_{gj})}\right)\frac{1}{\bar{c}_j}\left(1-\frac{\bar{\alpha}_j}{\bar{c}_j}\right)\left(1-\frac{\bar{b}_j}{\bar{c}_j}\right)\frac{\sqrt{\pi}}{\bar{c}_j\eta_{gj}}\exp\left(-\bar{u}_j^2\right)$$

Therefore, the dispersion law of the electrons of HD quantum well III–V SLs with graded interfacescan be expressed as [25]

$$\bar{k}_z^2 = \bar{G}_8 + i\bar{H}_8 \tag{6.2}$$

$$\bar{G}_8 = \left[\frac{\bar{C}_7^2 - D_7^2}{\bar{L}_0^2} - \bar{k}_s^2\right], \bar{C}_7 = \cos^{-1}(\omega_7), \omega_7 = (2)^{\frac{-1}{2}}\left[(1-\bar{G}_7^2-\bar{H}_7^2) - \sqrt{(1-\bar{G}_7^2-\bar{H}_7^2)^2+4\bar{G}_7^2}\right]^{\frac{1}{2}}$$

$$\bar{a}_{20} = \left[\sqrt{\frac{\bar{M}_{s2}(0,\eta_{g2})}{\bar{M}_{s1}(0,\eta_{g1})}+1}\right]^2\left[4\left(\frac{\bar{M}_{s2}(0,\eta_{g2})}{\bar{M}_{s1}(0,\eta_{g1})}\right)^{\frac{1}{2}}\right]^{-1}, \bar{a}_{21}$$

$$= \left[\sqrt{\frac{\bar{M}_{s2}(0,\eta_{g2})}{\bar{M}_{s1}(0,\eta_{g1})}-1}\right]^2\left[4\left(\frac{\bar{M}_{s2}(0,\eta_{g2})}{\bar{M}_{s1}(0,\eta_{g1})}\right)^{\frac{1}{2}}\right]^{-1}$$

$$\bar{C}_{40}\left(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g1}\right) = \left[1-\bar{P}_1\left(\bar{E},\eta_{g1}\right)\bar{k}_x^2 - \bar{Q}_2\left(\bar{E},\eta_{g1}\right)\bar{k}_y^2\right]^{1/2}\left[\bar{S}_1\left(\bar{E},\eta_{g1}\right)\right]^{-1/2}$$

$$\bar{D}_{40}\left(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g1}\right) = \left[1-\bar{P}_2\left(\bar{E},\eta_{g2}\right)\bar{k}_x^2 - \bar{Q}_2\left(\bar{E},\eta_{g2}\right)\bar{k}_y^2\right]^{1/2}\left[\bar{S}_1\left(\bar{E},\eta_{g2}\right)\right]^{-1/2}$$

$$\begin{aligned}\bar{G}_7 = {} & \left[\bar{G}_1 + \left(\rho_5\bar{G}_2/2\right) - \left(\rho_6\bar{H}_2/2\right) + (\Delta_0/2)\{\rho_6\bar{H}_2 - \rho_8\bar{H}_3 + \rho_9\bar{H}_4 - \rho_{10}\bar{H}_4\right. \\ & \left. + \rho_{11}\bar{H}_5 - \rho_{12}\bar{H}_5 + (1/12)\left(\rho_{12}\bar{G}_6 - \rho_{14}\bar{H}_6\right)\right], \bar{G}_1 \\ = {} & \left[\left(\cos(\bar{h}_1)\right)\left(\cos\left(\bar{h}_2\right)\right)\left(\cos\left(\bar{g}_1\right)\right)\left(\cos\left(\bar{g}_2\right)\right)\right. \\ & \left. + (\sin(\bar{h}_1))\left(\sin\left(\bar{h}_2\right)\right)(\sin(\bar{g}_1))(\sin(\bar{g}_2))\right],\end{aligned}$$

$$\bar{h}_1 = e_1(\bar{b}_0 - \Delta_0), e_1 2^{\frac{-1}{2}}\left(\sqrt{\bar{t}_1^2+\bar{t}_1^2}+\bar{t}_1\right)^{\frac{1}{2}},$$

$$\bar{t}_1 = [(2\bar{m}_{c1}^*/\hbar^2).\bar{T}_{11}(\bar{E},\bar{E}_{g1},\Delta_1,\eta_{g1}) - \bar{k}_s^2], \bar{t}_2 = [(2\bar{m}_{c1}^*/\hbar^2)T_{21}(\bar{E},\bar{E}_{g1},\Delta_1,\eta_{g1})]$$

$$\bar{h}_2 = e_2(\bar{b}_0 - \Delta_0), e_2 = 2^{\frac{-1}{2}}\left(\sqrt{\bar{t}_1^2+\bar{t}_1^2}-\bar{t}_1\right)^{\frac{1}{2}}, \bar{g}_1 = \bar{d}_1(\bar{a}_0 - \Delta_0), \bar{d}_1 = 2^{\frac{-1}{2}}\left(\sqrt{\bar{x}_1^2+\bar{y}_1^2}+\bar{x}_1\right)^{\frac{1}{2}},$$

$$\bar{x}_1 = [-(2\bar{m}_{c2}^*/\hbar^2).\bar{T}_{11}(\bar{E}-\bar{V}_0,\bar{E}_{g2},\Delta_2,\eta_{g2}) + \bar{k}_s^2], \bar{y}_1 = [(2\bar{m}_{c2}^*/\hbar^2)\bar{T}_{22}(\bar{E}-\bar{V}_0,\bar{E}_{g2},\Delta_2,\eta_{g2})]$$

$$\bar{g}_2 = \bar{d}_2(\bar{a}_0 - \Delta_0), \bar{d}_2 = 2^{\frac{-1}{2}}\left(\sqrt{\bar{x}_1^2+\bar{y}_1^2}-\bar{x}_1\right)^{\frac{1}{2}}, \rho_5 = (\rho_3^2+\rho_4^2)^{-1}[\rho_1\rho_3 - \rho_2\rho_4],$$

$$\rho_1 = [\bar{d}_1^2 + e_2^2 - \bar{d}_2^2 - e_1^2], \rho_3 = [\bar{d}_1 e_1 + \bar{d}_2 e_2], \rho_2 = 2[\bar{d}_1 \bar{d}_2 + e_1 e_2], \rho_4 = [\bar{d}_1 e_2 - e_1 \bar{d}_2],$$

$$\bar{G}_2 = [(\sin(\bar{h}_1))(\cos h(\bar{h}_2))(\sinh(\bar{g}_1))(\cos(\bar{g}_2)) + (\cos(\bar{h}_1))(\sinh(\bar{h}_2))(\cosh(\bar{g}_1))(\sin(\bar{g}_2))]$$

$$\rho_6 = (\rho_3^2 + \rho_4^2)^{-1}[\rho_1\rho_4 - \rho_2\rho_3],$$

$$\bar{H}_2 = [(\sin(\bar{h}_1))(\cosh(\bar{h}_2))(\sin(\bar{g}_2)(\cosh(\bar{g}_1)) - (\cos(\bar{h}_1))(\sinh(\bar{h}_2))(\sin(\bar{g}_1))(\cos(\bar{g}_2))]$$

$$\rho_7 = [(e_1^2 + e_2^2)^{-1}[e_1(\bar{d}_1^2 - \bar{d}_2^2) - 2\bar{d}_1\bar{d}_2 e_2] - 3e_1],$$

$$\bar{G}_3 = [(\sin(\bar{h}_1))(\cosh(\bar{h}_2))(\cosh(\bar{g}_1))(\cos(\bar{g}_2)) + (\cos(\bar{h}_1))(\sinh(\bar{h}_2))(\sin(\bar{g}_1))(\sin(\bar{g}_2)]$$

$$\rho_8 = [(e_1^2 + e_2^2)^{-1}[e_2(\bar{d}_1^2 - \bar{d}_2^2) + 2d_1 d_2 e_1] + 3e_2],$$

$$\bar{H}_3 = [(\sin(\bar{h}_1))(\cos\bar{h}(\bar{h}_2))(\sin(\bar{g}_2))(\sinh(\bar{g}_1)) - (\cos(\bar{h}_1))(\bar{s}\bar{i}\bar{n}\bar{h}(\bar{h}_2))(\cosh(\bar{g}_1))(\cos(\bar{g}_2))]$$

$$\rho_9 = [(\bar{d}_1^2 + \bar{d}_2^2)^{-1}[\bar{d}_2(e_2^2 - e_1^2) + 2e_2\bar{d}_2 e_1] + 3\bar{d}_1],$$

$$\bar{G}_4 = [(\cos(\bar{h}_1))(\cosh(\bar{h}_2))(\cos(\bar{g}_2))(\sinh(\bar{g}_1)) - (\sin(\bar{h}_1))(\sinh(\bar{h}_2))(\cosh(\bar{g}_1))(\sin(\bar{g}_2))]$$

$$\rho_{10} = [-(\bar{d}_1^2 + \bar{d}_2^2)^{-1}[\bar{d}_2(-e_2^2 + e_1^2) + 2e_2\bar{d}_2 e_1] + 3\bar{d}_2],$$

$$\bar{H}_4 = [(\cos(\bar{h}_1))(\cosh(\bar{h}_2))(\cosh(\bar{g}_1))(\sin(\bar{g}_2)) + (\sin(\bar{h}_1))(\sinh(\bar{h}_2))(\sinh(\bar{g}_1))(\cos(\bar{g}_2))]$$

$$\rho_{11} = 2[\bar{d}_1^2 + e_2^2 - \bar{d}_2^2 - e_1^2],$$

$$\bar{G}_5 = [(\cos(\bar{h}_1))(\cosh(\bar{h}_2))(\cos(\bar{g}_2))(\cosh(\bar{g}_1)) - (\sin(\bar{h}_1))(\sinh(\bar{h}_2))(\sinh(\bar{g}_1))(\sin(\bar{g}_2))]$$

$$\rho_{12} = 4[\bar{d}_1\bar{d}_2 + e_1 e_2],$$

$$\bar{H}_5 = [(\cos(\bar{h}_1))(\cosh(\bar{h}_2))(\sinh(\bar{g}_1))(\sin(\bar{g}_2)) + (\sin(\bar{h}_1))(\sinh(\bar{h}_2))(\cosh(\bar{g}_1))(\cos(\bar{g}_2))]$$

$$\rho_{13} = [\{5(\bar{d}_1 e_1^3 - 3\bar{e}_1\bar{e}_2^2\bar{d}_1) + 5\bar{d}_2(e_1^3 - 3e_1^2 e_2)\}(\bar{d}_1^2 + \bar{d}_2^2)^{-1} + (e_1^2 + e_2^2)^{-1}\{5(e_1\bar{d}_1^3 - 3\bar{d}_2 e_1^2\bar{d}_1) + 5(\bar{d}_2^3 e_2 - 3\bar{d}_1^2\bar{d}_2 e_2)\} - 34(\bar{d}_1\bar{e}_1 + \bar{d}_2\bar{e}_2)]$$

$$\bar{G}_6 = [(\sin(\bar{h}_1))(\cosh(\bar{h}_2))(\sinh(\bar{g}_1))(cos(\bar{g}_2)) + (cos(\bar{h}_1))(\sinh(h_2))(\cosh(\bar{g}_1))(\sin(\bar{g}_2))],$$

$$\rho_{14} = [\{5(\bar{d}_1\bar{e}_2^3 - 3\bar{e}_2\bar{e}_1^2\bar{d}_1) + 5\bar{d}_2(-e_1^3 + 3e_2^2 e_1)\}(\bar{d}_1^2 + \bar{d}_2^2)^{-1} + (e_1^2 + e_2^2)^{-1}(5(-e_1\bar{d}_2^3 + 3\bar{d}_1^2\bar{d}_2 e_1) + 5(-\bar{d}_1^3 e_2 + 3\bar{d}_2^2\bar{d}_1 e_2)) + 34(\bar{d}_1 e_2 - \bar{d}_2 e_1)],$$

$$\bar{H}_6 = [(\sin(\bar{h}_1))(\cosh(\bar{h}_2))(\cosh(\bar{g}_1))(sin(\bar{g}_2))$$
$$-(cos(\bar{h}_1))(\sinh(\bar{h}_2))(sinh(\bar{g}_1))(\cos(\bar{g}_2))],$$
$$\bar{H}_7 = [\bar{H}_1 + (\rho_5\bar{H}_2/2) + (\rho_6\bar{G}_2/2)$$
$$+(\Delta_0/2)\{\rho_8\bar{G}_3 + \rho_7\bar{H}_3 + \rho_{10}\bar{G}_4 + \rho_9\bar{H}_4 + \rho_{12}\bar{G}_5 + \rho_{11}\bar{H}_5 + (1/12)(\rho_{14}\bar{G}_6 + \rho_{14}\bar{H}_6)\}],$$
$$\bar{H}_1 = [(\sin(\bar{h}_1))(\sinh(\bar{h}_2))(\cosh(\bar{g}_1))(\cos(\bar{g}_2))$$
$$+(cos(\bar{h}_1))(\cosh(\bar{h}_2))(sinh(\bar{g}_1))(sin(\bar{g}_2))],$$
$$\bar{D}_7 = \sinh^{-1}(\bar{\omega}_7), \bar{H}_8 = (2\bar{C}_7\bar{D}_7/\bar{L}_0^2)$$

The simplified DR of HD quantum wire III–V SLs with graded interfaces can be expressed as

$$\bar{k}_z^2 = [\bar{G}_8 + i\bar{H}_8]|_{\bar{k}_x = \frac{\bar{n}_x\pi}{d_x}\, and\, \bar{k}_y = \frac{\bar{n}_y\pi}{d_y}} \tag{6.3a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\frac{\bar{H}(\bar{E}-\bar{E}_{13,1})\left[\overline{G'}_8 + i\overline{H'}_8\right]}{\sqrt{\bar{G}_8 + i\bar{H}_8}} \tag{6.3b}$$

where $\bar{E}_{13,1}$ is the sub band energy and the sub-band equation in this case can be expressed as

$$0 = [\bar{G}_8 + i\bar{H}_8]|_{\bar{k}_x = \frac{\bar{n}_x\pi}{d_x}\, and\, \bar{k}_y = \frac{\bar{n}_y\pi}{d_y}\, and\, \bar{E}-\bar{E}_{13,1}} \tag{6.3c}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\overline{G'} \tag{6.4}$$

The electron concentration can be written as

$$\bar{n}_{1D} = Real\, part\, of \sum_{\bar{n}=0}^{\bar{n}_{\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\tau_6 + \tau_7] \tag{6.5}$$

where

$$\tau_6 = \left[[\bar{G}_8 + i\bar{H}_8]|_{\bar{k}_z = \frac{\pi\bar{n}_z}{d_z},\ \bar{k}_y = \frac{\pi\bar{n}_y}{d_y}, \bar{E} = \bar{E}_{F61}}\right]^{1/2},$$

$$\tau_7 = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\tau_6]$$

and $\bar{E}_{F61}$ is the Fermi energy in this case

Using (1.31f) and (6.5), we can study the entropy in this case.

6.2.2 Entropy in II–VI quantum wire HD SLs with graded interfaces

The electron energy spectra of the HD constituent materials of II–VI SLs are given by

$$\gamma_3(\bar{E}, \eta_{g1}) = \frac{\hbar^2 \bar{k}_s^2}{2\bar{m}^*_{\perp,1}} + \frac{\hbar^2 \bar{k}_z^2}{2\bar{m}^*_{||,1}} \pm \bar{C}_0 \bar{k}_s \tag{6.6}$$

and

$$\frac{\hbar^2 \bar{k}^2}{2\bar{m}^*_{c2}} = \bar{T}_{12}(\bar{E}, \Delta_2, \bar{E}_{g2}\eta_{g2}) + i\bar{T}_{22}(\bar{E}, \Delta_2, \bar{E}_{g2}, \eta_{g2}) \tag{6.7}$$

where $\bar{m}^*_{\perp,1}$ and $\bar{m}^*_{||,1}$ are the transverse and longitudinal effective electron masses, respectively, at the edge of the conduction band for the first material. The energy-wave vector dispersion relation of the conduction electrons in HD quantum well II–VI SLs with graded interfaces can be expressed as

$$\bar{k}_z^2 = \bar{G}_{19} + i\bar{H}_{19} \tag{6.8}$$

where

$$\bar{G}_{19} = \left[\frac{\bar{C}_{18}^2 - \bar{D}_{18}^2}{\bar{L}_0^2} - \bar{k}_s^2\right],$$

$$\bar{C}_{18} = \cos^{-1}(\omega_{18}), \omega_{18} = (2)^{\frac{-1}{2}}[(1 - \bar{G}_{18}^2 - \bar{H}_{18}^2) - \sqrt{(1 - \bar{G}_{18}^2 - \bar{H}_{18}^2)^2 + 4\bar{G}_{18}^2}]^{\frac{1}{2}}$$

$$\bar{G}_{18} = \frac{1}{2}[\bar{G}_{11} + \bar{G}_{12} + \Delta_0(\bar{G}_{13} + \bar{G}_{14}) + \Delta_0(\bar{G}_{15} + \bar{G}_{16})], \bar{G}_{11} = 2(\cos(\bar{g}_1))(\cos(\bar{g}_2))(\cos\gamma_{11}(\bar{E}, \bar{k}_s))$$

$$\gamma_{11}(\bar{E}, \bar{k}_s) = \bar{k}_{21}(\bar{E}, \bar{k}_s)(b_0 - \Delta_0), \bar{k}_{21}(\bar{E}, \bar{k}_s) = \left\{\left[\gamma_3(\bar{E}, \eta_{g1}) - \frac{\hbar^2 \bar{k}_s^2}{2\bar{m}^*_{\perp,1}} \pm \bar{C}_0 \bar{k}_s\right] \frac{2\bar{m}^*_{||,1}}{\hbar^2}\right\}^{\frac{1}{2}}$$

$$\bar{C}_{18} = \cos^{-1}(\omega_{18}), \omega_{18} = (2)^{\frac{-1}{2}}[(1 - \bar{G}_{18}^2 - \bar{H}_{18}^2) - \sqrt{(1 - \bar{G}_{18}^2 - \bar{H}_{18}^2)^2 + 4\bar{G}_{18}^2}]^{\frac{1}{2}}$$

$$\bar{G}_{18} = \frac{1}{2}[\bar{G}_{11} + \bar{G}_{12} + \Delta_0(\bar{G}_{13} + \bar{G}_{14}) + \Delta_0(\bar{G}_{15} + \bar{G}_{16})], \bar{G}_{11} = 2(\cos(\bar{g}_1))(\cos(\bar{g}_2))(\cos\gamma_{11}(\bar{E}, \bar{k}_s))$$

$$\gamma_{11}(\bar{E},\bar{k}_s)=\bar{k}_{21}(\bar{E},\bar{k}_s)(\bar{b}_0-\Delta_0),\bar{k}_{21}(\bar{E},\bar{k}_s)=\left\{[\gamma_3(\bar{E},\eta_{g1})-\frac{\hbar^2\bar{k}_s^2}{2\bar{m}^*_{\perp,1}}\pm\bar{C}_0\bar{k}_s]\frac{2\bar{m}^*_{||,1}}{\hbar^2}\right\}^{\frac{1}{2}}$$

$$\bar{G}_{12}([\Omega_1(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\cos\bar{g}_2)-\Omega_2(\bar{E},\bar{k}_s)(\sin\bar{g}_2)(\cosh\bar{g}_1)](\sin\gamma_{11}(\bar{E},\bar{k}_s)))$$

$$\Omega_1(\bar{E},\bar{k}_s)=\left[\frac{\bar{d}_1}{\bar{k}_{21}(\bar{E},\bar{k}_s)}-\frac{\bar{k}_{21}(\bar{E},\bar{k}_s)\bar{d}_1}{\bar{d}_1^2+\bar{d}_2^2}\right]\ and\ \Omega_2(\bar{E},\bar{k}_s)=\left[\frac{\bar{d}_2}{\bar{k}_{21}(\bar{E},\bar{k}_s)}-\frac{\bar{k}_{21}(\bar{E},\bar{k}_s)\bar{d}_2}{\bar{d}_1^2+\bar{d}_2^2}\right]$$

$$\bar{G}_{13}([\Omega_3(\bar{E},\bar{k}_s)(\cosh\bar{g}_1)(\cos\bar{g}_2)-\Omega_4(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\sin\bar{g}_2)](\sin\gamma_{11}(\bar{E},\bar{k}_s)))$$

$$\Omega_3(\bar{E},\bar{k}_s)=\left[\frac{\bar{d}_1^2-\bar{d}_2^2}{\bar{k}_{21}(\bar{E},\bar{k}_s)}-3\bar{k}_{21}(\bar{E},\bar{k}_s)\right],\Omega_4(\bar{E},\bar{k}_s)=\left[\frac{2\bar{d}_1-\bar{d}_2}{\bar{k}_{21}(\bar{E},\bar{k}_s)}\right],$$

$$\bar{G}_{14}(\left[\Omega_5(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\cos\bar{g}_2)-\Omega_6(\bar{E},\bar{k}_s)(\sin\bar{g}_1)(\cosh\bar{g}_2)\right](\cos\gamma_{11}(\bar{E},\bar{k}_s)))$$

$$\Omega_5(\bar{E},\bar{k}_s)=\left[3\bar{d}_1-\frac{\bar{d}_1}{\bar{d}_1^2+\bar{d}_2^2}\bar{k}_{21}(\bar{E},\bar{k}_s)\right],\Omega_6(\bar{E},\bar{k}_s)=\left[3\bar{d}_2-\frac{\bar{d}_2}{\bar{d}_1^2+\bar{d}_2^2}\bar{k}_{21}(\bar{E},\bar{k}_s)\right]$$

$$\bar{G}_{15}(\left[\Omega_9(\bar{E},\bar{k}_s)(\cosh\bar{g}_1)(\cos\bar{g}_2)-\Omega_{10}(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\sin\bar{g}_2)\right](\cos\gamma_{11}(\bar{E},\bar{k}_s)))$$

$$\Omega_9(\bar{E},\bar{k}_s)=\left[2\bar{d}_1^2-2\bar{d}_2^2\bar{k}_{21}^2(\bar{E},\bar{k}_s)\right],\Omega_{10}(\bar{E},\bar{k}_s)=\left[2\bar{d}_1\bar{d}_2\right]$$

$$\bar{G}_{16}(\left[\Omega_7(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\cos\bar{g}_2)-\Omega_8(\bar{E},\bar{k}_s)(\sin\bar{g}_1)(\cosh\bar{g}_2)\right](\sin\gamma_{11}(\bar{E},\bar{k}_s)/12))$$

$$\Omega_7(\bar{E},\bar{k}_s)=\left[\frac{5d_2}{\bar{d}_1^2+\bar{d}_2^2}\bar{k}_{21}^3(\bar{E},\bar{k}_s)+\frac{5(\bar{d}_1^3-3\bar{d}_2^2\bar{d}_1)}{k_{21}(\bar{E},\bar{k}_s)}-34\bar{k}_{21}(\bar{E},\bar{k}_s)d_1\right],$$

$$\Omega_8(\bar{E},\bar{k}_s)=\left[\frac{5d_2}{\bar{d}_1^2+\bar{d}_2^2}\bar{k}_{21}^3(\bar{E},\bar{k}_s)+\frac{5(\bar{d}_1^3-3\bar{d}_2^2\bar{d}_2)}{k_{21}(\bar{E},\bar{k}_s)}+34\bar{k}_{21}(\bar{E},\bar{k}_s)\bar{d}_2\right],$$

$$\bar{H}_{18}=\frac{1}{2}[\bar{H}_{11}+\bar{H}_{12}+\Delta_0(\bar{H}_{13}+\bar{H}_{14})+\Delta_0(\bar{H}_{15}+\bar{H}_{16})],$$

$$\bar{H}_{12}=([\Omega_2(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\cos\bar{g}_2)+\Omega_1(\bar{E},\bar{k}_s)(\sin\bar{g}_2)(\cosh\bar{g}_1)](\sin\gamma_{11}(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{13}=([\Omega_4(\bar{E},\bar{k}_s)(cosh\bar{g}_1)(\cos\bar{g}_2)+\Omega_3(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\sin\bar{g}_2)](\sin\gamma_{11}(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{14}=([\Omega_6(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\cos\bar{g}_2)+\Omega_5(\bar{E},\bar{k}_s)(\sin\bar{g}_1)(\cosh\bar{g}_2)](\sin\gamma_{11}(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{15}=([\Omega_{10}(\bar{E},\bar{k}_s)(cosh\bar{g}_1)(\cos\bar{g}_2)+\Omega_9(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\sin\bar{g}_2)](\cos\gamma_{11}(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{16}=([\Omega_8(\bar{E},\bar{k}_s)(\sinh\bar{g}_1)(\cos\bar{g}_2)+\Omega_7(\bar{E},\bar{k}_s)(\sin\bar{g}_1)(\cosh\bar{g}_2)](\sin\gamma_{11}(\bar{E},\bar{k}_s)/12)),$$

$$\bar{H}_{19} = \left[\frac{2\bar{C}_{18}\bar{D}_{18}}{\bar{L}_0^2}\right] \text{ and } \bar{\mathrm{D}}_{18} = \sin^{-1}(\omega_{18})$$

The simplified DR of HD quantum wire III–V SLs with graded interfaces can be expressed as

$$\bar{k}_z^2 = [\bar{G}_{19} + \bar{i}\bar{H}_{19}]\Big|_{k_X = \frac{n_X\pi}{d_x} \text{ and } k_y = \frac{n_y\pi}{d_y}} \tag{6.9a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{g_v}{\pi}\sum_{n_x=1}^{n_{x\max}}\sum_{n_y=1}^{n_{y\max}}\frac{\bar{H}(\bar{E}-\bar{E}_{13,2})[\bar{G}'_{19} + \bar{i}\bar{H}'_{19}]}{\sqrt{\bar{G}_{19} + \bar{i}\bar{H}_{19}}} \tag{6.9b}$$

where $\bar{E}_{13,2}$ is the sub-band energy and the sub-band equation in this case can be expressed as

$$0 = [\bar{G}_{19} + i\bar{H}_{19}]\Big|_{\bar{k}_X = \frac{\bar{n}_X\pi}{\bar{d}_x} \text{ and } \bar{k}_y = \frac{\bar{n}_y\pi}{\bar{d}_y} \text{ and } \bar{E} - \bar{E}_{13,2}} \tag{6.9c}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\overline{G'}_{19} \tag{6.10}$$

The electron concentration can be written as

$$\bar{n}_{1D} = Real\,part\,of \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\tau_8 + \tau_9] \tag{6.11}$$

where

$$\tau_8 = \left[[\bar{G}_{19} + \bar{i}\bar{H}_{19}]\Big|_{\bar{k}_z = \frac{\pi\bar{n}_z}{\bar{d}_z},\ \bar{k}_y = \frac{\pi\bar{n}_y}{\bar{d}_y},\ \bar{E} = \bar{E}_{F62}}\right]^{1/2},$$

$$\tau_9 = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\tau_8]$$

and $\bar{E}_{F62}$ is the Fermi energy in this case

Using (1.31f) and (6.11), we can study the entropy in this case.

6.2.3 Entropy in IV–VI quantum wire HD SLs with graded interfaces

The **E-k** dispersion relation of the conduction electrons of the HD constituent materials of the IV–VI SLs can be expressed as

$$\bar{k}_z^2 = [2\bar{p}_{9,i}]^{-1}[-\bar{q}_{9,i}(\bar{E},\bar{k}_s,\eta_{gi}) + \left[[\bar{q}_{9,i}(\bar{E},\bar{k}_s,\eta_{gi})]^2 + 4\bar{p}_{9,i}\bar{R}_{9,1}(\bar{E},\bar{k}_s,\eta_{gi})\right]^{\frac{1}{2}}] \tag{6.12}$$

where,

$$\bar{p}_{9,i} = (\alpha_i\hbar^4)/\bar{p}_{9,i} = (\alpha_i\hbar^4)/(4\bar{m}_{l,i}^{-}\bar{m}_{l,i}^{+}), \bar{i} = 1,2,$$

$$\bar{q}_{9,1} = (\bar{E},\bar{k}_s,\eta_{gi}) = [(\hbar^2/2)((1/\bar{m}_{li}^{*}) + (1/\bar{m}_{li}^{-})) +$$

$$\alpha_i(\hbar^4/4)\bar{k}_s^2((1/\bar{m}_{li}^{+}\,\bar{m}_{li}^{-}) + (1/\bar{m}_{li}^{+}\,\bar{m}_{li}^{-})) - \alpha_i\gamma_3(\bar{E},\eta_{gi})((1/\bar{m}_{li}^{+}) - (1/\bar{m}_{li}^{-}))$$

and

$$\bar{R}_{9,i}(\bar{E},\bar{k}_s,\eta_{gi}) = [\gamma_2(\bar{E},\eta_{gi}) + \gamma_3(\bar{E},\eta_{gi})[(\hbar^2/2)\alpha_i k_s^2((1/\bar{m}_{ti}^{*}) - (1/\bar{m}_{ti}^{-}))]$$

$$-[(\hbar^2/2)\bar{k}_s^2((1/\bar{m}_{ti}^{*}) - (1/\bar{m}_{ti}^{-}))] = \alpha_i(\hbar^6/4)\bar{k}_s^4((1/\bar{m}_{ti}^{+}\,\bar{m}_{ti}^{-}))]$$

The electron dispersion law in HD quantum well IV–VI SLs with graded interfaces can be expressed as

$$\cos(\bar{L}_0\bar{k})\frac{1}{2}\Phi_2(\bar{E},\bar{k}_s) \tag{6.13}$$

$$\Phi_2(\bar{E},\bar{k}_s) \equiv [2\cos\{\beta_2(\bar{E},\bar{k}_s)\}\cos\{\gamma_2(\bar{E},\bar{k}_s)\} + \varepsilon_2(\bar{E},\bar{k}_s)\sinh\{\beta_2(\bar{E},\bar{k}_s)\}\sin\{\gamma_{22}(\bar{E},\bar{k}_s)\}$$

$$+\Delta_0\left[\left(\frac{\{\bar{K}_{112}(\bar{E},\bar{k}_s)\}^2}{\bar{K}_{212}(\bar{E},\bar{k}_s)} - 3\bar{K}_{212}(\bar{E},\bar{k}_s)\right)\cosh\{\beta_2(\bar{E},\bar{k}_s)\}\sin\{\gamma_{22}(\bar{E},\bar{k}_s)\}\right.$$

$$\left.+\left(3\bar{K}_{112}(\bar{E},\bar{k}_s) - \frac{\{\bar{K}_{212}(\bar{E},\bar{k}_s)\}^2}{\bar{K}_{112}(\bar{E},\bar{k}_s)}\right)\sinh\{\beta_2(\bar{E},\bar{k}_s)\}\cos\{\gamma_{22}(\bar{E},\bar{k}_s)\}\right]$$

$$+\Delta_0[2(\{\bar{K}_{112}(\bar{E},\bar{k}_s)\}^2 - \{\bar{K}_{212}(\bar{E},\bar{k}_s)\}^2)\cosh\{\beta_2(\bar{E},\bar{k}_s)\}\cos\{\gamma_{22}(\bar{E},\bar{k}_s)\}$$

$$+\frac{1}{12}\left[\frac{5\{\bar{K}_{112}(\bar{E},\bar{k}_s)\}^3}{\bar{K}_{212}(\bar{E},\bar{k}_s)} + \frac{5\{\bar{K}_{212}(\bar{E},\bar{k}_s)\}^3}{\bar{K}_{112}(\bar{E},\bar{k}_s)} - 34\bar{K}_{212}(\bar{E},\bar{k}_s)\bar{K}_{112}\right]$$

$$\sinh\{\beta_2(\bar{E},\bar{k}_s)\}\sin\{\gamma_{22}(\bar{E},\bar{k}_s)\}]],$$

$$\beta_2(\bar{E},\bar{k}_s) \equiv \bar{K}_{112}(\bar{E},\bar{k}_s)[\bar{a}_0 - \Delta_0],$$

$$\bar{k}_{112}^2(\bar{E},\bar{k}_s) = [2\bar{p}_{92}]^{-1}[-\bar{q}_{92}(\bar{E}-\bar{V}_0,\bar{k}_s\eta_{g2}) - \left[[\bar{q}_{92}(\bar{E}-\bar{V}_0,\bar{k}_s\eta_{g2})]^2 + 4\bar{p}_{92}\bar{R}_{92}(\bar{E}-\bar{V}_0,\bar{k}_s\eta_{g2})\right]^{\frac{1}{2}}],$$

$$\gamma_{22}(\bar{E},\bar{k}_s) \equiv \bar{K}_{212}(\bar{E},\bar{k}_s)[\bar{b}_0 - \Delta_0],$$

$$\bar{k}^2_{212}(\bar{E},\bar{k}_s) = [2\bar{p}_{9,1}]^{-1}\left[-\bar{q}_{9,1}(\bar{E},\bar{k}_s\eta_{g1}) + \left[[\bar{q}_{9,1}(\bar{E},\bar{k}_s\eta_{g1})]^2 + 4\bar{p}_{9,1}\bar{R}_{9,1}(\bar{E},\bar{k}_s\eta_{g1})\right]^{\frac{1}{2}}\right],$$

and

$$\varepsilon_2(\bar{E},\bar{k}_s) \equiv \left[\frac{\bar{K}_{112}(\bar{E},\bar{k}_s)}{\bar{K}_{212}(\bar{E},\bar{k}_s)} - \frac{\bar{K}_{212}(\bar{E},\bar{k}_s)}{\bar{K}_{112}(\bar{E},\bar{k}_s)}\right].$$

The simplified DR in HD quantum wire IV–VI SLs with graded interfaces can be expressed as

$$\bar{k}^2_z = \left[\frac{1}{\bar{L}^2_0}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_2(\bar{E},\bar{k}_s)\right\}\right]^2 - \bar{k}^2_s\right]\Bigg|_{\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x}\ and\ \bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y}} \tag{6.14a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi\bar{L}_0}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\frac{\cos^{-1}\{\frac{1}{2}\Phi_2(\bar{E},\bar{k}_s)\}\Phi_2(\bar{E},\bar{k}_s)\Phi'_2(\bar{E},\bar{k}_s)\bar{H}(\bar{E}-\bar{E}_{13,3})}{\left(\sqrt{\cos^{-1}\{\frac{1}{2}\Phi_2(\bar{E},\bar{k}_s)\}^2 - \bar{L}^2_0\{(\frac{\bar{n}_x\pi}{\bar{d}_x})^2 + (\frac{\bar{n}_x\pi}{\bar{d}_x})^2\}}\right)\sqrt{1-\frac{1}{4}\Phi^2_2(\bar{E},\bar{k}_s)}} \tag{6.14b}$$

where $\bar{E}_{13,3}$ is the sub-band energy and the sub-band equation in this case can be expressed as

$$0 = \left[\frac{1}{\bar{L}^2_0}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_2(\bar{E}_{13,3},\bar{k}_s)\right\}\right]^2 - \bar{k}^2_s\right]\Bigg|_{\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x}\ and\ \bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y}} \tag{6.14c}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y) = \frac{\hbar^2}{2\bar{L}^2_0}\cos^{-1}\left[\frac{1}{2}\Phi_2(\bar{E},\bar{k}_s)]\Phi'_2(\bar{E},\bar{k}_s)[1-\frac{1}{4}\Phi^2_2(\bar{E},\bar{k}_s)\right]^{-1/2} \tag{6.15}$$

The electron concentration can be written as

$$\bar{n}_{1D} = \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\tau_{10}+\tau_{11}] \tag{6.16}$$

where

$$\tau_{10} = \left[\left[\frac{1}{\bar{L}^2_0}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_2(\bar{E},\bar{k}_s)\right\}\right]^2 - k^2_s\right]\Bigg|_{\bar{k}_z=\frac{\pi\bar{n}_z}{\bar{d}_z},\ \bar{k}_y=\frac{\pi\bar{n}_y}{\bar{d}_y},\ \bar{E}=\bar{E}_{F63}}\right]^{1/2},$$

$$\tau_{11} = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\tau_{10}]$$

and $\bar{E}_{F63}$ is the Fermi energy in this case

Using (1.31f) and (6.16), we can study the entropy in this case.

6.2.4 Entropy in HgTe/CdTe quantum wire HD SLs with graded interfaces

The electron energy spectra of the constituent materials of HgTe/CdTe SLs are given by

$$\bar{k}^2 = \left[\frac{\bar{B}_{01}^2 + 4\bar{A}_1\bar{E} - \bar{B}_{01}\sqrt{\bar{B}_{01}^2 + 4\bar{A}_1\bar{E}}}{2\bar{A}_1^2}\right] \tag{6.17}$$

and

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_{c2}^*} = \bar{T}_{12}(\bar{E}, \Delta_2, \bar{E}_{g2}, \eta_{g2}) + i\bar{T}_{22}(\bar{E}, \Delta_2, \bar{E}_{g2}, \eta_{g2}) \tag{6.18}$$

where $\bar{B}_{01} = (3|e|^2/128\varepsilon_{sc1})$, $\bar{A}_1 = (\hbar^2/2\bar{m}_{c1}^*)$. $\varepsilon_{sc1}.\varepsilon_{sc1}$is the semiconductor permittivity of the first material. The energy-wave vector dispersion relation of the conduction electrons in HD quantum well HgTe/CdTe SLs with graded interfaces can be expressed as

$$\bar{k}_z^2 = \bar{G}_{192} + i\bar{H}_{192} \tag{6.19}$$

where,

$$\bar{G}_{192} = \left[\left((\bar{C}_{182}^2 - \bar{D}_{182}^2)/\bar{L}_0^2\right) - \bar{k}_s^2\right],$$

$$\bar{C}_{182} = \cos^{-1}(\omega_{182}), \omega_{182} = (2)^{\frac{-1}{2}}\left[(1 - \bar{G}_{182}^2 - \bar{H}_{182}^2) - \sqrt{(1 - \bar{G}_{182}^2 - \bar{H}_{182}^2)^2 + 4\bar{G}_{182}^2}\right]^{\frac{1}{2}}$$

$$\bar{G}_{182} = \frac{1}{2}[\bar{G}_{112} + \bar{G}_{122} + \Delta_0(\bar{G}_{132} + \bar{G}_{142}) + \Delta_0(\bar{G}_{152} + \bar{G}_{162})],$$

$$\bar{G}_{112} = 2(\cos(\bar{g}_{12}))(\cos(\bar{g}_{22}))(\cos\gamma_8(\bar{E}, \bar{k}_s))$$

$$\gamma_8(\bar{E}, \bar{k}_s) = \bar{k}_8(\bar{E}, \bar{k}_s)(\bar{b}_0 - \Delta_0), \bar{k}_8(\bar{E}, \bar{k}_s) = \left[\frac{\bar{B}_{01}^2 + 4\bar{A}_1\bar{E} - \bar{B}_{01}\sqrt{\bar{B}_{01}^2 + 4\bar{A}_1\bar{E}}}{2\bar{A}_1^2}\right]^{1/2}$$

$$\bar{G}_{122}([\Omega_{12}(\bar{E},\bar{k}_s)(\sinh\,\bar{g}_{12})(\cos\,\bar{g}_{22})-\Omega_{22}(\bar{E},\bar{k}_s)(\sin\,\bar{g}_{22})(\cosh\,\bar{g}_{12})](\sin\gamma_8(\bar{E},\bar{k}_s)))$$

$$\Omega_{12}(\bar{E},\bar{k}_s)=\left[\frac{\bar{d}_{12}}{\bar{k}_8(\bar{E},\bar{k}_s)}-\frac{\bar{k}_8(\bar{E},\bar{k}_s)\bar{d}_{12}}{\bar{d}_{12}^2+\bar{d}_{22}^2}\right],\Omega_{22}(\bar{E},\bar{k}_s)=\left[\frac{\bar{d}_{22}}{\bar{k}_8(\bar{E},\bar{k}_s)}-\frac{\bar{k}_8(\bar{E},\bar{k}_s)\bar{d}_{22}}{\bar{d}_{12}^2+\bar{d}_{22}^2}\right]$$

$$\bar{G}_{132}=([\Omega_{32}(\bar{E},\bar{k}_s)(\cosh\,\bar{g}_{12})(\cos\,\bar{g}_{22})-\Omega_{42}(\bar{E},\bar{k}_s)(\sinh\,\bar{g}_{12})(\sin\,\bar{g}_{22})](\sin\gamma_8(\bar{E},\bar{k}_s))),$$

$$\Omega_{32}(\bar{E},\bar{k}_s)=\left[\frac{\bar{d}_{12}^2-\bar{d}_{22}^2}{\bar{k}_8(\bar{E},\bar{k}_s)}-3\bar{k}_8(\bar{E},\bar{k}_s)\right],\Omega_{42}(\bar{E},\bar{k}_s)=\left[\frac{2\bar{d}_{12}\bar{d}_{22}}{\bar{k}_8(\bar{E},\bar{k}_s)}\right],$$

$$\bar{G}_{142}=([\Omega_{52}(\bar{E},\bar{k}_s)(\sinh\,\bar{g}_{12})(\cos\,\bar{g}_{22})-\Omega_{62}(\bar{E},\bar{k}_s)(\sin\,\bar{g}_{22})(\cosh\,\bar{g}_{22})](\cos\gamma_8(\bar{E},\bar{k}_s))),$$

$$\Omega_{52}(\bar{E},\bar{k}_s)=\left[3\bar{d}_{12}-\frac{\bar{d}_{12}}{\bar{d}_{12}^2+\bar{d}_{22}^2}\bar{k}_8^2(\bar{E},\bar{k}_s)\right],\Omega_{62}(\bar{E},\bar{k}_s)=\left[3\bar{d}_{22}+\frac{\bar{d}_{22}}{\bar{d}_{12}^2+\bar{d}_{22}^2}\bar{k}_8^2(\bar{E},\bar{k}_s)\right],$$

$$\bar{G}_{152}=([\Omega_{92}(\bar{E},\bar{k}_s)(\cosh\,\bar{g}_{12})(\cos\,\bar{g}_{22})-\Omega_{102}(\bar{E},\bar{k}_s)(\sinh\,\bar{g}_{12})(\sin\,\bar{g}_{22})](\cos\gamma_8(\bar{E},\bar{k}_s))),$$

$$\Omega_{92}(\bar{E},\bar{k}_s)=\left[2\bar{d}_{12}^2-2\bar{d}_{22}^2-\bar{k}_8^2(\bar{E},\bar{k}_s)\right],\Omega_{102}(\bar{E},\bar{k}_s)=\left[2\bar{d}_{12}\bar{d}_{22}\right],$$

$$\bar{G}_{162}([\Omega_{72}(\bar{E},\bar{k}_s)(\sinh\,\bar{g}_{12})(\cos\,\bar{g}_{22})-\Omega_{82}(\bar{E},\bar{k}_s)(\sin\,\bar{g}_{12})(\cosh\,\bar{g}_{22})](\sin\gamma_8(\bar{E},\bar{k}_s)/12))$$

$$\Omega_{72}(\bar{E},\bar{k}_s)=\left[\frac{5\bar{d}_{12}}{\bar{d}_{12}^2+\bar{d}_{22}^2}\bar{k}_8^3(\bar{E},\bar{k}_s)+\frac{5(\bar{d}_{12}^3-3\bar{d}_{22}^2\bar{d}_{12})}{\bar{k}_8(\bar{E},\bar{k}_s)}-34\bar{k}_8(\bar{E},\bar{k}_s)\bar{d}_{12}\right],$$

$$\Omega_{82}(\bar{E},\bar{k}_s)=\left[\frac{5\bar{d}_{12}}{\bar{d}_{12}^2+\bar{d}_{22}^2}\bar{k}_8^3(\bar{E},\bar{k}_s)+\frac{5(\bar{d}_{12}^3-3\bar{d}_{22}^2\bar{d}_{12})}{\bar{k}_8(\bar{E},\bar{k}_s)}+34\bar{k}_8(\bar{E},\bar{k}_s)\bar{d}_{12}\right],$$

$$\bar{H}_{182}=\frac{1}{2}\left[\bar{H}_{112}+\bar{H}_{122}+\Delta_0(\bar{H}_{132}+\bar{H}_{142})+\Delta_0(\bar{H}_{152}+\bar{H}_{162})\right]$$

$$\bar{H}_{112}=2(\sinh\,\bar{g}_{12}\sin\bar{g}_{22}\cos\gamma_8(\bar{E},\bar{k}_s)),$$

$$\bar{H}_{122}=([\Omega_{22}(\bar{E},\bar{k}_s)(\sinh\bar{g}_{12})(\cos\bar{g}_{22})+\Omega_{12}(\bar{E},\bar{k}_s)(\sin\bar{g}_{22})(\cosh\bar{g}_{12})](\sin\gamma_8(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{132}=([\Omega_{42}(\bar{E},\bar{k}_s)(\cosh\bar{g}_{12})(\cos\bar{g}_{22})+\Omega_{32}(\bar{E},\bar{k}_s)(\sinh\bar{g}_{12})(\sin\bar{g}_{22})](\sin\gamma_8(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{142}=([\Omega_{62}(\bar{E},\bar{k}_s)(\sinh\bar{g}_{12})(\cos\bar{g}_{22})+\Omega_{52}(\bar{E},\bar{k}_s)(\sin\bar{g}_{12})(\cosh\bar{g}_{22})](\cos\gamma_8(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{152}=([\Omega_{102}(\bar{E},\bar{k}_s)(\cosh\bar{g}_{12})(\cos\bar{g}_{22})+\Omega_{92}(\bar{E},\bar{k}_s)(\sinh\bar{g}_{12})(\sin\bar{g}_{22})](\cos\gamma_8(\bar{E},\bar{k}_s))),$$

$$\bar{H}_{162}=([\Omega_{82}(\bar{E},\bar{k}_s)(\sinh\bar{g}_{12})(\cos\bar{g}_{22})+\Omega_{72}(\bar{E},\bar{k}_s)(\sin\bar{g}_{12})(\cosh\bar{g}_{22})](\sin\gamma_8(\bar{E},\bar{k}_s)/12)),$$

$$\bar{H}_{192}=[((2\bar{C}_{182}\bar{D}_{182})/\bar{L}_0^2)]\ \textit{and}\ \bar{D}_{182}=\sinh^{-1}(\omega_{182})$$

The simplified entropy in HD quantum wire *HgTe*/*CdTe* superllatices with graded interfaces can be expressed as

$$\bar{k}_z^2 = [\bar{G}_{192} + i\bar{H}_{192}]\Big|_{\bar{k}_x = \frac{\bar{n}_x\pi}{d_x}\, and\, \bar{k}_y = \frac{\bar{n}_y\pi}{d_y}} \tag{6.20a}$$

The DOS function can be written a

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\frac{\bar{H}(\bar{E}-\bar{E}_{13,4})[\overline{G'}_{192} + i\bar{H}'_{192}]}{\sqrt{\bar{G}_{192} + i\bar{H}_{192}}} \tag{6.20b}$$

where $\bar{E}_{13,4}$ is the sub band energy and the sub – band equation in this case can be expressed as

$$0 = [\bar{G}_{192} + i\bar{H}_{192}]\Big|_{\bar{k}x = \frac{\bar{n}_x\pi}{d_x}, \bar{k}_y = \frac{\bar{n}_y\pi}{d_y}\, and\, \bar{E} = \bar{E}_{13,4}} \tag{6.20c}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\overline{G'}_{192} \tag{6.21}$$

The electron concentration can be written as

$$\bar{n}_{1D} = Real\, part\, of \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\tau_{12} + \tau_{13}] \tag{6.22}$$

where

$$\tau_{12} = \left[\left[\bar{G}_{192} + i\bar{H}_{192}\right]\Big|_{\bar{k}_z = \frac{\pi\bar{n}_z}{\bar{d}_z},\ k_y = \frac{\pi\bar{n}_y}{d_y}, \bar{E} = \bar{E}_{F64}}\right]^{1/2},$$

$$\tau_{13} = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\tau_{12}]$$

and $\bar{E}_{F64}$ is the Fermi energy in this case.

Using (1.31f) and (6.22), we can study the entropy in this case.

6.2.5 Entropy in strained layer quantum wire HD SLs with graded interfaces

The dispersion relation of the conduction electrons of the constituent materials of the strained layer super lattices can be expressed as

$$[\bar{E} - \bar{T}_{1i}]\bar{k}_x^2 + [\bar{E} - \bar{T}_{2i}]\bar{k}_y^2 + [\bar{E} - \bar{T}_{3i}]\bar{k}_z^2 = \bar{q}_i\bar{E}^3 - \bar{R}_i\bar{E}^2 + \bar{V}_i\bar{E} + \zeta_i \tag{6.23}$$

where

$$\bar{T}_{1i} = \theta_i, \theta_i = \left[\bar{E}_{gi} - \bar{C}^c_{1i}\varepsilon_i - (\bar{a}_i + \bar{C}^c_{1i})\varepsilon_i + \frac{3}{2}\bar{b}_i\varepsilon_{xxi} - \frac{\bar{b}_i\varepsilon_i}{2} + \frac{\sqrt{3\bar{d}_i\varepsilon_{xyi}}}{2}\right],$$

$$\bar{T}_{2i} = \omega_i, \omega_i = \left[\bar{E}_{gi} - \bar{C}^c_{1i}\varepsilon_i - (\bar{a}_i + \bar{C}^c_{1i})\varepsilon_i + \frac{3}{2}\bar{b}_i\varepsilon_{xxi} - \frac{\bar{b}_i\varepsilon_i}{2} - \frac{\sqrt{3\bar{d}_i\varepsilon_{xyi}}}{2}\right],$$

$$\bar{T}_{3i} = \delta_i, \delta_i = \left[\bar{E}_{gi} - \bar{C}^c_{1i}\varepsilon_i - (\bar{a}_i + \bar{C}^c_{1i})\varepsilon_i + \frac{3}{2}\bar{b}_i\varepsilon_{zzi} - \frac{\bar{b}_i\varepsilon_i}{2}\right],$$

$$\bar{R}_i = \bar{q}_i[2\bar{A}_i + \bar{C}^c_{1i}\varepsilon_i,\ \bar{q}_i = \frac{3}{2\bar{B}^2_{2i}}, \bar{A}_i = \bar{E}_{gi} - \bar{C}^c_{1i}\varepsilon_i,$$

$$\bar{V}_i = \bar{q}_i\left[\bar{A}^2_i - \frac{2\bar{C}^2_{1i}\varepsilon_{xyi}}{3} + 2\bar{A}_i\bar{C}^c_{1i}\varepsilon_i, \zeta_i = \bar{q}_i\left[\frac{2\bar{C}^2_{1i}\varepsilon_{xyi}}{3} - \bar{C}^c_{1i}\varepsilon_i\bar{A}^2_i\right]\right]$$

Therefore, the electron energy spectrum in HD stressed materials can be written as

$$\bar{P}_i(\bar{E}, \eta_{gi})\bar{k}^2_x + \bar{Q}_i(\bar{E}, \eta_{gi})\bar{k}^2_y + \bar{S}_i(\bar{E}, \eta_{gi})\bar{k}^2_z = 1 \tag{6.24}$$

where

$$\bar{P}_i(\bar{E}, \eta_{gi}) = \frac{[\gamma_0(\bar{E}, \eta_{gi}) - \bar{I}_0\bar{T}_{1i}]}{\bar{\Delta}_i(\bar{E}, \eta_{gi})},$$

$$\bar{\Delta}_i(\bar{E}, \eta_{gi}) = \left[\frac{-\bar{q}_i\eta^3_{gi}}{2\sqrt{\pi}}\exp\left(\frac{-\bar{E}^2}{\eta^2_{gi}}\right)\left[1 + \frac{\bar{E}^2}{\eta^2_{gi}}\right] - \bar{R}_i\theta_0(\bar{E}, \eta_{gi}) + \bar{V}_i\gamma_0(\bar{E}, \eta_{gi}) + \frac{\zeta_i}{2}\left[1 + Erf\left(\frac{\bar{E}}{\eta_{gi}}\right)\right]\right],$$

$$\bar{I}_0 = \frac{1}{2}[1 + Erf(\bar{E}/\eta_{gi})], \bar{Q}_i(\bar{E}, \eta_{gi}) = \frac{[\gamma_0(\bar{E}, \eta_{gi}) - \bar{I}_0\bar{T}_{2i}]}{\bar{\Delta}_i(\bar{E}, \eta_{gi})} and \bar{d}_i(\bar{E}, \eta_{gi}) = \frac{[\gamma_0(\bar{E}, \eta_{gi}) - \bar{I}_0\bar{T}_{3i}]}{\bar{\Delta}_i(\bar{E}, \eta_{gi})}$$

The energy-wave vector dispersion relation of the conduction electrons in heavily doped strained layer quantum well SLs with graded interfaces can be expressed as

$$\cos(\bar{L}_0\bar{k}) = \frac{1}{2}\bar{\phi}_6(\bar{E}, \bar{k}_s) \tag{6.25}$$

$$\bar{\phi}_6(\bar{E}, \bar{k}_s) = [2\cosh[\bar{T}_4(\bar{E}, \eta_{g2})]\cos[\bar{T}_5(\bar{E}, \eta_{g1})]] + [\bar{T}_6(\bar{E}, \bar{k}_s)]\sinh[\bar{T}_4(\bar{E}, \eta_{g2})]\sin[\bar{T}_5(\bar{E}, \eta_{g1})]$$

$$+ \Delta_0\left[\left(\frac{\bar{k}^2_0(\bar{E}, \eta_{g2})}{\bar{k}'(\bar{E}, \eta_{g1})} - 3\bar{k}'(\bar{E}, \eta_{g1})\right)\cosh\left[\bar{T}_4(\bar{E}, \eta_{g2})\right]\sin\left[\bar{T}_5(\bar{E}, \eta_{g1})\right]\right.$$

$$\left. + \left(3\bar{k}_0(\bar{E}, \eta_{g2}) - \frac{\bar{k}'^2(\bar{E}, \eta_{g1})}{\bar{k}_0(\bar{E}, \eta_{g2})}\right)\sinh\left[\bar{T}_4(\bar{E}, \eta_{g2})\right]\cos\left[\bar{T}_5(\bar{E}, \eta_{g1})\right]\right]$$

$$+\Delta_0[2(\bar{k}_0^2(\bar{E},\eta_{g2})-\bar{k}'^2(\bar{E},\eta_{g2}))\cosh[\bar{T}_4(\bar{E},\eta_{g2})]\sin[\bar{T}_5(\bar{E},\eta_{g1})]]$$

$$+\frac{1}{12}\left(\frac{5\bar{k}_0^3(\bar{E},\eta_{g2})}{\bar{k}'(\bar{E},\eta_{g1})}+\frac{5\bar{k}'^3(\bar{E},\eta_{g1})}{k_0(\bar{E},\eta_{g2})}-34\bar{k}_0(\bar{E},\eta_{g2})\bar{k}'(\bar{E},\eta_{g1})\right)\sinh[\bar{T}_4(\bar{E},\eta_{g2})]\sin[\bar{T}_5(\bar{E},\eta_{g1})]$$

$$[\bar{T}_4(\bar{E},\eta_{g2})]=\bar{k}_0(\bar{E},\eta_{g2})[\bar{a}_0-\Delta_0],$$

$$\bar{k}_0(\bar{E},\eta_{g2})=(\bar{S}_2(\bar{E}-\bar{V}_0,\eta_{g2}))^{-1/2}[\bar{P}_2(\bar{E}-\bar{V}_0,\eta_{g2})\bar{k}_x^2+\bar{Q}_2(\bar{E}-\bar{V}_0,\eta_{g2})\bar{k}_y^2-1]^{1/2},$$

$$\bar{T}_5(\bar{E},\eta_{g1})=\bar{k}'(\bar{E},\eta_{g1})[\bar{b}_0-\Delta_0],$$

$$\bar{k}'(\bar{E},\eta_{g1})=[\bar{S}_1(\bar{E},\eta_{g1})]^{-1/2}[1-\bar{P}_1(\bar{E},\eta_{g1})\bar{k}_x^2-\bar{Q}_2(\bar{E},\eta_{g1})\bar{k}_y^2]^{1/2}$$

and

$$\bar{T}_6(\bar{E},\bar{k}_s)=\left[\frac{\bar{k}_0(\bar{E},\eta_{g1})}{\bar{k}'(\bar{E},\eta_{g1})}-\frac{\bar{k}'(\bar{E},\eta_{g1})}{\bar{k}_0(\bar{E},\eta_{g1})}\right]$$

Therefore the entropy of the conduction electrons in HD strained layer quantum well SL with graded interfaces can be expressed as

$$\bar{k}_z^2=\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_6(\bar{E},\bar{k}_s)\right\}\right]^2-\bar{k}_s^2\right]\Bigg|_{\bar{k}_x=\frac{\bar{n}_x\pi}{d_x}\ and\ \bar{k}y=\frac{\bar{n}_y\pi}{d_y}} \tag{6.26a}$$

The DOS function can be written as

$$\bar{N}(\bar{E})=\frac{g_v}{\pi\bar{L}_0}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\frac{\cos^{-1}\{\frac{1}{2}\bar{\Phi}_6(\bar{E},\bar{k}_s)\}\bar{\Phi}_6(\bar{E},\bar{k}_s)[\bar{\Phi}_6(\bar{E},\bar{k}_s)]'\bar{H}(\bar{E}-\bar{E}_{13,5})}{\left(\sqrt{\cos^{-1}\{\frac{1}{2}\bar{\Phi}_6(\bar{E},\bar{k}_s)\}^2-\bar{L}_0^2\{(\frac{n_x\pi}{d_x})^2+(\frac{n_x\pi}{d_x})^2\}}\right)\sqrt{1-\frac{1}{4}[\bar{\Phi}_6(\bar{E},\bar{k}_s)]^2}} \tag{6.26b}$$

where $\bar{E}_{13,5}$ is the sub − band energy and the sub − band equation in this case can be expressed as

$$0=\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_6(\bar{E}_{13,3},\bar{k}_s)\right\}\right]^2-\bar{k}_s^2\right]\Bigg|\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x}\ \ and\ \bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y} \tag{6.26c}$$

EEM in this case is given

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)=\frac{\hbar^2}{2\bar{L}_0^2}\cos^{-1}\left[\frac{1}{2}\bar{\Phi}_6(\bar{E},\bar{k}_s)][\bar{\Phi}_6(\bar{E},\bar{k}_s)\right]'\left[1-\frac{1}{4}[\bar{\Phi}_6(\bar{E},\bar{k}_s)]^2\right]^{-1/2} \tag{6.27}$$

The electron concentration can be written as

$$\bar{n}_{1D} = \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} [\tau_{17} + \tau_{18}] \tag{6.28}$$

where

$$\tau_{17} = \left[\left[\frac{1}{\bar{L}_0^2} \left[\cos^{-1} \left\{ \frac{1}{2} \bar{\Phi}_6(\bar{E}, \bar{k}_s) \right\} \right]^2 - \bar{k}_s^2 \right] \Bigg|_{\bar{k}_z = \frac{\pi \bar{n}_z}{\bar{d}_z},\ \bar{k}_y = \frac{\pi \bar{n}_y}{\bar{d}_y},\ \bar{E} = \bar{E}_{F66}} \right]^{1/2},$$

$$\tau_{18} = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\tau_{17}]$$

and $\bar{E}_{F66}$ is the Fermi energy in this case.

Using (1.31f) and (6.28), we can study the entropy in this case.

6.2.6 Entropy in III–V quantum wire HD effective mass SLs

Following Sasaki [24], the electron dispersion law in III– V heavily doped effective mass superlattices (EMSLs) can be written as

$$\bar{k}_x^2 = \left[\frac{1}{\bar{L}_0^2} \left\{ \cos^{-1}(\bar{f}_{21}(\bar{E}, \bar{k}_y, \bar{k}_z)) \right\}^2 - \bar{k}_\perp^2 \right] \tag{6.29}$$

in which

$$(\bar{f}_{21}(\bar{E}, \bar{k}_y, \bar{k}_z) = \bar{a}_1 \cos[\bar{a}_0 \bar{C}_{21}(\bar{E}, \bar{k}_\perp, \eta_{g1}) + \bar{b}_0 \bar{D}_{21}(\bar{E}, \bar{k}_\perp, \eta_{g2})]$$

$$- \bar{a}_1 \cos[\bar{a}_0 C_{21}(\bar{E}, \bar{k}_\perp, \eta_{g1}) - \bar{b}_0 \bar{D}_{21}(\bar{E}, \bar{k}_\perp, \eta_{g2})],\ \bar{k}_\perp^2 = \bar{k}_y^2 + \bar{k}_z^2,$$

$$\bar{a}_1 = \left[\sqrt{\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})} + 1} \right]^2 \left[4 \left(\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})} \right)^{1/2} \right]^{-1}$$

$$\bar{a}_2 = \left[\sqrt{\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})} - 1} \right]^2 \left[4 \left(\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})} \right)^{1/2} \right]^{-1}$$

$$\bar{M}_{iz}(0, \eta_{gi}) = \bar{m}_{ci}^* \left[\frac{-2}{\sqrt{\pi}} \bar{T}(0, \eta_{gi}) + 2 \left[\frac{\alpha_i \bar{b}_i}{\bar{c}_i} \frac{\eta_{gi}}{\sqrt{\pi}} + \frac{1}{2} \left(\frac{\alpha_i \bar{c}_i + \bar{c}_i \bar{b}_i - \alpha_i \bar{b}_i}{\bar{c}_i^2} \right) + \frac{1}{\sqrt{\pi \bar{c}_i}} \left(1 - \frac{\alpha_i}{\bar{c}_i} \right) \left(1 - \frac{\bar{b}_i}{\bar{c}_i} \right) \right] \right.$$

$$-\frac{1}{\bar{c}_i}\left(1-\frac{\alpha_i}{\bar{c}_i}\right)\left(1-\frac{\bar{b}_i}{\bar{c}_i}\right)\frac{2}{\bar{c}_i\eta_{gi}\sqrt{\pi}}\left\{\frac{-2}{\bar{c}_i\eta_{gi}}\exp\left(\frac{1}{\bar{c}_i^2\eta_{gi}^2}\right)\left(\sum_{p=1}^{\alpha}\left(\exp\left(\frac{-\bar{p}^2}{4}\right)\right)\frac{1}{\bar{p}}\sinh\left(\frac{\bar{p}}{\bar{c}_i\eta_{gi}}\right)\right)\right.$$

$$\left.+\exp\left(\frac{-1}{\bar{c}_i^2\eta_{gi}^2}\right)\left(\sum_{p=1}^{\alpha}\left(\exp\left(\frac{-\bar{p}^2}{4}\right)\right)\frac{1}{\eta_{gi}}\cosh\left(\frac{\bar{p}}{\bar{c}_i\eta_{gi}}\right)\right)\right\}\Bigg]\Bigg],$$

$$\bar{T}(0,\eta_{gi})=2\left[\frac{\alpha_i\bar{b}_i}{\bar{c}_i}\frac{\eta_{gi}^2}{4}+\left(\frac{\alpha_i\bar{c}_i+\bar{b}_i\bar{c}_i-\alpha_i\bar{b}_i}{\bar{c}_i^2}\right)\frac{\eta_{gi}}{2\sqrt{\pi}}+\frac{1}{2\bar{c}_i}\left(1-\frac{\alpha_i}{\bar{c}_i}\right)\left(1-\frac{\bar{b}_i}{\bar{c}_i}\right)\right.$$

$$\left.-\frac{1}{\bar{c}_i}\left(1-\frac{\alpha_i}{\bar{c}_i}\right)\left(1-\frac{\bar{b}_i}{\bar{c}_i}\right)\frac{2}{\bar{c}_i\eta_{gi}\sqrt{\pi}}\exp\left(\frac{1}{\bar{c}_i^2\eta_{gi}^2}\right)\sum_{p=1}^{\alpha}\frac{\exp(-\bar{p}^2/4)}{\bar{p}}\sinh\left(\frac{\bar{p}}{\bar{c}_i\eta_{gi}}\right)\right],$$

$$\bar{C}_{21}(\bar{E},\bar{k}_\perp,\eta_{g1})=e_1+i\bar{e}_2,\bar{D}_{21}(\bar{E},\bar{k}_\perp,\eta_{g2})=e_3+ie_4,$$

$$e=\left[\left(\left(\sqrt{\bar{t}_1^2+\bar{t}_2^2+\bar{t}_1}\right)/2\right)\right]^{\frac{1}{2}},e_2=\left[\left(\left(\sqrt{\bar{t}_1^2+\bar{t}_2^2+\bar{t}_1}\right)/2\right)\right]^{\frac{1}{2}}$$

$$\bar{t}_1=\left[\frac{2\bar{m}_{c1}^*}{\hbar^2}\bar{T}_{11}(\bar{E},\Delta_1,\eta_{g1},\bar{E}_{g1})-\bar{k}_\perp^2\right],\bar{t}_2=\frac{2\bar{m}_{c1}^*}{\hbar^2}\bar{T}_{21}(\bar{E},\Delta_1,\eta_{g1},\bar{E}_{g1})$$

$$e=\left[\frac{\sqrt{\bar{t}_3^2+\bar{t}_4^2}+\bar{t}_3}{2}\right]^{1/2},e_4=\left[\frac{\sqrt{\bar{t}_3^2+\bar{t}_4^2}-\bar{t}_3}{2}\right]^{1/2}$$

$$\bar{t}_3=\left[\frac{2\bar{m}_{c2}^*}{\hbar^2}\bar{T}_{12}(\bar{E},\Delta_1,\eta_{g1},\bar{E}_{g2})-\bar{k}_\perp^2\right],\bar{t}_4=\frac{2\bar{m}_{c2}^*}{\hbar^2}\bar{T}_{22}(\bar{E},\Delta_1,\eta_{g1},\bar{E}_{g2}),$$

Therefore, (6.29) can be expressed as

$$k_z^2=\delta_7+i\delta_8 \tag{6.30}$$

where

$$\delta_7=\left[\frac{1}{\bar{L}_0^2}(\delta_5^2-\delta_6^2)-\bar{k}_\perp^2\right],\delta_5=\cos^{-1}p_5,$$

$$\bar{p}_5=\left[\frac{1-\delta_3^2-\delta_4^2\sqrt{\left(1-\delta_3^2-\delta_4^2\right)^2+4\delta_4^2}}{2}\right]^{1/2'}$$

$$\delta_3=(\bar{a}_1\cos\Delta_1\cosh\Delta_2-\bar{a}_2\cos\Delta_3\cosh\Delta_4),$$

$$\delta_4=(\bar{a}_1\sin\Delta_1 sinh\Delta_2-\bar{a}_2\sin\Delta_3 sinh\Delta_4),$$

$$\Delta_1=(\bar{a}_0e_1+\bar{b}_0e_3),\Delta_2=(\bar{a}_0e_2+\bar{b}_0e_4),\Delta_3=(\bar{a}_0e_1-\bar{b}_0e_3),\Delta_4=(\bar{a}_0e_1-\bar{b}_0e_4),$$

$$\delta_6 = \sinh^{-1}\bar{p}_5 \text{ and } \delta_8 = [2\delta_5\delta_6/\bar{L}_0^2]$$

The entropy in III–V HD effective mass quantum wire SLs can be written as

$$\bar{k}_z^2 = [\delta_7 + i\delta_8]\left|\bar{k}_x = \frac{\bar{n}_x\pi}{\bar{d}_x} \; and \; \bar{k}_y = \frac{\bar{n}_y\pi}{\bar{d}_y}\right| \tag{6.31a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\frac{\bar{H}(\bar{E}-\bar{E}_{13,6})[\delta'_7 + i\delta'_8]}{\sqrt{\delta_7 + i\delta_8}} \tag{6.31b}$$

where $E_{13,6}$ is the sub-band energy and the sub-band equation in this case can be expressed as

$$0 = [\delta_7 + i\delta_8]\left|\bar{k}_x = \frac{\bar{n}_x\pi}{\bar{d}_x}\;, \bar{k}_y = \frac{\bar{n}_y\pi}{\bar{d}_y} \; and \; \bar{E} - \bar{E}_{13,6}\right. \tag{6.31c}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\delta'_7 \tag{6.32}$$

The electron concentration can be written as

$$\bar{n}_{1D} = Real\,part\,of\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\tau_{15} + \tau_{16}] \tag{6.33}$$

where

$$\tau_{15} = \left[[\delta_7 + i\delta_8]\left|_{\bar{k}_z = \frac{\pi\bar{n}_z}{\bar{d}_z},\; \bar{k}_y = \frac{\pi\bar{n}_y}{\bar{d}_y}, \bar{E} = \bar{E}_{F67}}\right.\right]^{1/2},$$

$$\tau_{16} = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\tau_{15}]$$

and $\bar{E}_{F67}$ is the Fermi energy in this case.

Using (1.31f) and (6.33), we can study the entropy in this case.

6.2.7 Entropy in II–VI quantum wire HD effective mass SLs

Following Sasaki [24], the electron dispersion law in HD II–VI EMSLs can be written as

$$\bar{k}_z^2 = \Delta_{13} + i\Delta_{14}, \tag{6.34}$$

$$\Delta_{13} = \left[\frac{1}{\bar{L}_0^2}(\Delta_{11}^2 - \Delta_{12}^2) - \bar{k}_s^2\right],$$

$$\Delta_5 = \cos^{-1}\bar{p}_6,$$

$$\bar{p}_5 = \left[\frac{1 - \Delta_9^2 - \Delta_{10}^2\sqrt{(1 - \Delta_9^2 - \Delta_{10}^2)^2 + 4\Delta_{10}^2}}{2}\right]^{1/2\prime}$$

$$\Delta_9 = (\bar{a}_1 \cos\Delta_6 \cosh\Delta_7 - \bar{a}_2 \cos\Delta_8 \cosh\Delta_7),$$

$$\Delta_{10} = (\bar{a}_1 \sin\Delta_6 \sinh\Delta_7 + \bar{a}_2 \sin\Delta_8 \sinh\Delta_7),$$

$$\Delta_6 = [\bar{a}_0\bar{C}_{22}(\bar{E}, \bar{k}_s, \eta_{g1}) + \bar{b}_0\bar{e}_3], \Delta_7 = \bar{b}_0\bar{e}_4, \Delta_8 = [\bar{a}_0\bar{C}_{22}(\bar{E}, \bar{k}_s, \eta_{g1}) - \bar{b}_0\bar{e}_3]$$

$$\bar{C}_{22} = (\bar{E}, \bar{k}_s, \eta_{g1}) = \left[\frac{2m^*_{||,1}}{\hbar^2}\left\{\gamma_3(\bar{E}, \eta_{g1}) - \frac{\hbar^2\bar{k}_s^2}{2m^*_{\perp,1}} \mp \bar{C}_0 k_s\right\}\right]^{1/2},$$

$$\bar{a}_1 = \left[\sqrt{\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})} + 1}\right]^2 \left[4\left(\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})}\right)^{1/2}\right]^{-1}, \bar{M}_1(0, \eta_{g1}) = \bar{m}^*_{c1}\left(1 - \frac{2}{\pi}\right),$$

$$\bar{a}_2 = \left[\sqrt{\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})} - 1}\right]^2 \left[4\left(\frac{\bar{M}_2(0, \eta_{g2})}{\bar{M}_1(0, \eta_{g1})}\right)^{1/2}\right]^{-1}$$

$$\Delta_{12} = \cos^{-1}\bar{p}_6, \ \Delta_{14} = \frac{2\Delta_{11}\Delta_{12}}{\bar{L}_0^2}$$

Entropy in III–V HD effective mass quantum wire SLs can be written as

$$\bar{k}_z^2 = [\delta_{13} + i\delta_{14}]\Big|_{\bar{k}_X = \frac{\bar{n}_x\pi}{d_x} \text{ and } \bar{k}_y = \frac{\bar{n}_y\pi}{d_y}} \tag{6.35a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi}\sum_{n_x=1}^{n_{x\max}}\sum_{n_y=1}^{n_{y\max}}\frac{\bar{H}(\bar{E} - \bar{E}_{13,6})[\delta'_{13} + i\delta'_{14}]}{\sqrt{\delta_{13} + i\delta_{14}}} \tag{6.35b}$$

where $\bar{E}_{13,7}$ is the sub band energy and the sub – band equation in this case cane be expressed as

$$0 = [\delta_{13} + i\delta_{14}]\Big|_{\bar{k}_X = \frac{\bar{n}_x\pi}{d_x}, \bar{k}_y = \frac{\bar{n}_y\pi}{d_y} \text{ and } \bar{E} - \bar{E}_{13,71}} \tag{6.35c}$$

The EEM in this case is given by

$$\bar{m}^{*}(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y)=\frac{\hbar^2}{2}\delta' \tag{6.36}$$

The electron concentration can be written as

$$\bar{n}_{1D}=Real\,part\,of\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\tau_{19}+\tau_{20}] \tag{6.37}$$

where

$$\tau_{19}=\left[[\Delta_{13}+i\Delta_{14}]\Big|_{\bar{k}_z=\frac{\pi\bar{n}_z}{\bar{d}_z},\ \bar{k}_y=\frac{\pi\bar{n}_y}{\bar{d}_y},\ \bar{E}=\bar{E}_{F610}}\right]^{1/2},$$

$$\tau_{20}=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\tau_{19}]$$

and $\bar{E}_{F610}$ is the Fermi energy in this case

Using (1.31f) and (6.37), we can study the entropy in this case.

6.2.8 Entropy in IV–VI quantum wire HD effective mass SLs

Following Sasaki [24], the electron dispersion law in IV–VI, EMSLs can be written as

$$\bar{k}_z^2=\left[\frac{1}{\bar{L}_0^2}\{\cos^{-1}(\bar{f}_{23}(\bar{E},\bar{k}_x,\bar{k}_y))\}^2-\bar{k}_s^2\right] \tag{6.38}$$

where

$$\bar{f}_{23}(\bar{E},\bar{k}_x,\bar{k}_y)=\bar{a}_3\cos[\bar{a}_0\bar{C}_{23}(\bar{E},\bar{k}_x,\bar{k}_y\eta_{g1})+\bar{b}_0\bar{D}_{23}(\bar{E},\bar{k}_x,\bar{k}_y\eta_{g1})]$$

$$-\bar{a}_4\cos[\bar{a}_0\bar{C}_{23}(\bar{E},\bar{k}_x,\bar{k}_y\eta_{g2})-\bar{b}_0\bar{D}_{23}(\bar{E},\bar{k}_x,\bar{k}_y\eta_{g2})],$$

$$\bar{a}_3=\left[\sqrt{\frac{\bar{M}_3(0,\eta_{g2})}{\bar{M}_3(0,\eta_{g1})}}+1\right]^2\left[4\left(\frac{\bar{M}_3(0,\eta_{g2})}{\bar{M}_3(0,\eta_{g1})}\right)^{1/2}\right]^{-1},$$

$$\bar{a}_3=\left[\sqrt{\frac{\bar{M}_3(0,\eta_{g2})}{\bar{M}_3(0,\eta_{g1})}}-1\right]^2\left[4\left(\frac{\bar{M}_3(0,\eta_{g2})}{\bar{M}_3(0,\eta_{g1})}\right)^{1/2}\right]^{-1}$$

$$\bar{M}_3(0,\eta_{gi}) = (4\bar{p}_{9,1})^{-1}\left[\left\{\alpha_i\left(1-\frac{2}{\pi}\right)\left(\frac{1}{\bar{m}_{l,i}^{+}}-\frac{1}{\bar{m}_{l,i}^{-}}\right)\right\}+\left[\left[\bar{q}_{9,i}(0,\eta_{gi})\right]^2\right.\right.$$

$$\left.\left.+(4\bar{p}_{9,1})\bar{R}_{9,i}(0,\eta_{gi})\right]^{1/2}\left[\alpha_i\left(1-\frac{2}{\pi}\right)\left(\frac{1}{\bar{m}_{l,i}^{+}}-\frac{1}{\bar{m}_{l,i}^{-}}\right)\bar{q}_{9,i}(0,\eta_{gi})+2\bar{p}_{9,i}\left(1-\frac{2}{\pi}+\frac{\alpha_i\eta_{gi}}{\sqrt{\pi}}\right)\right]\right],$$

$$\bar{p}_{9,i} = \frac{\alpha_i\hbar^4}{4\bar{m}_{l,i}^{+}\bar{m}_{l,i}^{-}}, \bar{q}_{9,i}(0,\eta_{gi}) = \left[\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}_{l,i}^{+}}-\frac{1}{\bar{m}_{l,i}^{-}}\right)\right.$$

$$\left.-\frac{\alpha_i\eta_{gi}}{\sqrt{\pi}}\left(\frac{1}{\bar{m}_{l,i}^{+}}-\frac{1}{\bar{m}_{l,i}^{-}}\right)\right],\ \bar{\mathrm{R}}_{9,1}(0,\eta_{gi}) = \left[\frac{\eta_{gi}}{\sqrt{\pi}}+\frac{\alpha_i\eta_{gi}^2}{2}\right],$$

$$\bar{C}_{23}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g1}) = \left[\left[2\bar{p}_{9,1}\right]^{-1}\left[-\bar{q}_{9,1}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g1})+\left[(\bar{q}_{9,1}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g1}))^2\right.\right.\right.$$

$$\left.\left.\left.+(4\bar{p}_{9,1})\bar{R}_{9,1}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g1})\right]^{1/2}\right]\right]^{1/2},$$

$$\bar{D}_{23}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g2}) = \left[\left[2\bar{p}_{9,2}\right]^{-1}\left[-\bar{q}_{9,2}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g2})+\left[\left\{\bar{q}_{9,2}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g2})\right\}^2\right.\right.\right.$$

$$\left.\left.\left.+(4\bar{p}_{9,2})\bar{R}_{9,2}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{g2})\right]^{1/2}\right]\right]^{1/2},$$

$$\bar{q}_{9,i}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{gi}) = \left[\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}_{l,i}^{+}}+\frac{1}{\bar{m}_{l,i}^{-}}\right)+\alpha_i\frac{\hbar^4}{4}\bar{k}_s^2\left(\frac{1}{\bar{m}_{l,i}^{+}\bar{m}_{l,i}^{-}}+\frac{1}{\bar{m}_{l,i}^{+}\bar{m}_{l,i}^{-}}\right)\right.$$

$$\left.-\alpha_i\gamma_3(\bar{E},\eta_{gi})\left(\frac{1}{\bar{m}_{l,i}^{+}}-\frac{1}{\bar{m}_{l,i}^{-}}\right)\right],$$

$$\bar{R}_{9,i}(\bar{E},\bar{k}_x,\bar{k}_y,\eta_{gi}) = \left[\gamma_2(\bar{E},\eta_{gi})+\gamma_3(\bar{E},\eta_{gi})\alpha\frac{\hbar^2}{2}k_s^2\left(\frac{1}{\bar{m}_{l,i}^{+}}-\frac{1}{\bar{m}_{l,i}^{-}}\right)\right.$$

$$\left.-\frac{\hbar^2}{2}k_s^2\left(\frac{1}{\bar{m}_{l,i}^{+}}-\frac{1}{\bar{m}_{l,i}^{-}}\right)-\frac{\alpha\hbar^6}{4}\frac{k_s^4}{m_{t,i}^{-}m_{t,i}^{+}}\right],$$

$$\bar{a}_5 = \left[\sqrt{\frac{\bar{m}_2^*}{\bar{m}_1^*}+1}\right]^2\left[4\left(\frac{\bar{m}_2^*}{\bar{m}_1^*}\right)^{1/2}\right]^{-1}$$

Therefore, the entropy in HD IV–VI, quantum wire EMSLs can be written as

$$\bar{k}_z^2 = \left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left(\bar{f}_{23}(\bar{E},\bar{k}_x,\bar{k}_y)\right)\right]^2-\bar{k}_s^2\right]\Bigg|\bar{k}_x = \frac{\bar{n}_x\pi}{\bar{d}_x}\ \textit{and}\ \bar{k}_y = \frac{\bar{n}_y\pi}{\bar{d}_y} \tag{6.39a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi \bar{L}_0} \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} \frac{\cos^{-1}\left\{\frac{1}{2}\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right\}\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\left[\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]' \bar{H}(\bar{E}-\bar{E}_{13,8})}{\left(\sqrt{\cos^{-1}\left\{\frac{1}{2}\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right\}^2 - \bar{L}_0^2\left\{\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2\right\}}\right)\sqrt{1-\frac{1}{4}\left[\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]^2}} \tag{6.39b}$$

where $\bar{E}_{13,8}$ is the sub-band energy and the sub-band equation in this case can be expressed as

$$0 = \left[\frac{1}{\bar{L}_0^2}\{\cos^{-1}(\bar{f}_{23}(\bar{E}_{13,8}, \bar{k}_x, \bar{k}_y))\}^2 - \bar{k}_s^2\right]\Bigg|\, \bar{k}_x = \frac{\bar{n}_x\pi}{\bar{d}_x} \text{ and } \bar{k}_y = \frac{\bar{n}_y\pi}{\bar{d}_y} \tag{6.39c}$$

EEM in this case is given by

$$\bar{m}^*(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2\bar{L}_0^2}\cos^{-1}\left[\frac{1}{2}\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right] \left[\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]' \left[1-\frac{1}{4}\left[\bar{f}_{23}\left(\bar{E}, \frac{\bar{n}_x\pi}{\bar{d}_x}, \frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]^2\right]^{-1/2} \tag{6.40}$$

The electron concentration can be written as

$$\bar{n}_{1D} = \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}_y=1}^{\bar{n}_{y\max}} [\tau_{21} + \tau_{22}] \tag{6.41}$$

where

$$\tau_{21} = \left[\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\{\bar{f}_{23}(\bar{E}, \bar{k}_x, \bar{k}_y)\}\right]^2 - \bar{k}_s^2\right]\Bigg|_{\bar{k}_x=\frac{\pi\bar{n}_x}{\bar{d}_x},\ \bar{k}_y=\frac{\pi\bar{n}_y}{\bar{d}_y}, \bar{E}=\bar{E}_{F611}}\right]^{1/2},$$

$$\tau_{22} = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\tau_{21}]$$

and $\bar{E}_{F611}$ is the Fermi energy in this case.

Using (1.31f) and (6.41), we can study the entropy in this case.

6.2.9 Entropy in HgTe/CdTe quantum wire HD effective mass SLs

Following Sasaki [24], the electron dispersion law in HDHgTe/CdTeEMSLs can be written

$$\bar{k}_z^2 = \Delta_{13H} + i\Delta_{14H}, \tag{6.42}$$

where,

$$\Delta_{13H} = \left[\frac{1}{\bar{L}_0^2}(\Delta_{11H}^2 - \Delta_{12H}^2) - \bar{k}_s^2\right]$$

$$\Delta_{11H} = \cos^{-1}\bar{p}_{6H}, \bar{p}_{6H} = \left[\frac{1 - \Delta_{9H}^2 - \Delta_{10H}^2 - \sqrt{(1 - \Delta_{9H}^2 - \Delta_{10H}^2)^2 + 4\Delta_{10H}^2}}{2}\right]^{1/2},$$

$$\Delta_{9H} = (\bar{a}_{1H}\cos\Delta_{5H}\cosh\Delta_{6H} - \bar{a}_{2H}\cos\Delta_{7H}\cosh\Delta_{6H}),$$

$$\Delta_{10H} = (\bar{a}_{1H}\sin\Delta_{5H}\sinh\Delta_{6H} + \bar{a}_{2H}\sin\Delta_{7H}\sinh\Delta_{6H}),$$

$$\Delta_{5H} = [\bar{a}_0\bar{C}_{22H}(\bar{E}, \bar{k}_{s,}, \eta_{g1}) + \bar{b}_0\bar{e}_3], \Delta_{6H} = \bar{b}_0\bar{e}_4, \Delta_{7H} = [\bar{a}_0\bar{C}_{22H}(\bar{E}, \bar{k}_{s,}, \eta_{g1}) - \bar{b}_0\bar{e}_3]$$

$$\bar{C}_{22H}(\bar{E}, \bar{k}_{s,}, \eta_{g1}) = \left[\frac{\bar{B}_{01}^2 + 2\bar{A}_1\bar{E} - \bar{B}_{01}(\bar{B}_{01}^2 + 4\bar{A}_1\bar{E})}{2\bar{A}_1^2}\right]^{1/2},$$

$$\bar{a}_{1H} = \left[\sqrt{\frac{\bar{M}_2(0,\eta_{g2})}{m_{c1}^*}} + 1\right]^2, \left[4\left(\frac{\bar{M}_2(0,\eta_{g2})}{m_{c1}^*}\right)^{1/2}\right]^{-1},$$

$$\bar{a}_{2H} = \left[\sqrt{\frac{\bar{M}_2(0,\eta_{g2})}{m_{c1}^*}} + 1\right]^2, \left[4\left(\frac{\bar{M}_2(0,\eta_{g2})}{m_{c1}^*}\right)^{1/2}\right]^{-1}$$

$$\Delta_{12H} = \cos^{-1}\bar{p}_{6H}, \Delta_{14H} = \frac{2\Delta_{11H}\Delta_{12H}}{L_0^2}$$

The entropy in HDHgTe/CdTe QWEMSLs can be written as

$$\bar{k}_z^2 = [\Delta_{13H} + \Delta_{14H}]|_{\bar{k}_X = \frac{\bar{n}_X\pi}{d_x}\ and\ \bar{k}_Y = \frac{\bar{n}_Y\pi}{d_y}} \tag{6.43a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi}\sum_{n_X=1}^{n_{X\max}}\sum_{n_Y=1}^{n_{Y\max}}\frac{\bar{H}(\bar{E} - \bar{E}_{13,9})[\Delta'_{13H} + i\Delta'_{14H}]}{\sqrt{\Delta_{13H} + i\Delta_{14H}}} \tag{6.43b}$$

where $\bar{E}_{13,9}$ is the sub-band energy and the sub-band equation in this case can be expressed as

$$0 = \left[\Delta_{13H} + i\Delta_{14H}\right]\Big|_{\bar{k}_X = \frac{\bar{n}_X \pi}{\bar{d}_X},\ \bar{k}_Y = \frac{\bar{n}_Y \pi}{\bar{d}_Y}\ and\ \bar{E} = \bar{E}_{13,9}} \tag{6.43c}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E}, \eta_g, \bar{n}_x, \bar{n}_y) = \frac{\hbar^2}{2}\Delta'_{13H} \tag{6.44}$$

The electron concentration can be written as

$$\bar{n}_{1D} = \text{Real part of} \sum_{\bar{n}_X=1}^{\bar{n}_{X\max}} \sum_{\bar{n}_Y=1}^{\bar{n}_{Y\max}} [\tau_{23} + \tau_{24}] \tag{6.45}$$

where

$$\tau_{23} = \left[\left[\Delta_{13H} + i\Delta_{14H}\right]\Big|_{\bar{k}_X = \frac{\pi\bar{n}_X}{\bar{d}_X},\ \bar{k}_Y = \frac{\pi\bar{n}_Y}{\bar{d}_Y},\ \bar{E} = \bar{E}_{F614}}\right]^{1/2},$$

$$\tau_{24} = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\tau_{23}]$$

and $\bar{E}_{F614}$ is the Fermi energy in this case

Using (1.31f) and (6.45), we can study the entropy in this case.

6.2.10 Entropy in strained layer quantum wire HD effective mass SLs

The dispersion relation of the constituent materials of HD III–V SLs can be written as

$$\bar{P}_i(\bar{E}, \eta_{gi})k_x^2 + \bar{Q}_i(\bar{E}, \eta_{gi})\bar{k}_y^2 + \bar{S}_i(\bar{E}, \eta_{gi})k_z^2 = 1 \tag{6.46}$$

where

$$\bar{P}_i(\bar{E}, \eta_{gi}) = (\gamma_0(\bar{E}, \eta_{gi}) - \bar{I}_0\bar{T}_{1i})(\bar{\Delta}_i(\bar{E}, \eta_{gi}))^{-1},\ \ \bar{I}_0 = (1/2)[1 + Erf(\bar{E}/\eta_{gi})],$$

$$\bar{T}_{li} = [\bar{E}_{gi} - \bar{C}_{li}^c\varepsilon_i - (\bar{a}_i + \bar{C}_{li}^c)\varepsilon_i(3/2)\bar{b}_i\varepsilon_{xxi} - (\bar{b}\varepsilon_i/2) + (\sqrt{3\bar{d}_i\varepsilon_{xyi}}/2)],$$

$$\Delta_i(\bar{E}, \eta_{gi}) = [(-\bar{q}_i\eta_{gi}^3/2\sqrt{\pi})\exp(-(\bar{E}^2/\eta_{gi}^2))[1 + (E^2/\eta_{gi}^2)] - \bar{R}_i\theta_i(\bar{E}, \eta_{gi}) + \bar{V}_i\gamma_0(\bar{E}, \eta_{gi})$$

$$+ (\zeta_i/2)[1 + Erf(\bar{E}/\eta_{gi})]],\ \bar{q}_i = (3/2\bar{B}_{2i}^2),\ \bar{R}_i = \bar{q}_i[2\bar{A}_i + \bar{C}_{li}^c\varepsilon_i],\ \bar{A}_i = \bar{E}_{gi} - \bar{C}_{li}^c\varepsilon_i,$$

$$\bar{V}_i = \bar{q}_i[\bar{A}_i^2 - (2\bar{C}_{2i}^2\varepsilon_{xyi}/3) + 2\bar{A}_i\bar{C}_{li}^c\varepsilon_i],\ \zeta_i = \bar{q}_i[(2\bar{C}_{2i}^2\varepsilon_{xyi}/3) - \bar{C}_{li}^c\varepsilon_i\bar{A}_i^2],$$

$$\bar{Q}_i(\bar{E},\eta_{gi}) = (\gamma_0(\bar{E},\eta_{gi}) - \bar{I}_0\bar{T}_{2i})(\bar{\Delta}_i(\bar{E},\eta_{gi}))^{-1},$$

$$\bar{T}_{2i} = \left[\bar{E}_{gi} - \bar{C}^c_{li}\varepsilon_i - (\bar{a}_i + \bar{C}^c_{li})\varepsilon_i + (3/2)\bar{b}_i\varepsilon_{xyi} - (\bar{b}_i\varepsilon_i/2) - \left(\sqrt{3\bar{d}_i\varepsilon_{xyi}}/2\right)\right],$$

$$\bar{S}_i(\bar{E},\eta_{gi}) = (\gamma_0(\bar{E},\eta_{gi}) - \bar{I}_0\bar{T}_{3i})(\bar{\Delta}_i(\bar{E},\eta_{gi}))^{-1}$$

$$\bar{T}_{3i} = [\bar{E}_{gi} - \bar{C}^c_{li}\varepsilon_i + (\bar{a}_i + \bar{C}^c_{li})\varepsilon_i + (3/2)\bar{b}_i\varepsilon_{zzi} - (\bar{b}_i\varepsilon_i/2)],$$

Therefore entropy in HD IV–VI, quantum wire EMSLs can be written as

$$\bar{k}_z{}^2 = \left[\frac{1}{\bar{L}_0^2}\{\cos^{-1}(\bar{f}_{40}(\bar{E},\bar{k}_x,\bar{k}_y))\}^2 - \bar{k}_s^2\right]\Bigg|_{\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x}\ and\ \bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y}} \tag{6.47a}$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{\bar{g}_v}{\pi L_0}\sum_{\bar{n}_x=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_x=1}^{\bar{n}_{y\max}} \frac{\left(\cos^{-1}\left\{\frac{1}{2}\bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right\}\bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\left[\bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]'\bar{H}(\bar{E}-\bar{E}_{13,10})\right)}{\sqrt{\cos^{-1}\left\{\frac{1}{2}\bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right\}^2 - \bar{L}_0^2\left\{\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 + \left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2\right\}}\sqrt{1-\frac{1}{4}\left[\bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]^2}} \tag{6.47b}$$

where $\bar{E}_{13,10}$ is the sub-band energy and the sub-band equation in this case can be expressed as

$$0 = \left[\frac{1}{\bar{L}_0^2}\{\cos^{-1}(\bar{f}_{40}(\bar{E}_{13,10},\bar{k}_x,\bar{k}_y))\}^2 - k_s^2\right]\Bigg|_{\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x}\ and\ \bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y}} \tag{6.47c}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}_x,\bar{n}_y) = \frac{\hbar^2}{2\bar{L}_0^2}\cos^{-1}\left[\frac{1}{2}\ \bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right] \left[\bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]'\left[1-\frac{1}{4}\left[\bar{f}_{40}\left(\bar{E},\frac{\bar{n}_x\pi}{\bar{d}_x},\frac{\bar{n}_y\pi}{\bar{d}_y}\right)\right]^2\right]^{-1/2} \tag{6.48a}$$

The electron concentration can be written as

$$\bar{n}_{1D} = \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[\tau_{40}+\tau_{41}] \tag{6.48b}$$

where

$$\tau_{40} = \left[\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\{\bar{f}_{40}(\bar{E},\bar{k}_x,\bar{k}_y)\}\right]t^2 - k_s^2\right]\Bigg|_{\bar{k}_x=\frac{\pi\bar{n}_x}{d_x},\ \bar{k}_y=\frac{\pi\bar{n}_y}{d_y}\ and\ \bar{E}=\bar{E}_{F615}}\right]^{1/2},$$

$$\tau_{41} = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\tau_{40}]$$

and $\bar{E}_{F615}$ is the Fermi energy in this case.

Using (1.31f) and (6.48b), we can study the entropy in this case.

6.3 Results and discussion

Using the appropriate equations and the band constants from Appendix 15, the entropy in HD QW III–V SLs (taking GaAs/$Ga_{1-x}Al_xAs$ and $In_xGa_{1-x}As$/InP QW SLs) with graded interfaces has been plotted as functions of the film thickness and impurity concentration at 10 K, respectively, as shown in Figures 6.1 and 6.2, respectively.

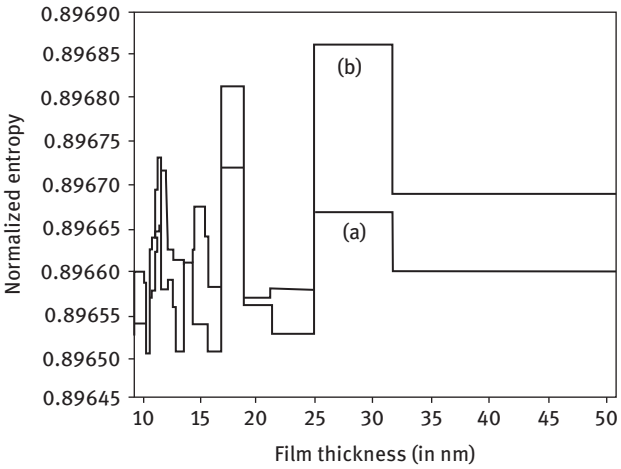

Figure 6.1: Plot of the normalized entropy in (a) GaAs/$Ga_{1-x}Al_xAs$ and (b) $In_xGa_{1-x}As$/InP HD quantum wire SLs with graded interfaces as a function of film thickness.

The normalized entropy has been plotted for (a) CdS/ZnSe with $\bar{\lambda}_o = 0$, (b) CdS/ZnSe with $\bar{\lambda}_o \neq 0$ (c) HgTe/CdTe and (d) PbSe/PbTe HD quantum wire SLs with graded interfaces as functions of film thickness and impurity concentration in Figures 6.3 and 6.4, respectively. The entropy in GaAs/$Ga_{1-x}Al_xAs$, HgTe/CdTe, CdS/ZnSe, HgTe/$Hg_{1-x}Cd_xTe$ and PbSe/PbTe quantum wire effective mass SLs have been plotted as functions of film thickness and impurity concentration in Figures 6.5 and 6.6, respectively.

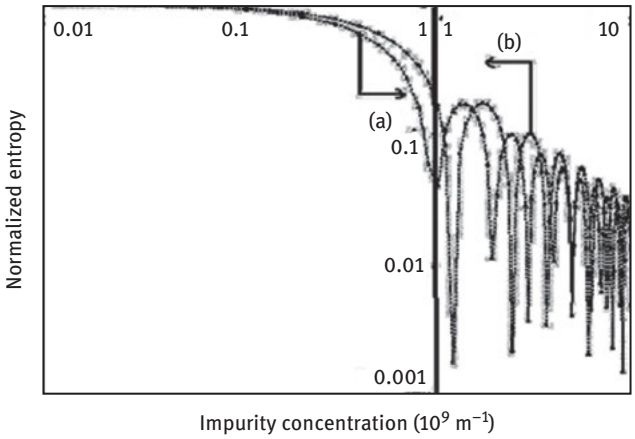

Figure 6.2: Plot of the normalized entropy in (a) GaAs/$Ga_{1-x}Al_xAs$ and (b) $In_xGa_{1-x}As$/InP HD quantum wire SLs with graded interfaces as a function of impurity concentration.

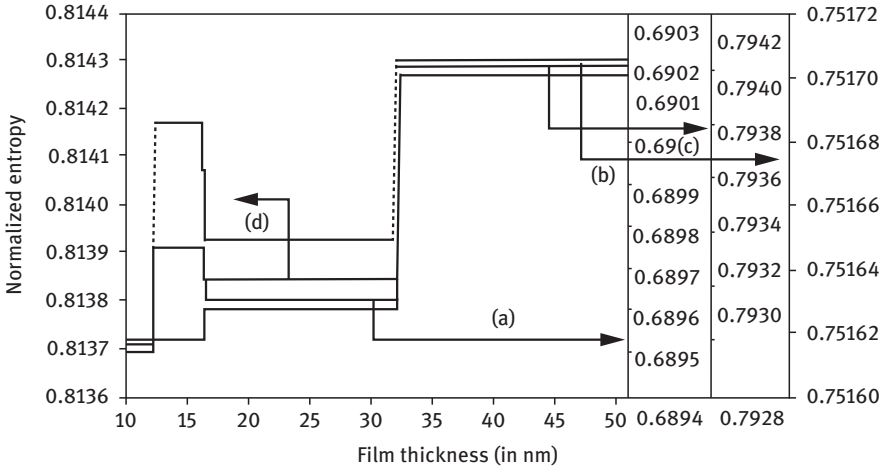

Figure 6.3: Plot of the entropy in (a) CdS/ZnSe with $\bar{\lambda}_o = 0$, (b) CdS/ZnSe with $\bar{\lambda}_o \neq 0$ (c) HgTe/CdTe and (d) PbSe/PbTe HD quantum wire SLswith graded interfaces as a function of film thickness.

The effect of size quantization is clearly exhibited by Figures 6.1 and 6.3, in which the composite fluctuations are due to the combined influence of the Landau quantization effect (due to magnetic field) with the size quantization effect. It also appears from the same figures that the entropy bears step functional dependency function of film thickness due to the Van Hove Singularity. Since the Fermi level decreases with the increase in the film thickness, the entropy increases. This physical fact

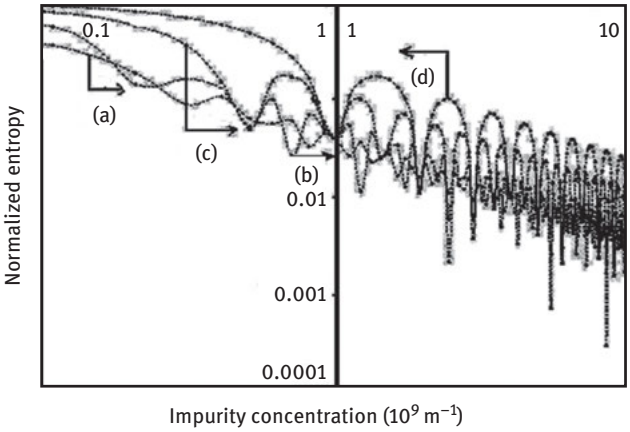

Figure 6.4: Plot of the entropy in (a) CdS/ZnSe with $\bar{\lambda}_o = 0$, (b) CdS/ZnSe with $\bar{\lambda}_o \neq 0$ (c) HgTe/CdTe and (d) PbSe/PbTe HD quantum wire SLs with graded interfaces as a function of impurity concentration.

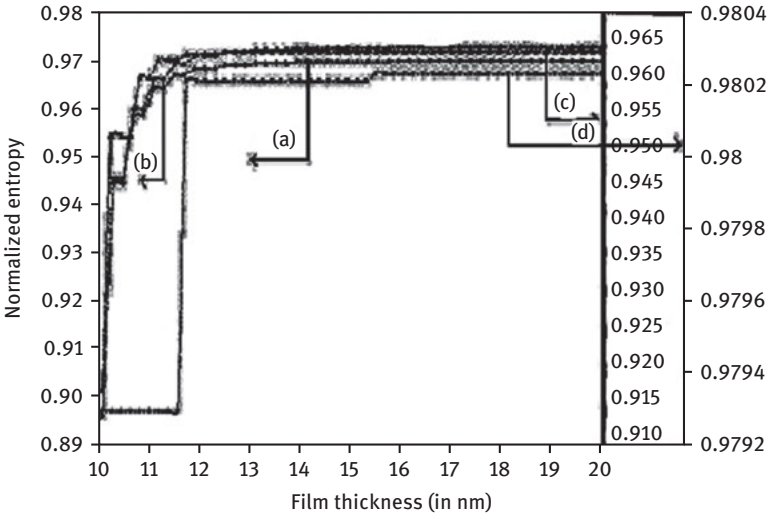

Figure 6.5: Plot of the entropy in (a) GaAs/$Ga_{1-x}Al_xAs$, (b) CdS/ZnSe, (c) HgTe/CdTe and (d) PbSe/PbTe HD quantum wire effective mass SLs as a function of film thickness.

also governs the nature of oscillatory variation of all the curves where the change in film thickness with respect to entropy for all type of SLs appears. The entropy changes with film thickness in oscillatory manner, where the nature of oscillations is totally different. It should also be noted that the entropy decreases with the increasing carrier degeneracy exhibiting different types of oscillations as is observed

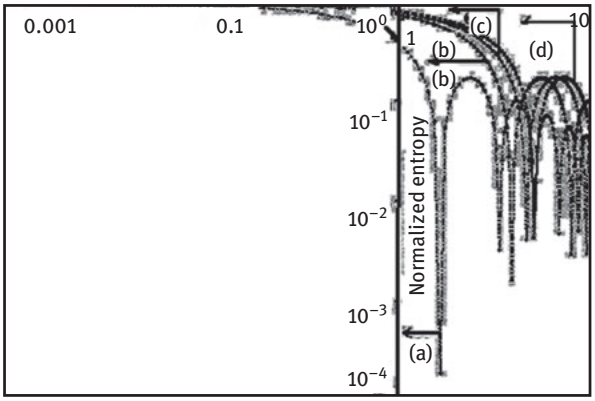

Figure 6.6: Plot of the entropy in (a) GaAs/$Ga_{1-x}Al_xAs$, (b) CdS/ZnSe, (c) HgTe/CdTe and (d) PbSe/PbTe HD quantum wire effective mass SLsas a function of impurity concentration.

from Figure 6.2. It may be also noted that due to the confinement of carriers along two orthogonal directions, the entropy exhibits the composite oscillations in Figures 6.1 and 6.3, while in Figures 6.2 and 6.4, the absence of composite oscillation are due to the suppression of the size quantization number along one direction by another. It appears from Figure 6.5 that the entropy in GaAs/$Ga_{1-x}Al_xAs$, CdS/ZnSe, HgTe/CdTe and PbSe/PbTe HD quantum wire effective mass SLs also exhibits such composite oscillations with increasing film thickness. The nature of oscillation in effective mass SLs are radically different than that of the corresponding graded interfaces which is the direct signature of the difference in band structure in the respective cases as found from all the respective corresponding figures.

From Figure 6.6, we observe that the entropy in the aforementioned case decreases with increasing impurity concentration and differ widely for large values of impurity concentration, whereas for relatively small values of the carrier degeneracy, the entropy converges to a single value in the whole range of the impurity concentration considered.

6.4 Open research problem

(R6.1) Investigate all the appropriate problems of Chapter 3 for all types of quantum wire SLs in the presence of strain.

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7 Entropy in quantum dot HDSLs

It is much better to know something about your own pin pointed topic of research than to know everything about one thing.

7.1 Introduction

In this chapter, the entropy from III–V, II–VI, IV–VI, HgTe/CdTe and strained layer quantum dot heavily doped superlattices (QDHDSLs) with graded interfaces [1–10] has been studied in Sections 7.2.1 to 7.2.5. From Sections 7.2.6 to 7.2.10, the entropy from III–V, II–VI, IV–VI, HgTe/CdTe and strained layer quantum dot heavily doped effective mass SLs [6–10], respectively, has been presented. Section 7.3 contains the summary and conclusion pertinent to this chapter. Section 7.4 presents 14 open research problems.

7.2 Theoretical background

7.2.1 Entropy in III–V quantum dot HD SLs with graded interfaces

The simplified DR of heavily doped quantum dot III–V SLs with graded interfaces can be expressed as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right) = \left[\bar{G}_8 + i\bar{H}_8\right]\Big|_{\bar{k}_X = \frac{\bar{n}_X\pi}{\bar{d}_x} \text{ and } \bar{k}_y = \frac{\bar{n}_y\pi}{\bar{d}_y}\ \bar{E} - \bar{E}_{14,1}} \tag{7.1}$$

where $\bar{E}_{14,1}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{n}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\delta'(\bar{E}-\bar{E}_{14,1}) \tag{7.2}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{7,1}) \tag{7.3}$$

where $\eta_{7,1} = \frac{\bar{E}_{F7,1}-\bar{E}_{14,1}}{k_B\bar{T}}$ and $\bar{E}_{F7,1}$ is the Fermi energy in this case.

Using (1.31f) and (7.3), we can study the entropy in this case.

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7.2.2 Entropy in II–VI quantum dot HD SLs with graded interfaces

The simplified DR of heavily doped quantum dot III–V SLs with graded interfaces can be expressed as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \left[\bar{G}_{19} + i\bar{H}_{19}\right]\Big|_{\bar{k}_X = \frac{\bar{n}_x\pi}{\bar{d}_x}\, and\, \bar{k}_Y = \frac{\bar{n}_y\pi}{\bar{d}_y}\, \bar{E} - \bar{E}_{14,2}} \tag{7.4}$$

where $\bar{E}_{14,2}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{n}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{max}}}\delta'(\bar{E} - \bar{E}_{14,2}) \tag{7.5}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{max}}}\bar{F}_{-1}(\eta_{7,2}) \tag{7.6}$$

where $\eta_{7,2} = \frac{\bar{E}_{F7,2} - \bar{E}_{14,2}}{k_B\bar{T}}$ and $\bar{E}_{F7,2}$ is the Fermi energy in this case.

Using (1.31f) and (7.6), we can study the entropy in this case.

7.2.3 Entropy in IV–VI quantum dot HD SLs with graded interfaces

The simplified DR in heavily doped quantum dot IV–VI SLs with graded interfaces can be expressed as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_2(\bar{E}_{14,3}, \bar{k}_s)\right\}\right]^2 - \bar{k}_s^2\right]\Big|_{\bar{k}_X = \frac{n_x\pi}{d_x}\, and\, \bar{k}_Y = \frac{\bar{n}_y\pi}{d_y}} \tag{7.7}$$

where $\bar{E}_{14,3}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{n}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{max}}}\delta'(\bar{E} - \bar{E}_{14,3}) \tag{7.8}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x_{max}}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y_{max}}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z_{max}}}\bar{F}_{-1}(\eta_{7,3}) \tag{7.9}$$

where $\eta_{7,3} = \frac{\bar{E}_{F7,3} - \bar{E}_{14,3}}{k_B \bar{T}}$ and $\bar{E}_{F7,3}$ is the Fermi energy in this case.

Using (1.31f) and (7.9), we can study the entropy in this case.

7.2.4 Entropy in HgTe/CdTe quantum dot HD SLs with graded interfaces

The simplified DR of heavily doped quantum dot III–V SLs with graded interfaces can be expressed as

$$\left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2 = [\bar{G}_{192} + \bar{i}\bar{H}_{192}]\Big|_{\bar{k}_X = \frac{\bar{n}_X \pi}{\bar{d}_x}, \bar{k}_Y = \frac{\bar{n}_Y \pi}{\bar{d}_y} \text{ and } \bar{E} - \bar{E}_{14,4}} \tag{7.10}$$

where $\bar{E}_{14,4}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{n}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \delta'(\bar{E} - \bar{E}_{14,4}) \tag{7.11}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}} \sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}} \sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}} \bar{F}_{-1}(\eta_{7,4}) \tag{7.12}$$

where $\eta_{7,4} = \frac{\bar{E}_{F7,4} - \bar{E}_{14,4}}{k_B \bar{T}}$ and $\bar{E}_{F7,4}$ is the Fermi energy in this case.

Using (1.31f) and (7.12), we can study the entropy in this case.

7.2.5 Entropy in strained layer quantum dot HD SLs with graded interfaces

DR of the conduction electrons in heavily doped strained layer quantum dot SL with graded interfaces can be expressed as

$$\left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right) = \left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_6(\bar{E}_{14,5}, \bar{k}_s)\right\}\right]^2 - \bar{k}_s^2\right]\Big|_{\bar{k}_X = \frac{\bar{n}_X \pi}{\bar{d}_x} \text{ and } \bar{k}_Y = \frac{\bar{n}_Y \pi}{\bar{d}_y}} \tag{7.13}$$

where $\bar{E}_{14,5}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{n}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x \bar{d}_y \bar{d}_z} \sum_{n_x=1}^{n_{x_{\max}}} \sum_{n_y=1}^{n_{y_{\max}}} \sum_{n_z=1}^{n_{z_{\max}}} \delta'(\bar{E} - \bar{E}_{14,5}) \tag{7.14}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{7,6}) \tag{7.15}$$

where $\eta_{7,5} = \frac{\bar{E}_{F7,6} - \bar{E}_{14,6}}{k_B\bar{T}}$ and $\bar{E}_{F7,6}$ is the Fermi energy in this case.

Using (1.31f) and (7.15), we can study the entropy in this case.

7.2.6 Entropy in III–V quantum dot HD effective mass SLs

DR in III–V heavily doped effective mass quantum dot SLs can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right) = [\delta_7 + i\delta_8]\Big|_{\bar{k}_X = \frac{\bar{n}_x\pi}{\bar{d}_x}, \bar{k}_Y = \frac{\bar{n}_y\pi}{\bar{d}_y}\ and\ \bar{E} - \bar{E}_{14,6}} \tag{7.16}$$

where $\bar{E}_{14,6}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{n}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\delta'(\bar{E} - \bar{E}_{14,6}) \tag{7.17}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{7,6}) \tag{7.18}$$

where $\eta_{7,6} = \frac{\bar{E}_{F7,6} - \bar{E}_{14,6}}{k_B\bar{T}}$ and $\bar{E}_{F7,6}$ is the Fermi energy in this case.

Using (1.31f) and (7.18), we can study the Entropy in this case.

7.2.7 Entropy in II–VI quantum dot HD effective mass SLs

DR in III–V heavily doped effective mass quantum dot SLs can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right) = [\delta_{13} + i\delta_{14}]\Big|_{\bar{k}_X = \frac{\bar{n}_x\pi}{\bar{d}_x}, \bar{k}_Y = \frac{\bar{n}_y\pi}{\bar{d}_y}\ and\ \bar{E} - \bar{E}_{14,6}} \tag{7.19}$$

where $\bar{E}_{14,7}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{n}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\delta'(\bar{E} - \bar{E}_{14,7}) \tag{7.20}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{7,7}) \tag{7.21}$$

where $\eta_{7,7} = \frac{\bar{E}_{F7,7} - \bar{E}_{14,7}}{k_B\bar{T}}$ and $\bar{E}_{F7,7}$ is the Fermi energy in this case.

Using (1.31f) and (7.21), we can study the entropy in this case.

7.2.8 Entropy in IV–VI quantum dot HD effective mass SLs

DR_in heavily doped IV–VI, quantum dot EMSLs can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\bar{f}_{23}(\bar{E}_{14,8},\bar{k}_x,\bar{k}_y)\right\}\right]^2 - \bar{k}_s^2\right]\Big|_{\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x}\,and\,\bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y}} \tag{7.22}$$

where $\bar{E}_{14,8}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{0QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\delta'(\bar{E}-\bar{E}_{14,8}) \tag{7.23}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x_{\max}}}\sum_{\bar{n}_y=1}^{\bar{n}_{y_{\max}}}\sum_{\bar{n}_z=1}^{\bar{n}_{z_{\max}}}\bar{F}_{-1}(\eta_{7,8}) \tag{7.24}$$

where

$$\eta_{7,8} = \frac{\bar{E}_{F7,8} - \bar{E}_{14,8}}{\bar{k}_B\bar{T}}$$

and $\bar{E}_{F7,8}$ is the Fermi energy in this case.

Using (1.31f) and (7.24), we can study the entropy in this case.

7.2.9 Entropy in HgTe/CdTe quantum dot HD effective mass SLs

DR in heavily doped HgTe/CdTe QWEMSLs can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \left[\Delta_{13H} + i\Delta_{14H}\right]\Big|_{\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x},\ \bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y}\ and\ \bar{E}=\bar{E}_{14,9}} \tag{7.25}$$

where $\bar{E}_{14,9}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x\max}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y\max}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z\max}}\delta'(\bar{E}-\bar{E}_{14,9}) \tag{7.26}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x\max}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y\max}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{7,9}) \tag{7.27}$$

where $\eta_{7,9} = \frac{\bar{E}_{F7,9}-\bar{E}_{14,9}}{k_B\bar{T}}$ and $\bar{E}_{F7,9}$ is the Fermi energy in this case.

Using (1.31f) and (7.27), we can study the entropy in this case.

7.2.10 Entropy in strained layer quantum dot HD effective mass SLs

DR in heavily doped IV–VI, quantum dot EMSLs can be written as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\bar{f}_{40}(\bar{E}_{14,10},\bar{k}_x,\bar{k}_y)\right\}\right]^2 - \bar{k}_s^2\right]\Bigg|_{\bar{k}_x=\frac{\bar{n}_x\pi}{\bar{d}_x}\,and\,\bar{k}_y=\frac{\bar{n}_y\pi}{\bar{d}_y}} \tag{7.28}$$

where $\bar{E}_{14,10}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{QDSL}(\bar{E}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x\max}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y\max}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z\max}}\delta'(\bar{E}-\bar{E}_{14,10}) \tag{7.29}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_{x=1}}^{\bar{n}_{x\max}}\sum_{\bar{n}_{y=1}}^{\bar{n}_{y\max}}\sum_{\bar{n}_{z=1}}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{7,10}) \tag{7.30}$$

where $\eta_{7,10} = \frac{\bar{E}_{F7,10}-\bar{E}_{14,10}}{k_B\bar{T}}$ and $\bar{E}_{F7,10}$ is the Fermi energy in this case.

Using (1.31f) and (7.30), we can study the entropy in this case.

7.3 Results and discussion

Using the band constants from appendix 15, the normalized entropy in this case in $HgTe/Hg_{1-x}Cd_xTe$, $CdS/ZnSe$, $PbSe/PbTe$ and $HgTe/CdTe$HD quantum dot SLs with graded interfaces have been plotted as a function of film thickness as shown by curves (a), (b), (c), and (d), respectively, in Figure 7.1. Figure 7.2 demonstrates the

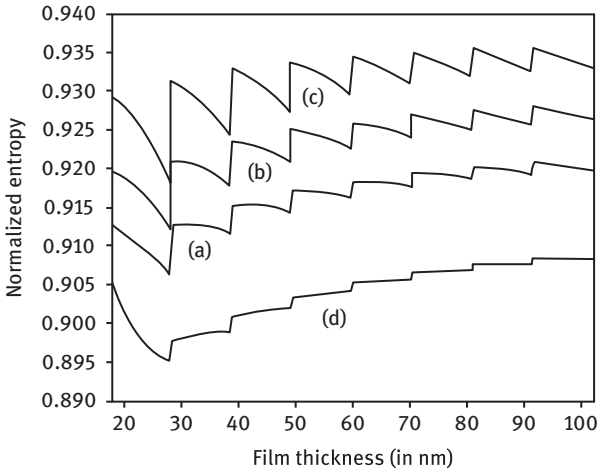

Figure 7.1: Plot of the entropy in (a) HgTe/$Hg_{1-x}Cd_xTe$, (b) CdS/ZnSe, (c) PbSe/PbTe, and (d) HgTe/CdTe HD quantum dot SLs with graded interfaces as a function offilm thickness.

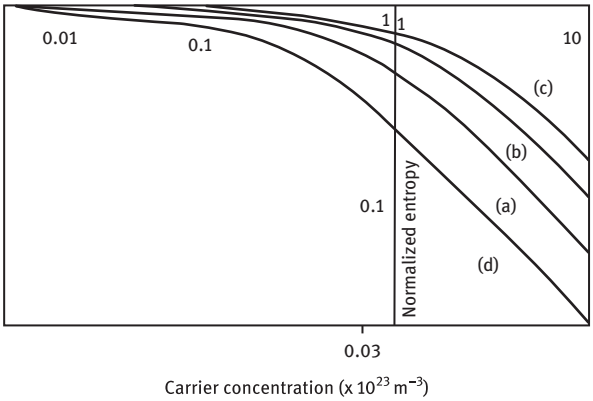

Figure 7.2: Plot of the entropy in (a) HgTe/$Hg_{1-x}Cd_xTe$, (b) CdS/ZnSe, (c) PbSe/PbTe, and (d) HgTe/CdTe HD quantum dot SLs with graded interfaces as a function of carrier concentration.

normalized entropy for the said quantized structures as a function of impurity concentration. Figure 7.3 exhibits the normalized entropy as a function of film thickness in $HgTe/Hg_{1-x}Cd_xTe$, $CdS/ZnSe$, $PbSe/PbTe$ and $HgTe/CdTe$ HD quantum dot effective mass SLs as shown by curves (a), (b), (c), and (d), respectively. The normalized entropy in $HgTe/Hg_{1-x}Cd_xTe$, $CdS/ZnSe$, $PbSe/PbTe$ and $HgTe/CdTe$HD quantum dot effective mass SLs has been plotted as a function of electron concentration in Figure 7.4.

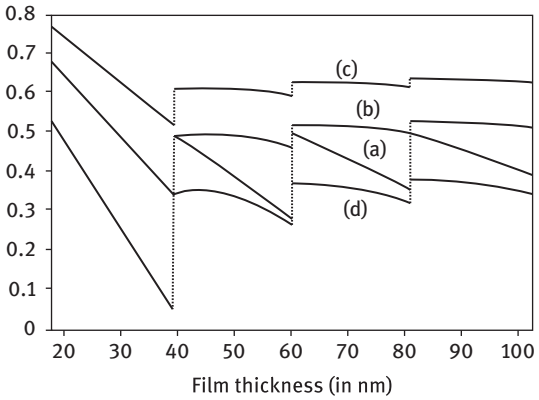

Figure 7.3: Plot of the entropy in (a) $HgTe/Hg_{1-x}Cd_xTe$, (b) CdS/ZnSe, (c) PbSe/PbTe, and (d) HgTe/CdTeHD quantum dot effective mass SLs as a function of film thickness.

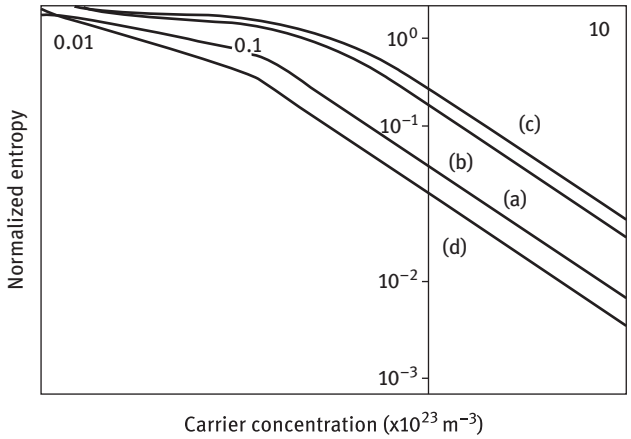

Figure 7.4: Plot of the entropy in (a) $HgTe/Hg_{1-x}Cd_xTe$, (b) CdS/ZnSe, (c) PbSe/PbTe, and (d) HgTe/CdTeHD quantum dot effective mass SLs as a function of carrier concentration.

It appears from Figure 7.1 that the entropy in $HgTe/Hg_{1-x}Cd_xTe$, $CdS/ZnSe$, $PbSe/PbTe$ and $HgTe/CdTe$ HD quantum dot SLs with graded interfaces increases with increasing film thickness exhibiting quantum jumps for fixed values of film thickness depending on the values of the energy band constants of the particular quantized structures. It is observed from Figure 7.2 that the entropy in quantum dots of aforementioned SLs decreases with increasing carrier degeneracy and differ widely for large values of same whereas for relatively small values of electron concentration, the entropy exhibits a converging behavior. From Figure 7.3, it is observed that the TPSM in $HgTe/Hg_{1-x}Cd_xTe$, $CdS/ZnSe$, $PbSe/PbTe$ and $HgTe/CdTe$ quantum dot effective

mass SLs oscillates with increasing film thickness. From Figure 7.4, it appears that the entropy of the aforementioned SLs decrease with increasing concentration. It should be noted that all types of variations of entropy with respect to thickness and concentration are basically band structure dependent.

It may further be noted that the entropy of a two-dimensional electron gas in the presence of a periodic potential has already been formulated in the literature. SL is a three-dimensional system under periodic potential. There is a radical difference in the dispersion relations of the 3D quantized structures and the corresponding carrier energy spectra of the 2D systems. From the dispersion relations of various SLs as discussed in this chapter, the energy spectra of the various other types of low-dimensional systems can be formulated and the corresponding entropy can also be investigated. The results will be fundamentally different in all cases due to system asymmetry together with the change in the respective wave functions exhibiting new physical features in the respective cases. Therefore, it appears that the dispersion law and the corresponding wave function

play a cardinal role in formulating any electronic property of any electronic material, since they change in a fundamental way in the presence of dimension reduction. Consequently, the derivations and the respective physical interpretations of the different transport quantities change radically.

It is imperative to state that our investigations excludes the many-body, hot electron, spin, broadening and the allied quantum dot and SL effects in this simplified theoretical formalism due to the absence of proper analytical techniques for including them for the generalized systems as considered here. Our simplified approach will be appropriate for the purpose of comparison when the methods of tackling the formidable problems after inclusion of the said effects for the generalized systems emerge. Finally, it may be noted that the inclusion of the said effects would certainly increase the accuracy of the results although the qualitative features of the entropy would not change in the presence of the aforementioned effects.

7.4 Open research problems

(R 7.1) Investigate the entropy in the absence of magnetic field by considering all types of scattering mechanisms for III–V, II–VI, IV–VI and HgTe/CdTe SLs with graded interfaces and also the effective mass SLs of the aforementioned materials with the appropriate dispersion relations as formulated in this chapter.

(R 7.2) Investigate the entropy in the absence of magnetic field by considering all types of scattering mechanisms for strained layer, random, short period, Fibonacci, polytype and saw-toothed SLs, respectively.

(R 7.3) Investigate the entropy in the absence of magnetic field by considering all types of scattering mechanisms for (R3.1) and (R3.2) under an arbitrarily

oriented (a) nonuniform electric field and (b) alternating electric field, respectively.

(R 7.4) Investigate the entropy by considering all types of scattering mechanisms for (R3.1) and (R3.2) under an arbitrarily oriented alternating magnetic field by including broadening and the electron spin, respectively.

(R 7.5) Investigate the entropy by considering all types of scattering mechanisms for (R3.1) and (R3.2) under an arbitrarily oriented alternating magnetic field and crossed alternating electric field by including broadening and the electron spin, respectively.

(R 7.6) Investigate the entropy by considering all types of scattering mechanisms for (R3.1) and (R3.2) under an arbitrarily oriented alternating magnetic field and crossed alternating non-uniform electric field by including broadening and the electron spin, respectively.

(R 7.7) Investigate the entropy in the absence of magnetic field for all types of SLs as considered in this chapter under exponential, Kane, Halperin, Lax and Bonch-Bruevich band tails [30], respectively.

(R 7.8) Investigate the entropy in the absence of magnetic field for the problem as defined in (R3.7) under an arbitrarily oriented (a) nonuniform electric field and (b) alternating electric field, respectively.

(R 7.9) Investigate the entropy for the problem as defined in (R3.7) under an arbitrarily oriented alternating magnetic field by including broadening and the electron spin, respectively.

(R 7.10) Investigate the entropy for the problem as defined in (R3.7) under an arbitrarily oriented alternating magnetic field and crossed alternating electric field by including broadening and the electron spin, respectively.

(R 7.11) Investigate the problems as defined in (R3.1) to (R3.10) for all types of quantum dot SLs as discussed in this chapter.

(R 7.12) Investigate the problems as defined in (R3.1) to (R3.10) for all types of quantum dot SLs as discussed in this chapter in the presence of strain.

(R 7.13) Introducing new theoretical formalisms, investigate all the problems of this chapter in the presence of hot electron effects.

(R 7.14) Investigate the influence of deep traps and surface states separately for all the appropriate problems of this chapter after proper modifications.

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8 Entropy in HDSLs under magnetic quantization

Real gentleness in a person is the power that sees, understands and yet interferes in a positive way.

8.1 Introduction

In this chapter, the magneto entropy in III–V, II–VI, IV–VI, HgTe/CdTe, and strained layerheavily doped superlattices (HDSLs) with graded interfaces [1–10] has been studied in Sections 8.2.1 to 8.2.5. From Sections 8.2.6 to 8.2.10, the magneto-entropy in III–V, II–VI, IV–VI, HgTe/CdTe and strained layer heavily doped (HD) effective mass superlattices (SL), respectively, has been presented. Section 8.3 contains the result and discussions pertinent to this chapter. Section 8.4 presents 14 open research problems.

8.2 Theoretical background

8.2.1 Entropy in III–VHD SLs with graded interfaces under magnetic quantization

The simplified DR of HD quantum well III–V SLs with graded interfaces under magnetic quantization can be expressed as

$$\bar{k}_z^2 = \bar{G}_{8,E,n} + i\bar{H}_{8E,n} \tag{8.1a}$$

where

$$\bar{G}_{8E,n} = \left[\frac{\bar{C}_{7E,n}^2 - \bar{D}_{7E,n}^2}{\bar{L}_0^2} - \left\{\frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right\}\right], \bar{C}_{7E,n} = \cos^{-1}(\omega_{7E,n}),$$

$$\omega_{7E,n} = (2)^{-\frac{1}{2}}\left[(1 - \bar{G}_{7E,n}^2 - \bar{H}_{7E,n}^2) - \sqrt{(1 - \bar{G}_{7E,n}^2 - \bar{H}_{7E,n}^2)^2 + 4\bar{G}_{7E,n}^2}\right]^{\frac{1}{2}}$$

$$\bar{G}_{7E,n} = \Big[\bar{G}_{1E,n} + (\rho_{5E,n}\bar{G}_{2E,n}/2) - (\rho_{6E,n}\bar{H}_{2E,n}/2)$$
$$+ (\Delta_0/2)\{\rho_{6E,n}\bar{H}_{2E,n} - \rho_{8E,n}\bar{H}_{3E,n} + \rho_{9E,n}\bar{H}_{4E,n} - \rho_{10E,n}\bar{H}_{4E,n}$$
$$\rho_{11E,n}\bar{H}_{5E,n} - \rho_{12E,n}\bar{H}_{5E,n} + (1/12)(\rho_{12E,n}\bar{G}_{6E,n} - \rho_{14E,n}\bar{H}_{6E,n})\}\Big],$$

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$$\bar{G}_{1E,n} = [(\cos(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))$$
$$+ (\sin(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))],$$

$$\bar{h}_{1E,n} = e_{1E,n}(\bar{b}_0 - \Delta_0), e_{1E,n=} 2^{-\frac{1}{2}}\left(\sqrt{\bar{t}_{1E,n}^2 + \bar{t}_2^2} + \bar{t}_{1E,n}\right)^{\frac{1}{2}}$$

$$\bar{t}_{1E,n} = \left[(2\bar{m}_{c1}^*/\hbar^2)\bar{T}_{11}(\bar{E}, \bar{E}_{g1}, \Delta_1\eta_{g1}) - \left\{\frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right\}\right],$$

$$\bar{t}_2 = (2\bar{m}_{c1}^*/\hbar^2)\bar{T}_{21}(\bar{E}, \bar{E}_{g1}, \Delta_1\eta_{g1})$$

$$\bar{h}_{2E,n} = e_{2E,n}(\bar{b}_0 - \Delta_0), e_{2E,n} = 2^{-\frac{1}{2}}\left(\sqrt{\bar{t}_{1E,n}^2 + \bar{t}_2^2} - \bar{t}_{1E,n}\right)^{\frac{1}{2}},$$

$$\bar{g}_{1E,n} = \bar{d}_{1E,n}(\bar{b}_0 - \Delta_0), \bar{d}_{1E,n} = 2^{-\frac{1}{2}}\left(\sqrt{\bar{x}_{1E,n}^2 + \bar{y}_1^2} - \bar{x}_{1E,n}\right)^{\frac{1}{2}}$$

$$\bar{x}_{1E,n} = \left[-(2\bar{m}_{c2}^*/\hbar^2)\bar{T}_{11}(\bar{E} - \bar{V}_0, \bar{E}_{g0}, \Delta_0\eta_{g2}) - \left\{\frac{2e\bar{B}}{\hbar}(\bar{n} + \frac{1}{2})\right\}\right],$$

$$\bar{y}_2 = (2\bar{m}_{c2}^*/\hbar^2)T_{22}(\bar{E} - \bar{V}_0, \bar{E}_{g2}, \Delta_2\eta_{g2})$$

$$\bar{g}_{2E,n} = \bar{d}_{2E,n}(\alpha_0 - \Delta_0), \bar{d}_{2E,n} = 2^{-\frac{1}{2}}\left(\sqrt{\bar{x}_{1E,n}^2 + \bar{y}_1^2} - \bar{x}_{1E,n}\right)^{\frac{1}{2}},$$

$$\rho_{5E,n} = (\rho_{3E,n}^2 + \rho_{4E,n}^2)^{-1}[\rho_{1E,n}\rho_{3E,n} - \rho_{2E,n}\rho_{4E,n}],$$

$$\rho_{1E,n} = [\bar{d}_{1E,n}^2 + e_{2E,n}^2 - \bar{d}_{2E,n}^2 - e_{1E,n}^2],\ \rho_{3E,n} = [\bar{d}_{1E,n}e_{1E,n} + \bar{d}_{2E,n}e_{2E,n}],$$

$$\rho_{2E,n} = 2[\bar{d}_{1E,n}\bar{d}_{2E,n} + e_{1E,n}e_{2E,n}],\ \rho_{4E,n} = [\bar{d}_{1E,n}e_{2E,n} - e_{1E,n}\bar{d}_{2E,n}],$$

$$\bar{G}_{2E,n} = [(\sin(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))$$
$$+ (\cos(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))],$$

$$\rho_{6E,n} = (\rho_{3E,n}^2 + \rho_{4E,n}^2)^{-1}[\rho_{1E,n}\rho_{4E,n} + \rho_{2E,n}\rho_{3E,n}],$$

$$\bar{H}_{2E,n} = [(\sin(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\sin(\bar{g}_{2E,n}))(\cosh(\bar{g}_{1E,n}))$$
$$- (\cos(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))],$$

$$\rho_{7E,n} = [(e_{1E,n}^2 + e_{2E,n}^2)^{-1}[e_{1E,n}(\bar{d}_{1E,n}^2 - \bar{d}_{2E,n}^2) - 2\bar{d}_{1E,n}\bar{d}_{2E,n}e_{2E,n}] - 3e_{1E,n}],$$

$$\bar{G}_{3E,n} = [(\sin(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))$$
$$+ (\cos(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))],$$

$$\rho_{8E,n} = [(e_{1E,n}^2 + e_{2E,n}^2)^{-1}[e_{2E,n}(\bar{d}_{1E,n}^2 - \bar{d}_{2E,n}^2) - 2\bar{d}_{1E,n}\bar{d}_{2E,n}e_{1E,n}] + 3e_{2E,n}],$$

$$\bar{H}_{3E,n} = [(\sin(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\sin(\bar{g}_{2E,n}))(\sinh(\bar{g}_{1E,n}))$$
$$-(\cos(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))],$$

$$\rho_{9E,n} = [(\bar{d}_{1E,n}^2 + \bar{d}_{2E,n}^2)^{-1}[\bar{d}_{2E,n}(e_{1E,n}^2 - e_{2E,n}^2) + 2e_{1E,n}\bar{d}_{2E,n}e_{1E,n}] + 3\bar{d}_{1E,n}],$$

$$\bar{G}_{4E,n} = [(\cos(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\cos(\bar{g}_{2E,n}))(\sinh(\bar{g}_{1E,n}))$$
$$-(\sin(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))],$$

$$\rho_{10E,n} = [-(\bar{d}_{1E,n}^2 + \bar{d}_{2E,n}^2)^{-1}\bar{d}_{2E,n}(-e_{1E,n}^2 + e_{2E,n}^2) + 2e_{1E,n}\bar{d}_{2E,n}e_{1E,n}] + 3\bar{d}_{2E,n}]],$$

$$\bar{H}_{4E,n} = [(\cos(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))$$
$$+(\sin(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))],$$

$$\rho_{11E,n} = 2[\bar{d}_{1E,n}^2 + e_{2E,n}^2 - e_{2E,n}^2 - \bar{d}_{1E,n}^2],$$

$$\bar{G}_{5E,n} = [(\cos(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\cos(\bar{g}_{2E,n}))(\cosh(\bar{g}_{1E,n}))$$
$$-(\sin(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))],$$

$$\rho_{12E,n} = 4[\bar{d}_{1E,n} + \bar{d}_{2E,n} - e_{1E,n} + e_{2E,n}],$$

$$\bar{H}_{5E,n} = [(\cos(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))$$
$$+(\sin(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\cosh(\bar{g}_1))(\cosh(\bar{g}_2))],$$

$$\rho_{13E,n} = [\{5(\bar{d}_{1E,n} + e_{1E,n}^3 - 3e_{1E,n}e_{2E,n}^2 + \bar{d}_{2E,n}) + 5\bar{d}_{2E,n}, (e_{2E,n}^3 - 3e_{1E,n}^2e_{2E,n})\}$$
$$(\bar{d}_{1E,n}^2 + \bar{d}_{2E,n}^2)^{-1} + (e_{1E,n}^2 + e_{2E,n}^2)^{-1}\{5(-e_{1E,n} + \bar{d}_{2E,n}^3 - 3e_{2E,n}e_{1E,n}^2 + \bar{d}_{1E,n})$$
$$+5\bar{d}_{2E,n}, (-e_{1E,n}^3 - 3e_{2E,n}^2e_{1E,n})\}(\bar{d}_{1E,n}^2 + \bar{d}_{2E,n}^2)^{-1}$$
$$+34(\bar{d}_{1E,n}e_{2E,n} - \bar{d}_{2E,n}e_{1E,n})]$$

$$\bar{H}_{6E,n} = [(\sin(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))$$
$$-(\cos(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))],$$

$$\bar{H}_{7E,n} = [\bar{H}_{1E,n} + (\rho_{5E,n}\bar{H}_{2E,n}/2)$$
$$+(\rho_{6E,n}\bar{G}_{2E,n}/2) + (\Delta_0/2)\{\rho_{8E,n}\bar{G}_{3E,n} + \rho_{7E,n}\bar{H}_{3E,n} + \rho_{10E,n}\bar{G}_{4E,n} + \rho_{9E,n}\bar{H}_{4E,n}$$
$$+\rho_{12E,n}\bar{G}_{5E,n} + \rho_{11E,n}\bar{H}_{5E,n} + (1/12)(\rho_{14E,n}\bar{G}_{6E,n} + \rho_{13E,n}\bar{H}_{6E,n})\}]$$

$$\bar{H}_{1E,n} = [(\sin(\bar{h}_{1E,n}))(\sinh(\bar{h}_{2E,n}))(\cosh(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))$$
$$+(\cos(\bar{h}_{1E,n}))(\cosh(\bar{h}_{2E,n}))(\sinh(\bar{g}_{1E,n}))(\sin(\bar{g}_{2E,n}))],$$

$$\bar{D}_{7E,n} = \sinh^{-1}(\omega_{7E,n}), \bar{H}_{8E,n} = (2\bar{C}_{7E,n}\bar{D}_{7E,n}/\bar{L}_0^2)$$

The DOS function can be written a

$$\bar{N}(\bar{E}) = \frac{e\bar{B}}{2\pi^2\hbar}\sum_{\bar{n}=0}^{\bar{n}\max}\frac{(\overline{G'}_{8E,n} + i\overline{H'}_{8E,n})\bar{H}(\bar{E}-\bar{E}_{15,1})}{\sqrt{\bar{G}_{8E,n} + i\bar{H}_{8E,n}}} \tag{8.1b}$$

where $\bar{E}_{15,1}$ is the sub-band energy in this case and is given by

$$0 = [\bar{G}_{8E,n} + \bar{i}\bar{H}_{8E,n}]\Big|_{E=E_{15,1}} \tag{8.1c}$$

EEM can be written as

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2}\overline{G'}_{8E,n} \tag{8.2}$$

The electron statistics can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v eB}{\pi^2\hbar}\,\mathrm{Re}al\,part\,of\sum_{n=0}^{n_{\max}}[(\bar{G}_{8,E,n} + \bar{i}\bar{H}_{8,E,n})^{1/2}\Big|_{E_{F1321}}\sum_{r=1}^{s}L(r)[(\bar{G}_{8,E,n} + \bar{i}\bar{H}_{8,E,n})^{1/2}\Big|_{E_{F1321}}$$

where E_{F1321} is the fermi energy in this case.

Using (1.31f) and (8.4), we can study the entropy in this case.

8.2.2 Entropy in II–VI HD SLs with graded interfaces under magnetic quantization

The simplified DR in HD II–VI SLs with graded interfaces under magnetic quantization can be expressed as

$$\bar{k}_z^2 = \bar{G}_{19E,n} + \bar{i}\bar{H}_{19E,n} \tag{8.3a}$$

where

$$\bar{G}_{19E,n} = \left[\frac{\bar{C}_{18E,n}^2 - \bar{D}_{18E,n}^2}{\bar{L}_0^2} - \left(\frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)\right]$$

$$\bar{C}_{18E,n} = \cos^{-1}(\omega_{18E,n}),$$

$$\omega_{18E,n} = (2)^{\frac{-1}{2}}[(1-\bar{G}_{18E,n}^2 - \bar{H}_{18E,n}^2) - \sqrt{(1-\bar{G}_{18E,n}^2 - \bar{H}_{18E,n}^2)^2 + 4\bar{G}_{180D}^2}]^{\frac{1}{2}},$$

$$\bar{G}_{18E,n} = \frac{1}{2}[\bar{G}_{11E,n} + \bar{G}_{12E,n} + \Delta_0(\bar{G}_{13E,n} + \bar{G}_{14E,n}) + \Delta_0(\bar{G}_{15E,n} + \bar{G}_{16E,n})],$$

$$\bar{G}_{11E,n} = 2(\cos(\bar{g}_{1E,n}))(\cos(\bar{g}_{2E,n}))(\cos\gamma_{11}(\bar{E},\bar{n})),\ \gamma_{11}(\bar{E},\bar{n}) = \bar{k}_{21}(\bar{E},\bar{n})(\bar{b}_0 - \Delta_0)$$

$$\bar{k}_{21}(\bar{E},\bar{n}) = \left\{\left[\gamma_3(\bar{E},\eta_{g1}) - \frac{\hbar^2}{2\bar{m}_{\perp,1}^*}\left\{\frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right\} \pm \bar{C}_0\left\{\frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right\}^{\frac{1}{2}}\right]\frac{2m_{||,1}^*}{\hbar^2}\right\}^{1/2},$$

$$\bar{G}_{12E,n} = ([\Omega_1(\bar{E},\bar{n})(\sinh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) - \Omega_2(\bar{E},\bar{n})(\sin \bar{g}_{2E,n})(\cosh \bar{g}_{1E,n})])(\sin \gamma_{11}(\bar{E},\bar{n})))$$

$$\Omega_1(\bar{E},\bar{n}) = \left[\frac{\bar{d}_{1E,n}}{\bar{k}_{21}(\bar{E},\bar{n})} - \frac{\bar{k}_{21}(\bar{E},\bar{n})\bar{d}_{1E,n}}{\bar{d}^2_{1E,n}+\bar{d}^2_{2E,n}}\right], \Omega_2(\bar{E},\bar{n}) = \left[\frac{\bar{d}_{1E,n}}{\bar{k}_{21}(\bar{E},\bar{n})} - \frac{\bar{k}_{21}(\bar{E},\bar{n})d_{1E,n}}{\bar{d}^2_{1E,n}+\bar{d}^2_{2E,n}}\right]$$

$$\bar{G}_{13E,n} = ([\Omega_3(\bar{E},\bar{n})(\cosh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) - \Omega_4(\bar{E},\bar{n})(\sin \bar{g}_{2E,n})(\cosh \bar{g}_{1E,n})])(\sin \gamma_{11}(\bar{E},\bar{n})))$$

$$\Omega_3(\bar{E},\bar{n}) = \left[\frac{\bar{d}^2_{1E,n}-\bar{d}^2_{2E,n}}{\bar{k}_{21}(\bar{E},\bar{n})} - 3\bar{k}_{21}(\bar{E},\bar{n})\right], \Omega_4(\bar{E},\bar{n}) = \left[\frac{2\bar{d}_{1E,n}\bar{d}_{2E,n}}{\bar{k}_{21}(\bar{E},\bar{n})}\right]$$

$$\bar{G}_{14E,n} = ([\Omega_5(\bar{E},\bar{n})(\sinh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) - \Omega_6(\bar{E},\bar{n})(\sin \bar{g}_{2E,n})(\cosh \bar{g}_{1E,n})])(\cos \gamma_{11}(\bar{E},\bar{n})))$$

$$\Omega_5(\bar{E},\bar{n}) = \left[3\bar{d}_{1E,n}\frac{\bar{d}_{1E,n}}{\bar{d}^2_{1E,n}-\bar{d}^2_{2E,n}} - \bar{k}^2_{21}(\bar{E},\bar{n})\right], \Omega_6(\bar{E},\bar{n}) = \left[3\bar{d}_{2E,n}\frac{\bar{d}_{2E,n}}{\bar{d}^2_{1E,n}-\bar{d}^2_{2E,n}} - \bar{k}^2_{21}(\bar{E},\bar{n})\right]$$

$$\bar{G}_{15E,n} = ([\Omega_9(\bar{E},\bar{n})(\cosh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) - \Omega_{10}(\bar{E},\bar{n})(\sinh \bar{g}_{1E,n})(\sinh \bar{g}_{2E,n})])(\cos \gamma_{11}(\bar{E},\bar{n})))$$

$$\Omega_9(\bar{E},\bar{n}) = [2\bar{d}^2_{1E,n} - 2\bar{d}^2_{2E,n} - \bar{k}_{21}(\bar{E},\bar{n})], \Omega_{10}(\bar{E},\bar{n}) = [2\bar{d}_{1E,n}\bar{d}_{2E,n}]$$

$$\bar{G}_{16E,n} = ([\Omega_7(\bar{E},\bar{n})(\sinh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) - \Omega_8(\bar{E},\bar{n})(\sin \bar{g}_{1E,n})(\cosh \bar{g}_{2E,n})])(\sin \gamma_{11}(\bar{E},\bar{n})/12))$$

$$\Omega_7(\bar{E},\bar{n}) = \left[\frac{5\bar{d}_{1E,n}}{\bar{d}^2_{1E,n}+\bar{d}^2_{2E,n}}\bar{k}^3_{21}(\bar{E},\bar{n}) + \frac{5(\bar{d}^3_{1E,n}-3\bar{d}^2_{2E,n}\bar{d}_{1E,n}}{\bar{k}_{21}(\bar{E},\bar{n})} - 34\bar{k}_{21}(\bar{E},\bar{n})\bar{d}_{1E,n}\right],$$

$$\Omega_8(\bar{E},\bar{n}) = \left[\frac{5\bar{d}_{2E,n}}{\bar{d}^2_{1E,n}+\bar{d}^2_{2E,n}}\bar{k}^3_{21}(\bar{E},\bar{n}) + \frac{5(\bar{d}^3_{2E,n}-3\bar{d}^2_{2E,n}\bar{d}_{1E,n}}{\bar{k}_{21}(\bar{E},\bar{n})} - 34\bar{k}_{21}(\bar{E},\bar{n})\bar{d}_{1E,n}\right],$$

$$\bar{H}_{18,E,n} = \frac{1}{2}\left[\bar{H}_{11,E,n} + \bar{H}_{12E,n} + \Delta_0(\bar{H}_{13,E,n} + \bar{H}_{14E,n}) + \Delta_0(\bar{H}_{15E,n} + \bar{H}_{16E,n})\right]$$

$$\bar{H}_{11E,n} = 2(\sinh \bar{g}_{1E,n})(\sin \bar{g}_{2E,n})(\cos \gamma_{11}(\bar{E},\bar{n})))$$

$$\bar{H}_{12E,n} = ([\Omega_2(\bar{E},\bar{n})(\sinh\ \bar{g}_{1E,n})(\cos\ \bar{g}_{2E,n}) + \Omega_1(\bar{E},\bar{n})(\sin\ \bar{g}_{2E,n})(\cosh\ \bar{g}_{1E,n})](\sin \gamma_{11}(\bar{E},\bar{n}))),$$

$$\bar{H}_{13E,n} = ([\Omega_4(\bar{E},\bar{n})(\cosh\ \bar{g}_{1E,n})(\cos\ \bar{g}_{2E,n}) + \Omega_3(\bar{E},\bar{n})(\sinh\ \bar{g}_{1E,n})(\sin\ \bar{g}_{2E,n})](\sin \gamma_{11}(\bar{E},\bar{n}))),$$

$$\bar{H}_{14E,n} = ([\Omega_6(\bar{E},\bar{n})(\sinh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) + \Omega_5(\bar{E},\bar{n})(\sin \bar{g}_{1E,n})(\cosh \bar{g}_{2E,n})](\cos \gamma_{11}(\bar{E},\bar{n})))$$

$$\bar{H}_{15E,n} = ([\Omega_{10}(\bar{E},\bar{n})(\cosh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) + \Omega_9(\bar{E},\bar{n})(\sin \bar{g}_{1E,n})(\sin \bar{g}_{2E,n})](\cos \gamma_{11}(\bar{E},\bar{n}))),$$

$$\bar{H}_{19E,n} = ([\Omega_8(\bar{E},\bar{n})(\sinh \bar{g}_{1E,n})(\cos \bar{g}_{2E,n}) + \Omega_7(\bar{E},\bar{n})(\sin \bar{g}_{1E,n})(\cosh \bar{g}_{2E,n})](\sin \gamma_{11}(\bar{E},\bar{n})/2))$$

$$\bar{H}_{19E,n} = \left[\frac{2\bar{C}_{18E,n}\bar{D}_{18E,n}}{\bar{L}_0^2}\right] \textit{and}\ \bar{D}_{18E,n} = \sinh^{-1}(\omega_{18E,n})$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{eB}{2\pi^2\hbar}\sum_{n=0}^{n_{\max}} \frac{(\bar{G}'_{19E,n} + \bar{i}\bar{H}'_{19E,n})\bar{H}(E - E_{15,2})}{\sqrt{G_{19E,n} + iH_{19E,n}}} \tag{8.3b}$$

where $E_{15,2}$ is the sub-band energy in this case and is given by

$$0 = [\bar{G}_{19E,n} + \bar{H}_{19E,n}]\Big|_{E=E_{15,2}} \tag{8.3c}$$

EEM can be written as

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2}\overline{G'}_{19E,n} \tag{8.4}$$

The electron statistics can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v eB}{\pi^2\hbar}\,\text{Re}\textit{al part of} \sum_{n=0}^{n_{\max}}\left[\left(\bar{G}_{19,E,n} + + \bar{i}\bar{H}_{19,E,n}\right)^{1/2}\Big|_{E_{F1322}}\sum_{r=1}^{s}L(r)\left[\left(\bar{G}_{19,E,n} + + \bar{i}\bar{H}_{19,E,n}\right)^{1/2}|_{E_{F1322}}\right]\right] \tag{8.5}$$

where $\bar{E}_{F1322}$ is the fermi energy in this case.

Using (1.31f) and (8.7), we can study the entropy in this case.

8.2.3 Entropy in IV–VI HD SLs with graded interfaces under magnetic quantization

The simplified DR in HD IV–VI SLs with graded interfaces under magnetic quantization can be expressed as

$$\bar{k}_z^2 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_2(\bar{E},\bar{n})\right\}\right]^2 - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \tag{8.6}$$

where

$$\begin{aligned}
\Phi_2(\bar{E},\bar{n}) \equiv{}& [2\cosh\{\beta_2(\bar{E},\bar{n})\}\cos\{\gamma_2(\bar{E},\bar{n})\} + \varepsilon_2(\bar{E},\bar{n})\sinh\{\beta_2(\bar{E},\bar{n})\}\sin\{\gamma_{22}(\bar{E},\bar{n})\} \\
&+ \Delta_0[((\{\bar{K}_{112}(\bar{E},\bar{n})\}^2/\bar{K}_{212}(\bar{E},\bar{n})) - 3\bar{K}_{212}(\bar{E},\bar{n}))\cosh\{\beta_2(\bar{E},\bar{n})\}\sin\{\gamma_{22}(\bar{E},\bar{n})\} \\
&+ (3\bar{K}_{112}(\bar{E},\bar{n}) - \frac{\{\bar{K}_{112}(\bar{E},\bar{n})\}^2}{\bar{K}_{112}(\bar{E},\bar{n})}\sinh\{\beta_2(\bar{E},\bar{n})\}\cos\{\gamma_{22}(\bar{E},\bar{n})\}] \\
&+ \Delta_0[2\{\bar{K}_{112}(\bar{E},\bar{n})\}^2 - \{\bar{K}_{212}(\bar{E},\bar{n})\}^2\cosh\{\beta_2(\bar{E},\bar{n})\}\cos\{\gamma_{22}(\bar{E},\bar{n})\} \\
&+ \frac{1}{12}\left[\frac{5\{\bar{K}_{112}(\bar{E},\bar{n})\}^3}{\bar{K}_{212}(\bar{E},\bar{n})} + \frac{5\{\bar{K}_{212}(\bar{E},\bar{n})\}^3}{\bar{K}_{112}(\bar{E},\bar{n})}\right. \\
&\left. - 34\bar{K}_{212}(\bar{E},\bar{n})\bar{K}_{112}(\bar{E},\bar{n})\sinh\{\beta_2(\bar{E},\bar{n})\sin\{\gamma_{22}(\bar{E},\bar{n})\}\}\right]]
\end{aligned}$$

$$\beta_2(\bar{E},\bar{n}) \equiv \bar{K}_{112}(\bar{E},\bar{n})[\bar{a}_0 - \Delta_0],$$

$$\begin{aligned}
\bar{k}_{112}^2(\bar{E},\bar{n}) = {}& [2\bar{p}_{9,2n}]^{-1}[-\bar{q}_{9,2n}(\bar{E}-\bar{V}_0\eta_{g2}) - [[\bar{q}_{9,2n}(\bar{E}-\bar{V}_0\eta_{g2})]^2 \\
&+ 4\bar{p}_{9,2n}\bar{R}_{9,2n}(\bar{E}-\bar{V}_0\eta_{g2})]^{\frac{1}{2}}]
\end{aligned}$$

$$\begin{aligned}
&\bar{q}_{9,2n}(\bar{E}-\bar{V}_0\eta_{g2})[(\hbar^2/2)((1/\bar{m}_{l2}^-)) + \bar{a}_2(\hbar^2/4)\frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)((1/\bar{m}_{l2}^+\bar{m}_{t2}^-) \\
&\quad + (1/\bar{m}_{t2}^+\bar{m}_{l2}^-)) - \alpha_2\gamma_3(\bar{E}-\bar{V}_0\eta_{g2})((1/\bar{m}_{l2}^+) - (1/\bar{m}_{t2}^-)]
\end{aligned}$$

$$\begin{aligned}
&\bar{R}_{9,2n}(\bar{E},\eta_{g2}) + [\gamma_2(\bar{E}-\bar{V}_0\eta_{g2}) + \gamma_3(\bar{E}-\bar{V}_0\eta_{g2})\left[\left(\frac{\hbar^2}{2}\right)\alpha_2\frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)((1/\bar{m}_{t2}^*)\right. \\
&\qquad \left. - (1/\bar{m}_{t2}^-))] - \left[\left(\frac{\hbar^2}{2}\right)k_{s0}^2((1/\bar{m}_{t2}^*) + (1/\bar{m}_{t2}^-)))\right] \\
&\qquad - \alpha_2\left(\frac{\hbar^6}{4}\right)\left[\frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^2((1/\bar{m}_{t2}^+\bar{m}_{t2}^-))],
\end{aligned}$$

$$\begin{aligned}
\gamma_2(\bar{E},\bar{n}) = {}& \bar{K}_{212}(\bar{E},\bar{n})[\bar{b}_0 - \Delta_0], \bar{K}_{212}^2(\bar{E},\bar{n}) \\
&= [2\bar{p}_{9,1n}]^{-1}[-\bar{q}_{9,1n}(\bar{E},\eta_{g1}) + [[\bar{q}_{9,1n}(\bar{E},\eta_{g1})]^2 + 4\bar{p}_{9,1n}\bar{R}_{9,1n}(\bar{E},\eta_{g1})]^{\frac{1}{2}}]
\end{aligned}$$

$$\begin{aligned}
\bar{q}_{9,1n}(\bar{E},\eta_{g1}) = {}& \left[\left(\frac{\hbar^2}{2}\right)((1/\bar{m}_{l1}^*) + (1/\bar{m}_{l1}^-)) + \alpha_1\left(\frac{\hbar^6}{4}\right)\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)((1/\bar{m}_{l1}^+\bar{m}_{t1}^-)\right. \\
&\left. + (1/\bar{m}_{l1}^+\bar{m}_{t1}^-) - \alpha_1\gamma_3(\bar{E},\eta_{g1})((1/\bar{m}_{l1}^+) - (1/\bar{m}_{t1}^-))\right],
\end{aligned}$$

$$\bar{R}_{9,1n}(\bar{E},\eta_{g1}) = [\gamma_2(\bar{E},\eta_{g1}) + \gamma_2(\bar{E},\eta_{g1})\left[\left(\frac{\hbar^2}{2}\right)\alpha_1(2e\bar{B}/\hbar)\left(\bar{n}+\frac{1}{2}\right)((1/\bar{m}^{*}_{t1}) - (1/\bar{m}^{-}_{t1}))] - \left[\left(\frac{\hbar^2}{2}\right)\bar{k}^2_{s0}((1/\bar{m}^{*}_{t2}) + (1/\bar{m}^{-}_{t2}))] - \alpha_1\left(\frac{\hbar^6}{4}\right)\left(\left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)^2((1/\bar{m}^{+}_{t2}\bar{m}^{-}_{t2}))\right]$$

and

$$\varepsilon_2(\bar{E},n) \equiv \left[\frac{\bar{K}_{112}(\bar{E},n)}{\bar{K}_{212}(\bar{E},n)} - \frac{\bar{K}_{212}(\bar{E},n)}{\bar{K}_{112}(\bar{E},n)}\right]$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{e\bar{B}\bar{g}_v}{2\pi^2\hbar\bar{L}_0}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{\cos^{-1}[\frac{1}{2}\varphi_2(\bar{E},\bar{n})(1-\frac{1}{4}\varphi_2{}^2(\bar{E},\bar{n})]^{-1/2}\varphi_2'(\bar{E},\bar{n})\bar{H}(\bar{E}-\bar{E}_{15,3})}{[[\cos^{-1}[\frac{1}{2}\varphi_2(\bar{E},\bar{n})]]^2 - \bar{L}_0{}^2\frac{2e\bar{B}}{\hbar}(1+\frac{1}{2})]^{1/2}} \tag{8.7}$$

where $\bar{E}_{15,3}$ is the sub-band energy in this case and is given by

$$0 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\Phi_2(\bar{E}_{15,3},\bar{n})\right\}\right]^2 - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \tag{8.8}$$

EEM can be written as

$$\bar{m}^{*}(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2\bar{L}_0{}^2}\cos^{-1}\left[\frac{1}{2}\varphi_2(\bar{E},\bar{n})(1-\frac{1}{4}\varphi_2{}^2(\bar{E},\bar{n})\right]^{-1/2}\varphi_2'(\bar{E},\bar{n}) \tag{8.9}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar}\ \text{Real Part of}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left(\frac{1}{2}\phi_2(\bar{E},\bar{n})\right]^2 - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2}\right|_{\bar{E}_{F1323}}$$
$$\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left(\frac{1}{2}\phi_2(\bar{E},\bar{n})\right]^2 - \frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2}\right|_{\bar{E}_{F1323}}\right]\right] \tag{8.10}$$

where $\bar{E}_{F1323}$ is the fermi energy in this case.

Using (1.31f) and (8.10) we can study the entropy in this case.

8.2.4 Entropy in HgTe/CdTe HD SLs with graded interfaces under magnetic quantization

The simplified DR in HD*HgTe*/*CdTe*SLs with graded interfaces under magnetic quantization can be expressed as

$$(\bar{k}_z)^2 = \bar{G}_{192E,n} + i\bar{H}_{192E,n} \tag{8.11a}$$

where

$$\bar{G}_{192E,n} = \left[\frac{\bar{C}^2_{182E,n} - \bar{D}^2_{182E,n}}{\bar{L}_0^2} - \left(\frac{2e\bar{B}}{\hbar}\right)\left(\bar{n} + \frac{1}{2}\right)\right],$$

$$\bar{C}_{1820D} = \cos^{-1}(\omega_{182E,n}), \omega_{182E,n} = (2)^{-\frac{1}{2}}[(1 - \bar{G}^2_{182E,n} - \bar{H}^2_{182E,n}) - \sqrt{(1 - \bar{G}^2_{182E,n} - \bar{H}^2_{182E,n})^2 + 4\bar{G}^2_{182E,n}}]^{\frac{1}{2}}$$

$$\bar{G}_{112E,n} = 2(\cos(\bar{g}_{12}))(\cos(\bar{g}_{22}))(\cos\gamma_8(\bar{E},\bar{n})), \gamma_8(\bar{E},\bar{n}) = k_8(\bar{E},\bar{n})(\bar{b}_0 - \Delta_0),$$

$$\bar{k}_8(\bar{E},\bar{n}) = \left[\frac{\bar{B}^2_{01} + 4\bar{A}_1\bar{E} - \bar{B}_{01}\sqrt{\bar{B}^2_{01} + 4\bar{A}_1\bar{E}}}{2\bar{A}_1^2} - \left(\frac{2e\bar{B}}{\hbar}\right)\left(\bar{n} + \frac{1}{2}\right)\right]^{1/2},$$

$$\bar{G}_{120D} = ([\Omega_{12}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{12E,n}) - \Omega_{22}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{12E,n})](\sin\gamma_8(\bar{E},\bar{n}))),$$

$$\Omega_{12}(\bar{E},\bar{n}) = \left[\frac{\bar{d}_{12E,n}}{\bar{k}_8(\bar{E},\bar{n})} - \frac{\bar{k}_8(\bar{E},\bar{n})\bar{d}_{12E,n}}{\bar{d}_{12E,n} + \bar{d}_{22E,n}}\right], \Omega_{22}(\bar{E},\bar{n}) = \left[\frac{\bar{d}_{22E,n}}{\bar{k}_8(\bar{E},\bar{n})} - \frac{\bar{k}_8(\bar{E},\bar{n})\bar{d}_{22E,n}}{\bar{d}_{12E,n} + \bar{d}_{22E,n}}\right],$$

$$\bar{G}_{1320D} = ([\Omega_{32}(\bar{E},\bar{n})(\cosh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) - \Omega_{42}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{12E,n})](\sin\gamma_8(\bar{E},\bar{n}))),$$

$$\Omega_{32}(\bar{E},\bar{n}) = \left[\frac{d^2_{12E,n} - d^2_{2E,n}}{\bar{k}_8(\bar{E},\bar{n})} - 3\bar{k}_8(\bar{E},\bar{n})\right],\ \Omega_{42}(\bar{E},\bar{n}) = \left[\frac{2d_{12E,n}d_{22E,n}}{k_8(\bar{E},\bar{n})}\right]$$

$$\bar{G}_{1420D} = ([\Omega_{52}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) - \Omega_{62}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cosh\ \bar{g}_{22E,n})](\cos\gamma_8(\bar{E},\bar{n}))),$$

$$\Omega_{52}(\bar{E},\bar{n}) = \left[3d_{12E,n} - \frac{d_{12E,n}}{d^2_{12E,n} + d^2_{22E,n}}\bar{k}_8^2(\bar{E},\bar{n})\right], \Omega_{62}(\bar{E},\bar{n}) = \left[3\bar{d}_{22E,n} + \frac{d_{22E,n}}{d^2_{12E,n} + d^2_{22E,n}}\bar{k}_8^2(\bar{E},\bar{n})\right],$$

$$\bar{G}_{1520D} = ([\Omega_{72}(\bar{E},\bar{n})(\cosh\bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) - \Omega_{102}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cosh\ \bar{g}_{22E,n})](\sin\ \gamma_{80D}(\bar{E},\bar{n})/12)),$$

$$\Omega_{92}(\bar{E},\bar{n}) = [2d^2_{12E,n} - 2d^2_{22E,n} - \bar{k}_8^2(\bar{E},\bar{n})], \Omega_{102}(\bar{E},\bar{n}) = [2d_{12E,n}d_{22E,n}]$$

$$\bar{G}_{162E,n} = ([\Omega_{72}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) - \Omega_{82}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cosh\ \bar{g}_{22E,n})](\sin\ \gamma_{80D}(\bar{E},\bar{n})/12)),$$

$$\Omega_{72}(\bar{E},\bar{n}) = \left[\frac{5d_{12E,n}}{d_{12E,n}^2 + \bar{d}_{22E,n}^2}\bar{k}_8^3(\bar{E},\bar{n}) + \frac{5(d_{12E,n}^3 - 3d_{22E,n}^2 d_{12E,n})}{\bar{k}_8(\bar{E},\bar{n})} - 34\bar{k}_8(\bar{E},\bar{n})d_{12E,n}\right]$$

$$\Omega_{82}(\bar{E},\bar{n}) = \left[\frac{5d_{22E,n}}{d_{12E,n}^2 + d_{22E,n}^2}\bar{k}_8^3(\bar{E},\bar{n}) + \frac{5(d_{12E,n}^3 - 3d_{22E,n}^2 d_{12E,n})}{\bar{k}_8(\bar{E},\bar{n})} - 34\bar{k}_8(\bar{E},\bar{n})d_{12E,n}\right]$$

$$\bar{H}_{182E,n} = \frac{1}{2}\left[\bar{H}_{112E,n} + \bar{H}_{122E,n} + \Delta_0(\bar{H}_{132E,n} + \bar{H}_{142E,n}) + \Delta_0(\bar{H}_{152E,n} + \bar{H}_{162E,n})\right],$$

$$\bar{H}_{112E,n} = 2(\sinh\ \bar{g}_{12E,n})(\sinh\ \bar{g}_{22E,n})(\cos\gamma_8(\bar{E},\bar{n}))),$$

$$\bar{H}_{1220D} = ([\Omega_{22}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) + \Omega_{12}(\bar{E},\bar{n})(\sinh\ \bar{g}_{22E,n})(\cosh\ \bar{g}_{12E,n})](\sin\ \gamma_8(\bar{E},\bar{n}))),$$

$$\bar{H}_{132E,n} = ([\Omega_{42}(\bar{E},\bar{n})(\cosh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) + \Omega_{32}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\sinh\ \bar{g}_{22E,n})](\sin\ \gamma_8(\bar{E},\bar{n}))),$$

$$\bar{H}_{132E,n} = \left([\Omega_{42}(\bar{E},\bar{n})(\cosh\bar{g}_{12E,n})(\cos\bar{g}_{22E,n}) + \Omega_{32}(\bar{E},\bar{n})(\sinh\bar{g}_{12E,n})(\sinh\bar{g}_{22E,n})](\sin\gamma_8(\bar{E},\bar{n}))\right),$$

$$\bar{H}_{142E,n} = \left([\Omega_{62}(\bar{E},\bar{n})(\sinh\bar{g}_{12E,n})(\cos\bar{g}_{22E,n}) + \Omega_{52}(\bar{E},\bar{n})(\sinh\bar{g}_{12E,n})(\cosh\bar{g}_{22E,n})]\left(\cos\gamma_8(\bar{E},\bar{n})\right)\right),$$

$$\bar{H}_{142E,n} = ([\Omega_{62}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) + \Omega_{52}(\bar{E},\bar{n})(\sinh\ \bar{g}_{12E,n})(\cosh\ \bar{g}_{22E,n})](\cos\ \gamma_8(\bar{E},\bar{n}))),$$

$$\bar{H}_{1520D} = ([\Omega_{102}(\bar{E},\bar{n})(\cosh\ \bar{g}_{12E,n})(\cos\ \bar{g}_{22E,n}) + \Omega_{92}(\bar{E},\bar{n})(\sinh\ \bar{g}_{22E,n})(c\sinh\ \bar{g}_{12E,n})](\sin\ \gamma_8(\bar{E},\bar{n}))),$$

$$\bar{H}_{192E,n} = [((2\bar{C}_{182E,n}d_{182E,n})/\bar{L}_0^2)]\ \textit{and}\ \bar{D}_{182E,n} = \sinh^{-1}(\omega_{182E,n})$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{e\bar{B}}{2\pi^2\hbar}\sum_{n=0}^{n_{\max}}\frac{(\overline{G'}_{192E,n} + i\overline{H'}_{192E,n})\bar{H}(\bar{E}-\bar{E}_{15,4})}{\sqrt{\bar{G}_{192E,n} + i\bar{H}_{192E,n}}} \tag{8.11b}$$

where $\bar{E}_{15,4}$ is the sub-band energy in this case and is given by

$$0 = [\bar{G}_{192E,n} + \bar{H}_{192E,n}]|_{\bar{E}=\bar{E}_{15,4}} \tag{8.11c}$$

EEM can be written as

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2}\overline{G'}_{192E,n} \tag{8.12}$$

The electron statistics can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v eB}{\pi^2\hbar}\text{Re}al\,part\,of \sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\bar{G}_{192,E,n}++i\bar{H}_{192,E,n})^{1/2}\Big|_{\bar{E}_{F1324}}\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[(\bar{G}_{192,E,n}++i\bar{H}_{192,E,n})^{1/2}\Big|_{\bar{E}_{F1324}}\right]\right] \tag{8.13}$$

where $\bar{E}_{F1324}$ is the fermi energy in this case.

Using (1.31f) and (8.13), we can study the entropy in this case.

8.2.5 Entropy in strained layer HD SLs with graded interfaces under magnetic quantization

DR of the conduction electrons in HD strained layer SL with graded interfaces can be expressed as

$$\bar{k}_z^2 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\bar{\varphi}_6(\bar{E},\bar{n})\right\}\right]^2 - \frac{2|e|\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \tag{8.14a}$$

Where

$$\begin{aligned}\bar{\phi}_6(\bar{E},\bar{n}) &= [2\cosh[\bar{T}_4(\bar{E},\bar{n},\eta_{g2})]\cos[\bar{T}_5(\bar{E},\bar{n},\eta_{g1})]]\\ &+[\bar{T}_6(\bar{E},\bar{n})]\sinh[\bar{T}_4(\bar{E},\bar{n},\eta_{g2})]\sin[\bar{T}_5(\bar{E},\bar{n},\eta_{g1})]\\ &+\Delta_0\left[\left(\frac{\bar{k}_0^2(\bar{E},\bar{n},\eta_{g2})}{\bar{k}_0^{'2}(\bar{E},\bar{n},\eta_{g1})}-3\bar{k}_0{}'(\bar{E},\bar{n},\eta_{g1})\right)\cos[\bar{T}_4(\bar{E},\bar{n},\eta_{g2})]\sin[T_1(\bar{E},\bar{n},\eta_{g1})]\right]\\ &+\left(3\bar{k}_0(\bar{E},\bar{n},\eta_{g2})-\frac{\bar{k}_0^{'2}(\bar{E},\bar{n},\eta_{g1})}{\bar{k}_0(\bar{E},\bar{n},\eta_{g2})}\right)\sin[\bar{T}_4(\bar{E},\bar{n},\eta_{g2})]\cos[\bar{T}_5(\bar{E},\bar{n},\eta_{g1})]\\ &+\Delta_0[2(\bar{k}_0^2(\bar{E},\bar{n},\eta_{g1})-\bar{k}_{0D}^{'2}(\bar{E},\bar{n},\eta_{g1}))\cos[\bar{T}_4(\bar{E},\bar{n},\eta_{g2})]\cos[\bar{T}_5(\bar{E},\bar{n},\eta_{g1})]]\\ &+\frac{1}{12}\left(\frac{5\bar{k}_0^3(\bar{E},\bar{n},\eta_{g2})}{\bar{k}_0{}'(\bar{E},\bar{n},\eta_{g1})}+\frac{5\bar{k}_0^{'3}(\bar{E},\bar{n},\eta_{g1})}{\bar{k}_0(\bar{E},\bar{n},\eta_{g2})}\right.\\ &\left.-34\bar{k}_0(\bar{E},\bar{n},\eta_{g2})k_0{}'(\bar{E},\bar{n},\eta_{g1})\right)\sinh[\bar{T}_4(\bar{E},\bar{n},\eta_{g2})\sin(\bar{E},\bar{n},\eta_{g1})]\end{aligned}$$

$$[\bar{T}_4(\bar{E},\bar{n},\eta_{g2})] = \bar{k}_0(\bar{E},\bar{n},\eta_{g2})[\bar{a}_0-\Delta_0],$$

$$\bar{k}_0(\bar{E},\bar{n},\eta_{g2}) = [\bar{S}_2(\bar{E},\bar{n},\eta_{g2})]^{-1/2}.\left[\left[\left(\bar{n}+\frac{1}{2}\right)\hbar eb/(\sqrt{\rho_1}(\bar{E})\rho_2(\bar{E}))\right]-1\right]^{1/2}$$

$$\rho_1(\bar{E}) = \hbar^2/(2\bar{p}_2(\bar{E}-\bar{V}_0,\eta_{g2})), \rho_2(\bar{E}) = \hbar^2/(2\bar{Q}_2(\bar{E}-\bar{V}_0,\eta_{g2}))$$

$$\bar{T}_5(\bar{E},\bar{n},\eta_{g1}) = \bar{k}_0'(\bar{E},\bar{n},\eta_{g1})[\bar{b}_0-\Delta_0],$$

$$\bar{k}_0'(\bar{E},\bar{n},\eta_{g1}) = [\bar{S}_1(\bar{E},\bar{n},\eta_{g1})]^{-1/2}\left[1-\left[(\bar{n}+1/2)\hbar eB/\left(\sqrt{\rho_3(\bar{E})\rho_4(\bar{E})}\right)\right]\right]^{1/2}$$

$$\rho_3(\bar{E}) = \hbar^2/(2\bar{p}_1(\bar{E},\eta_{g2})), \rho_4(\bar{E}) = \hbar^2/(2\bar{Q}_1(\bar{E},\eta_{g1}))$$

$$\bar{T}_6(\bar{E},\bar{n}) = \left[\frac{\bar{k}_0(\bar{E},\bar{n},\eta_{g2})}{\bar{k}_0'(\bar{E},\bar{n},\eta_{g1})} - \frac{\bar{k}_0'(\bar{E},\bar{n},\eta_{g1})}{\bar{k}_0(\bar{E},\bar{n},\eta_{g2})}\right]$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{e\bar{B}\bar{g}_v}{2\pi^2\hbar\bar{L}_0}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{\cos^{-1}\left[\frac{1}{2}\overline{\varphi}_6(\bar{E},\bar{n})(1-\frac{1}{4}\left[\overline{\varphi}_6(\bar{E},\bar{n})\right]^2\right]^{-1/2}\left[\overline{\varphi}_6(\bar{E},\bar{n})\right]'\bar{H}(\bar{E}-\bar{E}_{15,5})}{\left[\left[\cos^{-1}\left[\frac{1}{2}\overline{\varphi}_6(\bar{E},\bar{n})\right]\right]^2-\bar{L}_0{}^2\frac{2e\bar{B}}{\hbar}(1+\frac{1}{2})\right]^{1/2}} \tag{8.14b}$$

where $\bar{E}_{15,5}$ is the sub-band energy in this case and is given by

$$0 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\bar{\varphi}_6(\bar{E}_{15,5},\bar{n})\right\}\right]^2 - \frac{2|e|\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \tag{8.14c}$$

EEM can be written as

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2\bar{L}_0{}^2}\cos^{-1}\left[\frac{1}{2}\bar{\varphi}_6(\bar{E},\bar{n})\left(1-\frac{1}{4}[\bar{\varphi}_6(\bar{E},\bar{n})]^2\right]^{-1/2}[\bar{\varphi}_6(\bar{E},\bar{n})]' \tag{8.15}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar}\text{Real Part of}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left(\frac{1}{2}\phi_2(\bar{E},\bar{n})\right]^2-\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2}\right|_{\bar{E}_{F1325}}$$

$$\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[\left[\frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left(\frac{1}{2}\phi_2(\bar{E},\bar{n})\right]^2-\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2}\right|_{\bar{E}_{F1325}}\right]\right] \tag{8.16}$$

where $\bar{E}_{F1325}$ is the Fermi energy in this case.

Using (1.31f) and (8.16), we can study the entropy in this case.

8.2.6 Entropy in III–V HD effective mass SLs under magnetic quantization

DR in this case assumes the form

$$-(\bar{k}_x)^2 = \delta_{7E,n} + i\delta_{8E,n} \tag{8.17a}$$

Where

$$\delta_{5E,n} = \left[\frac{1}{\bar{L}_0^2}(\delta_{5E,n}^2 - \delta_{6E,n}^2) - \left\{\frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right\}\right],\ \delta_{5E,n} = \cos^{-1} p_{5E,n},$$

$$\bar{p}_{5E,n} = \left[\frac{1 - \delta_{3E,n}^2 - \delta_{4E,n}^2 - \sqrt{(1 - \delta_{3E,n}^2 - \delta_{4E,n}^2) + 4\delta_{4E,n}^2}}{2}\right]^{1/2},$$

$$\delta_{3E,n} = (\bar{a}_1 \cos\Delta_{1E,n} \cos\Delta_{2E,n} - \bar{a}_2 \cos\Delta_{3E,n} \cos\Delta_{4E,n})$$

$$\delta_{4E,n} = (\bar{a}_2 \sin\Delta_{1E,n} \sin\Delta_{2E,n} - \bar{a}_2 \sin\Delta_{3E,n} \sin\Delta_{4E,n})$$

$$\Delta_{1E,n} = (\bar{a}_0 e_{1E,n} + \bar{b}_0 e_{3E,n}), \Delta_{2E,n} = (\bar{a}_0 e_{2E,n} + \bar{b}_0 e_{4E,n}), \Delta_{3E,n}$$

$$= (\bar{a}_0 e_{1E,n} - \bar{b}_0 e_{3E,n}), \Delta_{4E,n} = (\bar{a}_0 e_{2E,n} - \bar{b}_0 e_{4E,n}),$$

$$\delta_{6E,n} = \sinh^{-1}\bar{p}_{5E,n} \text{ and } \delta_{8E,n} = [2\delta_{5E,n}\delta_{6E,n}/\bar{L}_0^2],$$

$$e_{1E,n} = \left[\left(\left(\sqrt{\bar{t}_{1E,n}^2 + \bar{t}_2^2} + \bar{t}_{1E,n}\right)/2\right)\right]^{\frac{1}{2}}, e_{2E,n} = \left[\left(\left(\sqrt{\bar{t}_{1E,n}^2 + \bar{t}_2^2} - \bar{t}_{1E,n}\right)/2\right)\right]^{\frac{1}{2}}$$

$$e_{3E,n} = \left[\frac{\sqrt{\bar{t}_{3E,n}^2 + \bar{t}_4^2} + \bar{t}_{3E,n}}{2}\right]^{1/2}, e_{4E,n} = \left[\frac{\sqrt{\bar{t}_{3E,n}^2 + \bar{t}_4^2} - \bar{t}_{3E,n}}{2}\right]^{1/2},$$

$$\bar{t}_{1E,n}\left[\frac{2\bar{m}_{c1}^*}{\hbar^2}\bar{T}_{11}(\bar{E}, \Delta_1, \eta_{g1}, \bar{E}_{g1}) - \frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right],$$

$$\bar{t}_{3E,n}\left[\frac{2\bar{m}_{c2}^*}{\hbar^2}\bar{T}_{12}(\bar{E}, \Delta_2, \eta_{g2}, \bar{E}_{g2}) - \frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right]$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{eB}{2\pi^2\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}} \frac{(\delta'_{7E,n} + i\delta'_{8E,n})\bar{H}(\bar{E} - \bar{E}_{15,6})}{\sqrt{\delta_{7E,n} + i\delta_{8E,n}}} \tag{8.17b}$$

where $\bar{E}_{15,6}$ is the sub-band energy in this case and is given by

$$0 = \delta_{7E_{15,6},n} + i\delta_{8E_{15,6},n} \tag{8.17c}$$

EEM can be written as

$$\bar{m}^{*}(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2}\delta'_{7E,n} \tag{8.18}$$

The electron statistics can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar}\text{Real part of}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\delta_{8,E,n}++\delta_{8,E,n})^{1/2}|_{\bar{E}_{F1326}}\right.$$
$$\left.\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[(\delta_{8,E,n}+\delta_{8,E,n})^{1/2}|_{\bar{E}_{F1326}}]\right] \tag{8.19}$$

where $\bar{E}_{F1326}$ is the Fermi energy in this case.

Using (1.31f) and (8.19) we can study the entropy in this case.

8.2.7 Entropy in II–VI HD effective mass SLs under magnetic quantization

DR in HD II–VI EMSL can be written as

$$(\bar{k}_z)^2 = \Delta_{13E,n} + i\Delta_{14E,n}, \tag{8.20a}$$

where,

$$\Delta_{13E,n} = \left[\frac{1}{\bar{L}_0^2}(\Delta_{11E,n}^2 - \Delta_{12E,n}^2) - \left\{\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right\}\right]$$

$$\Delta_{11E,n} = \cos^{-1}\bar{p}_{6E,n}, \bar{p}_{6E,n} = \left[\frac{1-\Delta_{9E,n}^2-\Delta_{10E,n}^2-\sqrt{(1-\Delta_{9E,n}^2-\Delta_{10E,n}^2)^2+4\Delta_{10E,n}^2}}{2}\right]^{1/2}$$

$$\Delta_{9E,n} = (\bar{a}_1\cos\Delta_{6E,n}\cosh\Delta_{7E,n} - \bar{a}_2\cos\Delta_{8E,n}\cosh\Delta_{7E,n}),$$

$$\Delta_{10E,n} = (\bar{a}_1\sin\Delta_{6E,n}\sinh\Delta_{7E,n} + \bar{a}_2\sin\Delta_{8E,n}\sinh\Delta_{7E,n}),$$

$$\Delta_{6E,n} = [\bar{a}_0\bar{C}_{22E,n}(\bar{E}_{E,n},\eta_{g1}) + \bar{b}_0\bar{e}_{3E,n}], \Delta_{7E,n} = \bar{b}_0\bar{e}_{4E,n}, \Delta_{8E,n}$$
$$= [\bar{a}_0\bar{C}_{22E,n}(\bar{E}_{E,n},\eta_{g1}) - \bar{b}_0\bar{e}_{3E,n}],$$

$$\bar{C}_{22E,n}(\bar{E}_{E,n,\eta_{g1}}) = \left[\frac{2\bar{m}^{*}_{||,1}}{\hbar^2}\left\{\gamma_3(\bar{E}_{E,n,\eta_{g1}}) - \frac{\hbar^2}{2\bar{m}^{*}_{\perp,1}}\left\{\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right\}\right.\right.$$
$$\left.\left.\mp\bar{C}_0\left[\left\{\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right\}\right]^{1/2}\right\}\right]^{1/2},$$

$$\Delta_{12E,n} = \cos^{-1}\bar{p}_{6E,n}, \Delta_{14E,n} = \frac{2\Delta_{11E,n}\Delta_{12E,n}}{L_0^2},$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{e\bar{B}}{2\pi^2\hbar}\sum_{n=0}^{n_{\max}} \frac{(\Delta'_{13E,n} + i\Delta'_{14E,n})\bar{H}(\bar{E} - \bar{E}_{15,7})}{\sqrt{\Delta_{13E,n} + i\Delta_{14E,n}}} \tag{8.20b}$$

where $\bar{E}_{15,7}$ is the sub-band energy in this case and is given by

$$0 = \Delta_{13E_{15,7,n}} + i\Delta_{14E_{15,7,n}} \tag{8.20c}$$

EEM can be written as

$$\bar{m}^*(\bar{E}, \eta_g, \bar{n}) = \frac{\hbar^2}{2}\Delta'_{13E,n} \tag{8.20d}$$

The electron statistics can be expressed a

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar}\text{Real part of}$$
$$\sum_{\bar{n}=0}^{\bar{n}_{\max}}\left[(\Delta_{13,E,n} + + \Delta_{14,E,n})^{1/2}|_{\bar{E}_{F1327}}\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[(\Delta_{13,E,n} + + \Delta_{14,E,n})^{1/2}|_{\bar{E}_{F1327}}]\right] \tag{8.21}$$

where $\bar{E}_{F1327}$ is the Fermi energy in this case.

Using (1.31f) and (8.21), we can study the entropy in this case.

8.2.8 Entropy in IV–VI HD effective mass SLs under magnetic quantization

DR in HD IV–VI, EMSL sunder magnetic quantization can be written as

$$(\bar{k}_z)^2 = \left[[1/\bar{L}_0^2]\{\cos^{-1}(\bar{f}_{23}(\bar{E}, \bar{n}))\}^2 - \left(\frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right)\right] \tag{8.22a}$$

where,

$$\bar{f}_{23}(\bar{E}, \bar{n}) = \bar{a}_3\cos[\bar{a}_0\bar{C}_{23E,n}(\bar{E}, \bar{n}, \eta_{g1}) + \bar{b}_0\bar{D}_{23E,n}(\bar{E}, \bar{n}, \eta_{g1})]$$
$$- \bar{a}_4\cos[\bar{a}_0\bar{C}_{23E,n}(\bar{E}, \bar{n}, \eta_{g2}) - \bar{b}_0\bar{D}_{23E,n}(E, n, \eta_{g2})],$$

$$\bar{C}_{23}(\bar{E}, \bar{n}, \eta_{g1}) = [[2\bar{p}_{9,1}]^{-1}[-\bar{q}_{9,1}(\bar{E}, \bar{n}, \eta_{g1}) + [\{\bar{q}_{9,1}(\bar{E}, \bar{n}, \eta_{g1})\}^2$$
$$+ (4\bar{p}_{9,1})\bar{R}_{9,1}(\bar{E}, \bar{n}, \eta_{g1})]^{1/2}]]^{1/2},$$

$$\bar{D}_{23}(\bar{E}, \bar{n}, \eta_{g2}) = [[2\bar{p}_{9,2}]^{-1}[-\bar{q}_{9,2}(E, n, \eta_{g2})$$
$$+ [\{\bar{q}_{9,2}(E, n, \eta_{g2})\}^2 + (4\bar{p}_{9,2})\bar{R}_{9,2}(E, n, \eta_{g2})]^{1/2}]]^{1/2},$$

$$\bar{q}_{9,i}(\bar{E},\bar{n},\eta_{gi}) = \left[\frac{\hbar^2}{2}\left(\frac{1}{\bar{m}^{+}_{l,i}} - \frac{1}{\bar{m}^{-}_{l,i}}\right) + \alpha_i \frac{\hbar^4}{4}\left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)\left(\frac{1}{\bar{m}^{+}_{l,i}\bar{m}^{-}_{t,i}} + \frac{1}{\bar{m}^{+}_{t,i}\bar{m}^{-}_{l,i}}\right) - \alpha_i \gamma_3(\bar{E},\eta_{gi})\left(\frac{1}{\bar{m}^{+}_{l,i}} - \frac{1}{\bar{m}^{-}_{l,i}}\right)\right],$$

$$\bar{R}_{9,i}(\bar{E},\bar{n},\eta_{gi}) = \left[\gamma_2(\bar{E},\eta_{gi}) + \gamma_3(\bar{E},\eta_{gi}) + \alpha_i \frac{\hbar^2}{2}\left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)\left(\frac{1}{\bar{m}^{+}_{t,i}} - \frac{1}{\bar{m}^{+}_{t,i}}\right) - \frac{\hbar^2}{2}\left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)\left(\frac{1}{\bar{m}^{+}_{t,i}} - \frac{1}{\bar{m}^{+}_{t,i}}\right) - \frac{\alpha\hbar^6}{4}\frac{\left(\frac{2e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\right)^2}{\bar{m}^{-}_{t,i}\bar{m}^{+}_{t,i}}\right]$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{e\bar{B}\bar{g}_v}{2\pi^2\hbar\bar{L}_0}\sum_{\bar{n}=0}^{\bar{n}_{\max}} \frac{\cos^{-1}[\frac{1}{2}\bar{f}_{23}(\bar{E},\bar{n})(1-\frac{1}{4}\bar{f}_{23}{}^2(\bar{E},\bar{n})]^{-1/2}\bar{f}'_{23}(\bar{E},\bar{n})\bar{H}(\bar{E}-\bar{E}_{15,8})}{[[\cos^{-1}[\frac{1}{2}\bar{f}_{23}(\bar{E},\bar{n})]]^2 - \bar{L}_0{}^2\frac{2e\bar{B}}{\hbar}(1+\frac{1}{2})]^{1/2}} \tag{8.22b}$$

where $\bar{E}_{15,8}$ is the sub-band energy in this case and is given by

$$0 = [[1/\bar{L}_0{}^2]\{\cos^{-1}(\bar{f}_{23}(\bar{E}_{15,8},\bar{n}))\}^2 - \left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)\Bigg] \tag{8.22c}$$

EEM can be written as

$$\bar{m}^{*}(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2\bar{L}_0{}^2}\cos^{-1}\left[\frac{1}{2}\bar{f}_{23}(\bar{E},\bar{n})\left(1-\frac{1}{4}\bar{f}_{23}{}^2(\bar{E},\bar{n})\right]^{-1/2}\bar{f}'_{23}(\bar{E},\bar{n}) \tag{8.23}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{e\bar{B}}{\pi^2\hbar}\ \ \mathrm{Re}al\ Part\ of \sum_{\bar{n}=0}^{\bar{n}_{\max}}[\Theta_{8,15}+\Theta_{8,16}] \tag{8.24}$$

where

$$\Theta_{8,15} = \left[\frac{1}{\bar{L}_0^2}[\cos^{-1}\{\bar{f}_{23}(\bar{E}_{F8,8},\bar{n})\}]^{1/2} - \left(\frac{2e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\right]^{1/2},$$

$$\Theta_{8,16} = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\Theta_{8,15}]$$

and $\bar{E}_{F8,8}$ is the Fermi energy in this case.

Using (1.31f) and (8.24), we can study the entropy in this case.

8.2.9 Entropy in HgTe/CdTe HD effective mass SLs under magnetic quantization

DR in HDHgTe/CdTe EMSLs under magnetic quantization can be written as

$$(\bar{k}_z)^2 = \Delta_{13HE,n} + i\Delta_{14HE,n} \tag{8.25a}$$

where

$$\Delta_{13HE,n} = \left[\frac{1}{\bar{L}_0^2}(\Delta_{11HE,n}^2 - \Delta_{12HE,n}^2) - \left\{\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right\}\right]$$

$$\Delta_{11HE,n} = \cos^{-1} p_{6HE,n}, p_{6HE,n} = \left[\frac{1-\Delta_{9HE,n}^2-\Delta_{10HE,n}^2-\sqrt{(1-\Delta_{9HE,n}^2-\Delta_{10HE,n}^2)^2+4\Delta_{10HE,n}^2}}{2}\right]^{1/2},$$

$$\Delta_{9HE,n} = (\bar{a}_{1H}\cos\Delta_{5HE,n}\cosh\Delta_{6HE,n} - \bar{a}_{2H}\cos\Delta_{7HE,n}\cosh\Delta_{6HE,n}),$$

$$\Delta_{10HE,n} = (\bar{a}_{1H}\sin\Delta_{5HE,n}\sinh\Delta_{6HE,n} + \bar{a}_{2H}\sin\Delta_{7HE,n}\sinh\Delta_{6HE,n}),$$

$$\Delta_{5HE,n} = [\bar{a}_0\bar{C}_{22HE,n}(\bar{E}_{E,n},\eta_{g1}) + \bar{b}_0\bar{e}_3], \Delta_{6HE,n} = \bar{b}_0\bar{e}_4, \Delta_{7HE,n} = [\bar{a}_0\bar{C}_{22HE,n}(\bar{E}_{E,n},\eta_{g1}) - \bar{b}_0\bar{e}_3],$$

$$\bar{C}_{22HE,n}(\bar{E}_{E,n,\eta_{g1}}) = \left[\frac{\bar{B}_{01}^2+2\bar{A}_1E_{E,n}-\bar{B}_{01}(\bar{B}_{01}^2+4\bar{A}_1E_{E,n})}{2\bar{A}_1^2} - \left[\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]\right]^{1/2},$$

$$\Delta_{12HE,n} = \cos^{-1}\bar{p}_{6HE,n}, \Delta_{14HE,n} = \frac{2\Delta_{11HE,n}\Delta_{12HE,n}}{\bar{L}_0^2},$$

The DOS function can be written as

$$\bar{N}(\bar{E}) = \frac{e\bar{B}}{2\pi^2\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{(\Delta'_{13HE,n}+i\Delta'_{14HE,n})\bar{H}(\bar{E}-\bar{E}_{15,9})}{\sqrt{\Delta_{13HE,n}+i\Delta_{14HE,n}}} \tag{8.25b}$$

where $\bar{E}_{15,9}$ is the sub-band energy in this case and is given by

$$0 = \Delta_{13HE_{15,9},n} + i\Delta_{14HE_{15,9},n} \tag{8.26a}$$

The EEM can be written as

$$\bar{m}^*(\bar{E},\eta_g,\bar{n}) = \frac{\hbar^2}{2}\Delta'_{13HE,n} \tag{8.26b}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{e\bar{B}}{\pi^2\hbar}\,\mathrm{Re}al\,part\ of\ \sum_{\bar{n}=0}^{\bar{n}_{\max}}[\Theta_{8,17}+\Theta_{8,18}] \tag{8.27}$$

where

$$\Theta_{8,17} = [\Delta_{13HE_{F8,9},n} + i\Delta_{14HE_{F8,9},n}]^{1/2},\ \Theta_{8,18} = \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})[\Theta_{8,17}]$$

and $\bar{E}_{F8,9}$ is the Fermi energy in this case.

Using (1.31f) and (8.27) we can study the entropy in this case.

8.2.10 Entropy in strained layer HD effective mass SLs under magnetic quantization

DR in HD strained layer effective mass SLs under magnetic quantizationcan be expressed as

$$(\bar{k}_z)^2 = \left[\frac{1}{\bar{L}_0^2}\left\{\cos^{-1}(\bar{f}_{40}(\bar{E},\bar{n}))\right\}^2 - \left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)\right] \tag{8.28a}$$

where

$$\bar{f}_{40}(\bar{E},\bar{n}) = \bar{a}_{20}\cos[\bar{a}_{20}\bar{C}_{40}(\bar{E},\bar{n},\eta_{g1}) + \bar{b}_0\bar{D}_{40}(\bar{E},\bar{n},\eta_{g1})] - a_{21}\cos[\bar{a}_0\bar{C}_{40}(E,n,\eta_{g2}) - \bar{b}_0\bar{D}_{40}(\bar{E},\bar{n},\eta_{g2})],$$

$$\bar{C}_{40}(\bar{E},\bar{n},\eta_{g1}) = \left[1 - \frac{\hbar e\bar{B}}{\phi_{50}(\bar{E},\eta_{g1})}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2}[\bar{S}_1(\bar{E},\eta_{g1})]^{=1/2},$$

$$\phi_{50}(\bar{E},\eta_{g1}) = \sqrt{\psi_{50}(\bar{E},\eta_{g1})\psi_{51}\eta_{g1}},$$

$$\psi_{50}(\bar{E},\eta_{g1}) = \frac{\hbar^2}{2\bar{P}_1(\bar{E},\eta_{g1})},\ \psi_{51}(\bar{E},\eta_{g1}) = \frac{\hbar^2}{2\bar{Q}_1(\bar{E},\eta_{g1})}$$

$$\bar{D}_{40}(\bar{E},\bar{n},\eta_{g2}) = \left[1 - \frac{\hbar e\bar{B}}{\phi_{50}(\bar{E},\eta_{g2})}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2}[\bar{S}_2(\bar{E},\eta_{g2})]^{-1/2},$$

$$\phi_{501}(\bar{E},\eta_{g2}) = \sqrt{\psi_{501}(\bar{E},\eta_{g2})\psi_{511}\eta_{g2}}$$

$$\psi_{501}(\bar{E},\eta_{g2})=\frac{\hbar^2}{2\bar{P}_1(\bar{E},\eta_{g2})},\psi_{511}(\bar{E},\eta_{g2})=\frac{\hbar^2}{2\bar{Q}_2(\bar{E},\eta_{g2})}$$

The DOS function can be written as

$$\bar{N}(\bar{E})=\frac{e\bar{B}\bar{g}_v}{2\pi^2\hbar\bar{L}_0}\text{Re}al\ Part\ of \sum_{\bar{n}=0}^{\bar{n}_{\max}}\frac{\cos^{-1}[\frac{1}{2}\bar{f}_{40}(\bar{E},\bar{n})(1-\frac{1}{4}\bar{f}_{40}{}^2(E,n)]^{-1/2}\bar{f}'_{40}(\bar{E},\bar{n})\bar{H}(\bar{E}-\bar{E}_{15,10})}{[[\cos^{-1}[\frac{1}{2}\bar{f}_{40}(\bar{E},\bar{n})]]^2-\bar{L}_0{}^2\frac{2e\bar{B}}{\hbar}(1+\frac{1}{2})]^{1/2}} \tag{8.28b}$$

where $\bar{E}_{15,10}$ is the sub-band energy in this case and is given by

$$0=\left[[1/\bar{L}_0{}^2]\{\cos^{-1}(\bar{f}_{40}(\bar{E}_{15,10},\bar{n}))\}^2-\left(\frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right)\right] \tag{8.28c}$$

EEM can be written as

$$\bar{m}^*(\bar{E},\eta_g,\bar{n})=\frac{\hbar^2}{2\bar{L}_0{}^2}\cos^{-1}\left[\frac{1}{2}\bar{f}_{40}(\bar{E},\bar{n})\left(1-\frac{1}{4}\bar{f}_{40}{}^2(\bar{E},\bar{n})\right]^{-1/2}\bar{f}'_{40}(\bar{E},\bar{n})\right. \tag{8.29}$$

The electron concentration can be written as

$$\bar{n}_0=\frac{e\bar{B}}{\pi^2\hbar}\text{Re}al\ Part\ of\ \sum_{\bar{n}=0}^{\bar{n}_{\max}}[\Theta_{8,19}+\Theta_{8,20}] \tag{8.30}$$

where

$$\Theta_{8,19}=\left[\frac{1}{\bar{L}_0^2}[\cos^{-1}\{\bar{f}_{40}(\bar{E}_{F8,10},n)\}]^{1/2}-\frac{2eB}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{1/2},\Theta_{8,20}=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\Theta_{8,19}]$$

and $\bar{E}_{F8,10}$ is the Fermi energy in this case.

Using (1.31f) and (8.30) we can study the entropy in this case.

8.3 Results and discussion

Using Appendix 15, we have plotted in Figures 8.1 and 8.2 the entropy as functions of inverse quantizing magnetic field and impurity concentration, respectively, for HgTe/CdTe, PbTe/PbSnTe, CdS/CdTe, and GaAs/$Ga_{1-x}Al_xAs$ HD SLs with graded interfaces. With decreasing magnetic field intensity, the thermoelectric power increases periodically as a result of SdH periodicity. However, with increasing impurity concentration, the thermoelectric power increases to some extent exhibiting spikes for higher values,

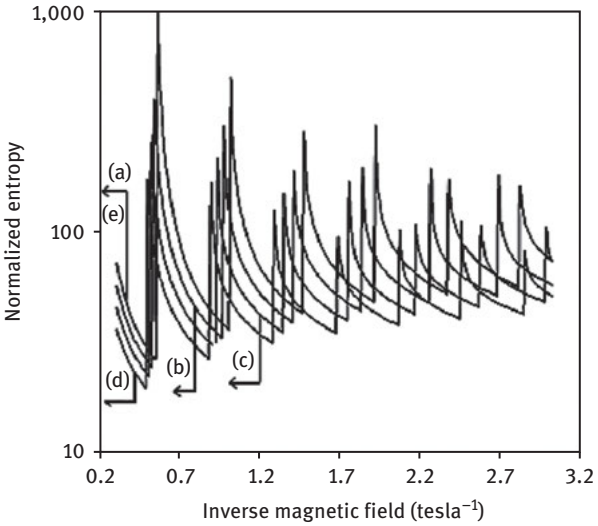

Figure 8.1: The plot of the entropy as a function of inverse quantizing magnetic field for (a) HgTe/CdTe, (b) PbTe/PbSnTe, (c) CdS/CdTe, and (d) GaAs/$Ga_{1-x}Al_xAs$ HDSLs with graded interfaces.

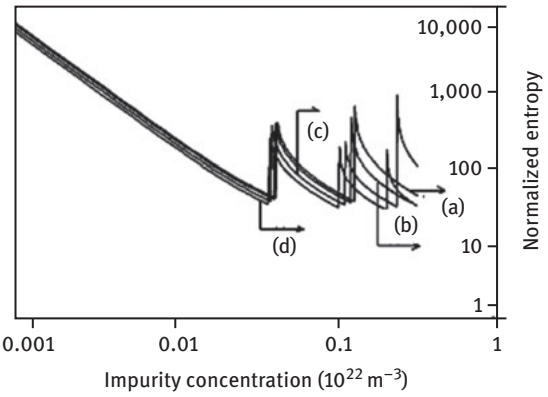

Figure 8.2: Plot of the entropy as a function of impurity concentration for all the cases of Figure 8.1.

a result which already been discussed in previous chapter. It appears that the entropy is lower in magnitude for HD GaAs/$Ga_{1-x}Al_xAs$ and higher in magnitude for HD HgTe/CdTe for all the cases. In Figures 8.3 and 8.4, the entropy as functions of inverse quantizing magnetic field and impurity concentration for HgTe/CdTe, PbTe/PbSnTe, CdS/CdTe, and GaAs/$Ga_{1-x}Al_xAs$ effective mass HDSLs structures. The concentration has been fixed at a value $10^{22}m^{-3}$ for varying magnetic field intensity, while 10 tesla

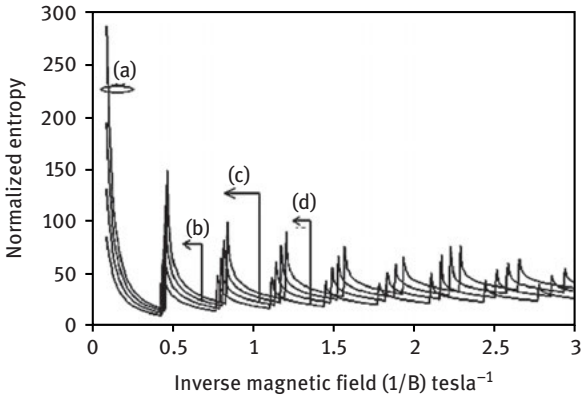

Figure 8.3: Plot of the entropy as a function of inverse quantizing magnetic field for (a) HgTe/CdTe, (b) PbTe/PbSnTe, (c) CdS/CdTe, and (d) GaAs/$Ga_{1-x}Al_xAs$ effective mass HD SLs.

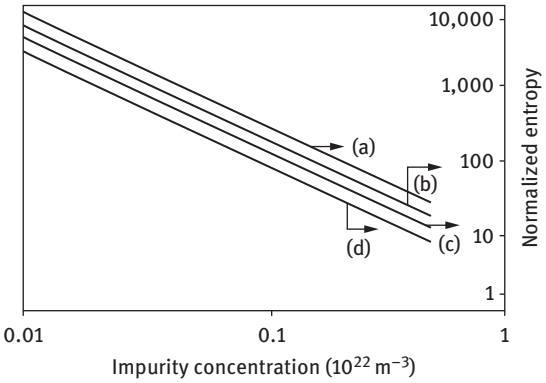

Figure 8.4: Plot of the entropy as a function of impurity concentration for all the cases of Figure 8.3.

was fixed for varying impurity concentration. With decreasing magnetic field intensity, the thermoelectric power increases periodically as a result of SdH periodicity. However, with increasing impurity concentration, the entropy decreases.

In Figures 8.5 and 8.6, the entropy as functions of film thickness and 2D carrier concentration for HgTe/CdTe, PbTe/PbSnTe, CdS/CdTe, and GaAs/$Ga_{1-x}Al_xAs$ for HD QWSLs with graded interfaces. It appears that the entropy in this case signatures an increasing step like variation with increasing film thickness and decreases with increasing 2D carrier concentration. In Figures 8.7 and 8.8, the magneto thermoelectric power as function of film thickness and 2D carrier concentration for HgTe/CdTe, PbTe/PbSnTe, CdS/CdTe, and GaAs/$Ga_{1-x}Al_xAs$ for HD QW effective mass SLs.

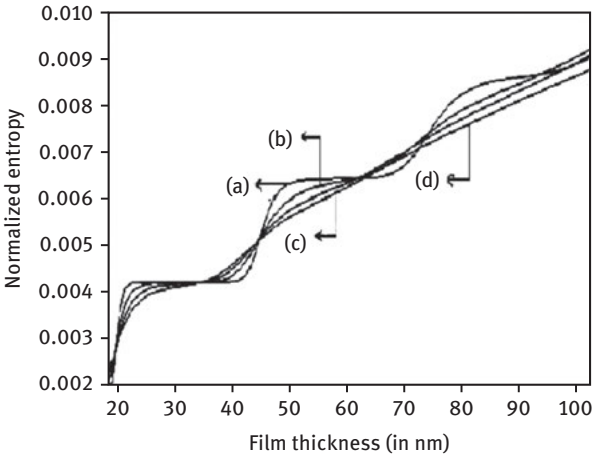

Figure 8.5: Plot of the normalized entropy as a function of film thickness for (a) HgTe/CdTe, (b) PbTe/PbSnTe, (c) CdS/CdTe, and (d) GaAs/$Ga_{1-x}Al_x$Asquantum well HD SLs with graded interfaces.

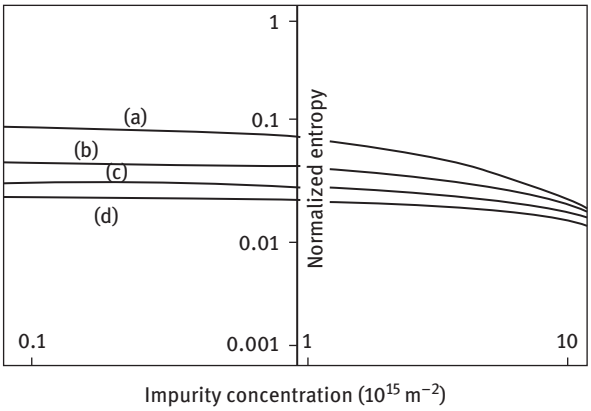

Figure 8.6: Plot of the normalized entropy as a function of impurity concentration for all the cases of Figure 8.6.

Finally, it may be remarked from the Figures 8.7 and 8.8 and Figures 8.5 and 8.6 that the nature of variations of the entropy for all types of HD QW effective mass SLs does not differ widely as compared with the corresponding HD QWSLs with graded interfaces.

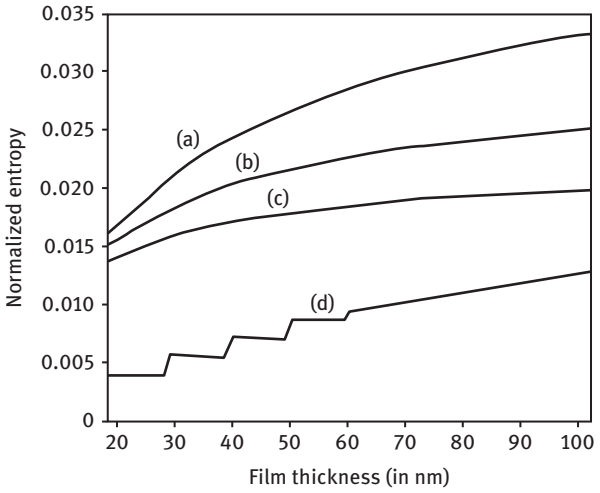

Figure 8.7: Plot of the normalized entropy as a function of film thickness for (a) HgTe/CdTe, (b) PbTe/PbSnTe, (c) CdS/CdTe, and (d) GaAs/$Ga_{1-x}Al_x$Asquantum well effective mass HD SLs.

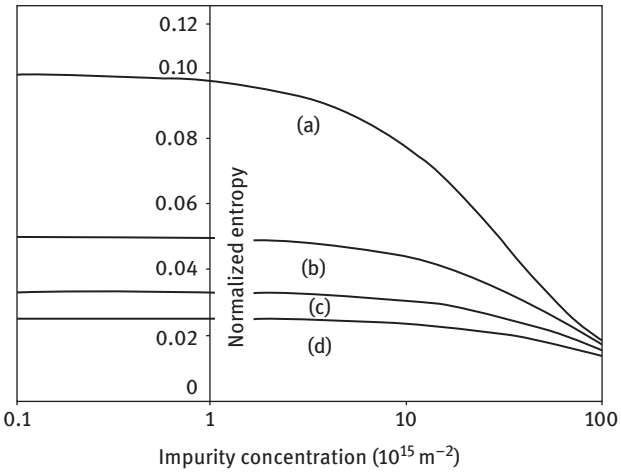

Figure 8.8: Plot of the normalized entropy as a function of impurity concentration for all the cases of Figure 8.7.

8.4 Open research problems

(R8.1) Investigate the entropy in the absence of magnetic field by considering all types of scattering mechanisms for HD III–V, II–VI, IV–VI, and HgTe/CdTe quantum well and quantum wire SLs with graded interfaces and also the effective mass SLs of the aforementioned materials.

(R8.2) Investigate the entropy in the absence of magnetic field by considering all types of scattering mechanisms for HD strained layer, random, short period and Fibonacci, polytype and saw-tooth quantum well and quantum wire SLs.

(R8.3) Investigate the entropy in the presence of an arbitrarily oriented quantizing magnetic field in the presence of spin and broadening by considering all types of scattering mechanisms for (R8.1) and (R8.2) under an arbitrarily oriented (a) nonuniform electric field and (b) alternating electric field respectively.

(R8.4) Investigate the entropy by considering all types of scattering mechanisms for (R8.1) and (R8.2) under an arbitrarily oriented alternating magnetic field by including broadening and the electron spin, respectively.

(R8.5) Investigate the entropy by considering all types of scattering mechanisms for (R8.1) and (R8.2) under an arbitrarily oriented quantizing alternating magnetic field and crossed alternating electric field by including broadening and the electron spin, respectively.

(R8.6) Investigate the entropy by considering all types of scattering mechanisms for (R8.1) and (R8.2) under an arbitrarily oriented alternating quantizing magnetic field and crossed alternating non-uniform electric field by including broadening and the electron spin respectively.

(R8.7) Investigate the entropy in the absence of magnetic field for all types of quantum well and quantum wire SLs as considered in this chapter under exponential, Kane, Halperin, Lax, and Bonch-Bruevich band tails [2], respectively.

(R8.8) Investigate the entropy in the presence of quantizing magnetic field including spin and broadening for the problem as defined in (R8.7) under an arbitrarily oriented (a) nonuniform electric field and (b) alternating electric field, respectively.

(R8.9) Investigate the entropy for the problem as defined in (R8.7) under an arbitrarily oriented alternating quantizing magnetic field by including broadening and the electron spin, respectively.

(R8.10) Investigate the entropy for the problem as defined in (R8.7) under an arbitrarily oriented alternating quantizing magnetic field and crossed alternating electric field by including broadening and the electron spin, respectively.

(R8.11) Investigate all the appropriate problems as defined in (R8.1) to (R8.10) for all types of quantum dot SLs.

(R8.12) Investigate all the appropriate problems as defined in (R8.1) to (R8.10) for all types of quantum dot SLs in the presence of strain.

(R8.13) Introducing new theoretical formalisms, investigate all the problems of this chapter in the presence of hot electron effects.

(R8.14) Investigate the influence of deep traps and surface states separately for all the appropriate problems of this chapter after proper modifications.

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9 Conclusion and scope for future research

The greatest pleasure in life is doing what people say we cannot do.

This monograph deals with the entropy in various types of HD materials and their quantized counter parts. The quantization and strong electric field alter profoundly the basic band structures, which, in turn, generate pinpointed knowledge regarding entropy in various HDS and their nanostructures. The in-depth experimental investigations covering the whole spectrum of nano materials and allied science in general, are extremely important to uncover the underlying physics and the related mathematics in this particular aspect. We have formulated the simplified expressions of entropy for few HD quantized structures together with the fact that our investigations are based on the simplified $\vec{k}.\vec{p}$ formalism of solid-state science without incorporating the advanced-field theoretic techniques. In spite of such constraints, the role of band structure, which generates, in turn, new concepts are truly amazing and discussed throughout the text.

We present the last bouquet of open research problem in this pin-pointed topic of research of modern physics.

(R9.1) Investigate the entropy in the presence of a quantizing magnetic field under exponential, Kane, Halperin, Lax and Bonch-Bruevich band tails [1] for all the problems of this monograph of all the HD materials whose unperturbed carrier energy spectra are defined in Chapter 1 by including spin and broadening effects.

(R9.2) Investigate all the appropriate problems after proper modifications introducing new theoretical formalisms for the problems as defined in (R9.1) for HD negative refractive index, macro molecular, nitride and organic materials.

(R9.3) Investigate all the appropriate problems of this monograph for all types of HD quantum confined p-InSb, p-CuCl and materials having diamond structure valence bands whose dispersion relations of the carriers in bulk materials are given by Cunningham [2], Yekimov et. al. [3] and Roman et. al. [4], respectively.

(R9.4) Investigate the influence of defect traps and surface states separately on the entropy of the HD materials for all the appropriate problems of all the chapters after proper modifications.

(R9.5) Investigate the entropy of the HD materials under the condition of non-equilibrium of the carrier states for all the appropriate problems of this monograph.

(R9.6) Investigate the entropy for all the appropriate problems of this monograph for the corresponding HD p-type materials and their nanostructures.

(R9.7) Investigate the entropy for all the appropriate problems of this monograph for all types of HD materials and their nanostructures under mixed conduction in the presence of strain.

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(R9.8) Investigate the entropy for all the appropriate problems of this monograph for all types of HD materials and their nanostructures in the presence of hot electron effects.

(R9.9) Investigate the entropy for all the appropriate problems of this monograph for all types of HD materials and their nanostructures for nonlinear charge transport.

(R9.10) Investigate the entropy for all the appropriate problems of this monograph for all types of HD materials and their nanostructures in the presence of strain in an arbitrary direction.

(R9.11) Investigate all the appropriate problems of this monograph for strongly correlated electronic HD systems in the presence of strain.

(R9.12) Investigate all the appropriate problems of this chapter in the presence of arbitrarily oriented photon field and strain.

(R9.13) Investigate all the appropriate problems of this monograph for all types of HD nanotubes in the presence of strain.

(R9.14) Investigate all the appropriate problems of this monograph for HD Bi_2Te_3-Sb_2Te_3 superlattices in the presence of strain.

(R9.15) Investigate the influence of the localization of carriers on the entropy in HDS for all the appropriate problems of this monograph in the presence of crossed fields.

(R9.16) Investigate entropy for HD p-type SiGe under different appropriate physical conditions as discussed in this monograph in the presence of strain and crossed fields.

(R9.17) Investigate entropy for HD GaN under different appropriate physical conditions as discussed in this monograph in the presence of strain and crossed fields.

(R9.18) Investigate entropy for different disordered HD conductors under different appropriate physical conditions as discussed in this monograph in the presence of strain and crossed fields.

(R9.19) Investigate all the appropriate problems of this monograph for HD $Bi_2Te_{3-x}Se_x$ and $Bi_{2-x}Sb_xTe_3$, Respectively, in the presence of strain and crossed fields.

(R9.20) Investigate all the appropriate problems of this monograph in the presence of crossed electric and alternating quantizing magnetic fields.

(R9.21) Investigate all the appropriate problems of this monograph in the presence of crossed alternating electric and quantizing magnetic fields.

(R9.22) Investigate all the appropriate problems of this monograph in the presence of crossed alternating non uniform electric and alternating quantizing magnetic fields.

(R9.23) Investigate all the appropriate problems of this monograph in the presence of alternating crossed electric and alternating quantizing magnetic fields.

(R9.24) Investigate all the appropriate problems of this monograph in the presence of arbitrarily oriented pulsed electric and quantizing magnetic fields.

(R9.25) Investigate all the appropriate problems of this monograph in the presence of arbitrarily oriented alternating electric and quantizing magnetic fields.

(R9.26) Investigate all the appropriate problems of this monograph in the presence of crossed in homogeneous electric and alternating quantizing magnetic fields.

(R9.27) Investigate all the appropriate problems of this monograph in the presence of arbitrarily oriented electric and alternating quantizing magnetic fields under strain.

(R9.28) Investigate all the appropriate problems of this monograph in the presence of arbitrarily oriented electric and alternating quantizing magnetic fields under light waves.

(R9.29) (a) ***Investigate the entropy for all types of HD materials of this monograph in the presence of many body effects, strain and arbitrarily oriented alternating light waves, respectively.***

(b) ***Investigate all the appropriate problems of this chapter for the Dirac electron.***

(c) ***Investigate all the problems of this monograph by removing all the physical and mathematical approximations and establishing the respective appropriate uniqueness conditions.***

The formulation of* entropy *for all types of HD materials and their quantum-confined counterparts considering the influence of all the bands created due to all types of quantizations after removing all the assumptions and establishing the respective appropriate uniqueness conditions is, in general, an extremely difficult problem. **Around 200 open research problems** have been presented in this monograph and we hope that the readers will not only solve them but also generate new concepts, both theoretical and experimental. Incidentally, we can easily infer how little is presented and how much more is yet to be investigated in this exciting topic which is the signature of coexistence of new physics, advanced mathematics combined with the inner fire for performing creative researches in this context from the young scientists since like Kikoin [5] we firmly believe that ***"A young scientist is no good if his teacher learns nothing from him and gives his teacher nothing to be proud of."*** In the mean time, our research interest has been shifted and we are leaving this particular beautiful topic with the hope that (R9.29) alone is sufficient to draw the attention of the researchers from diverse fields and our readers are surely in tune with the fact that ***"Exposition, criticism, appreciation is the work for second-rate minds"*** [6].

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10 Appendix A: The entropy under intense electric field in HD Kane type materials

My life equation is Mission = Vision = Passion = Creation

10.1 Introduction

With the advent of modern nano devices, there has been considerable interest in studying the electric field-induced processes in materials having different band structures. It appears from the literature that the studies have been made on the assumption that the carrier dispersion laws are invariant quantities in the presence of intense electric field, which is not fundamentally true. In this chapter, we shall study the entropy in quantum-confined optoelectronic materials under strong electric field. In Section 10.2.1, an attempt is made to investigate the entropy in the presence of intense electric field in HD III–V, ternary and quaternary materials Section 10.2.2, contains the investigation of the entropy under magnetic quantization in HD Kane-type materials in the presence of intense electric field. In Section 10.2.3, entropy in QWs of HD Kane-type materials in the presence of intense electric field has been studied. In Section 10.2.4, we investigatethe entropy in NWs of HD Kane-type materials in the presence of intense electric field. In Section 10.2.5, the magneto entropy in QWs in HD Kane-type materials in the presence of intense electric field has been studied. In Section 10.2.6, the entropy in accumulation and inversion layers of Kane-type materials in the presence of intense electric field has been studied. In Section 10.2.7,the entropy in doping superlattices of HD Kane-type materials in the presence of intense electric field has been studied. In Section 10.2.8, the entropy in QWHD effective mass superlattices of Kane-type materials in the presence of intense electric field has been investigated. In Section 10.2.9, the entropy in NWHD effective mass superlattices of Kane type materials in the presence of intense electric field has been studied. In Section 10.2.10, the magneto entropy in QWHD effective mass superlattices of Kane-type materials in the presence of intense electric field has been studied. In Section 10.2.11, the entropy in QWHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field has been studied. In Section 10.2.12, the entropy in NWHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field has been investigated. In Section 10.2.13, the entropy in Quantum dot HD superlattices of Kane-Type materials with graded interfaces in the presence of intense electric field is studied. In Section 10.2.14, the magneto entropy in HD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field has been investigated. In Section 10.2.15, the magneto

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entropy in QWHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field has been investigated. Section 10.3 presents Six open research problems that challenge the first-order creativity of the readers from diverse fields.

10.2 Theoretical background

10.2.1 Entropy in the presence of intense electric field in HD III–V, ternary, and quaternary materials

The expression of the inter-band transition matrix element $(\bar{X}_{12})$ in this case can be written as

$$\bar{X}_{12} = i\int \bar{u}^{*}_{\bar{k}1}(\bar{r}).\frac{\partial}{\partial \bar{k}_x}\bar{u}_{\bar{k}2}(\bar{r})\bar{d}^3\bar{r} \tag{10.1}$$

where $\bar{u}_{\bar{k}1}(\bar{r}) \equiv \bar{u}_1(\bar{k},\bar{r})$ and $\bar{u}_{\bar{k}2}(\bar{r}) \equiv \bar{u}_2(\bar{k},\bar{r})$ in which $\bar{u}_1(\bar{k},\bar{r})$ and $\bar{u}_2(\bar{k},\bar{r})$are given by

In the case of the presence of an external electric field, $\bar{F}_s$ along *x*-axis, the inter-band transition matrix-element, $\bar{X}_{12}$, has finite interaction band same band, e.g.,

$$\acute{a}\bar{S}\left|\bar{S}\check{n}\right. = \acute{a}\bar{X}\left|\bar{X}\check{n}\right. = \acute{a}\bar{Y}\left|\bar{Y}\check{n}\right. = \acute{a}\bar{Z}\left|\bar{Z}\check{n}\right. = 1$$

$$\acute{a}\bar{X}\left|\bar{Y}\check{n}\right. = \acute{a}\bar{Y}\left|\bar{Z}\check{n}\right. = \acute{a}\bar{Z}\left|\bar{X}\check{n}\right. = 0$$

$$\acute{a}\bar{S}\left|\bar{X}\check{n}\right. = \acute{a}\bar{X}\left|\bar{S}\check{n}\right. = 0;$$

$$\acute{a}\bar{S}\left|\bar{Y}\check{n}\right. = \acute{a}\bar{Y}\left|\bar{S}\check{n}\right. = 0 \; and \; \acute{a}\bar{S}\left|\bar{Z}\check{n}\right. = \acute{a}\bar{Z}\left|\bar{S}\check{n}\right. = 0.$$

Using the appropriate equations, we can write

$$\begin{aligned}
\bar{X}_{12} = i\int \bar{d}^3\bar{r}\Bigg\{ & \bar{a}_{k_+}\left[(i\bar{S})\downarrow'\right] + \bar{b}_{k_+}\left[\left(\frac{\bar{X}' - i\bar{Y}'}{\sqrt{2}}\right)\uparrow'\right] + \bar{c}_{k_+}\left[\bar{Z}'\downarrow'\right]\Bigg\}^{*}\frac{\partial}{\partial \bar{k}_x} \\
& \left\{\bar{a}_{k_-}\left[(i\bar{S})\uparrow'\right] - \bar{b}_{k_-}\left[\left(\frac{\bar{X}' - i\bar{Y}'}{\sqrt{2}}\right)\downarrow'\right] + \bar{c}_{k_-}\left[\bar{Z}'\uparrow'\right]\right\} \\
= i\int \bar{d}^3\bar{r}\Bigg[& \left\{\left(\bar{a}_{k_+}\frac{\partial}{\partial \bar{k}_x}\bar{a}_{k_-}\right).\left(\left[(i\bar{S})\downarrow'\right]\left[(i\bar{S})\uparrow'\right]\right)\right. \\
& + \left(\frac{\bar{b}_{k_+}}{\sqrt{2}}\frac{\partial}{\partial \bar{k}_x}\bar{a}_{k_-}\right)\left[\left(\bar{X}' - i\bar{Y}'\right)\uparrow'\right]^{*}.\left[(i\bar{S})\uparrow'\right] \\
& \left. + \left(\bar{c}_{k_+}\frac{\partial}{\partial \bar{k}_x}\bar{a}_{k_-}\right)\left[\bar{Z}'\downarrow'\right]^{*}.\left[(i\bar{S})\uparrow'\right]\right\}\Bigg]
\end{aligned}$$

$$
\begin{aligned}
&- \left(\frac{\bar{b}_{k_+} \frac{\partial}{\partial k_x} \bar{b}_{k_-}}{2} \right) [(\bar{X}' - i\bar{Y}') \uparrow']^* . [(\bar{X}' - i\bar{Y}') \downarrow'] \\
&- \left(\frac{\bar{c}_{k_+} \frac{\partial}{\partial k_x} \bar{b}_{k_-}}{\sqrt{2}} \right) [(\bar{Z}' \downarrow')]^* . [(\bar{X}' - i\bar{Y}') \downarrow']\}] \\
&= i \int \bar{d}^3 \bar{r} \left[\left\{ \left(- \bar{a}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{c}_{k_-} \right) . [(i\bar{S}) \downarrow']^* . [\bar{Z}' \uparrow'] - \left(\frac{\bar{b}_{k_+}}{\sqrt{2}} \frac{\partial}{\partial \bar{k}_x} \bar{c}_{k_-} \right) [(\bar{X}' - i\bar{Y}') \uparrow']^* . [\bar{Z}' \uparrow'] \right. \right. \\
&\left. \left. + \left(\bar{c}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{c}_{k_-} \right) [\bar{Z}' \downarrow']^* . [\bar{Z}' \uparrow'] \right\} \right]
\end{aligned} \tag{10.2}
$$

Therefore,

$$
\begin{aligned}
\frac{\bar{X}_{12}}{i} = &\left[\left\{ \left[\left(\bar{a}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{a}_{k_-} \right) . \langle i\bar{S} | i\bar{S} \rangle \langle \downarrow' | \uparrow' \rangle \right] + \left[\left(\frac{\bar{b}_{k_+}}{\sqrt{2}} \frac{\partial}{\partial \bar{k}_x} \bar{a}_{k_-} \right) \langle (\bar{X}' - i\bar{Y}') | i\bar{S} \rangle \langle \uparrow' | \downarrow' \rangle \right] \right. \\
&\left. + \left[\left(\bar{c}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{a}_{k_-} \right) \langle \bar{Z}' | i\bar{S} \rangle \langle \downarrow' | \uparrow' \rangle \right] \right\} \\
&- \left[\left\{ \left[\left(\frac{\bar{a}_{k_+}}{\sqrt{2}} \frac{\partial}{\partial \bar{k}_x} \bar{b}_{k_-} \right) . \langle i\bar{S} | (\bar{X}' - i\bar{Y}') \rangle \langle \downarrow' | \downarrow' \rangle \right] \right. \right. \\
&+ \left[\left(\frac{\bar{b}_{k_+}}{2} \frac{\partial}{\partial \bar{k}_x} \bar{b}_{k_+} \right) \langle (\bar{X}' - i\bar{Y}') | (\bar{X}' + i\bar{Y}') \rangle \langle \uparrow' | \downarrow' \rangle \right] \\
&\left. \left. + \left[\left(\frac{\bar{c}_{k_+}}{\sqrt{2}} \frac{\partial}{\partial \bar{k}_x} \bar{a}_{k_-} \right) \langle \bar{Z}' | (\bar{X}' - i\bar{Y}') \rangle \langle \downarrow' | \uparrow' \rangle \right] \right\} \right] \\
&+ \left\{ \left[\left(\bar{a}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{c}_{k_-} \right) . \langle i\bar{S} | \bar{Z}' \rangle \langle \downarrow' | \uparrow' \rangle \right] + \left[\left(\frac{\bar{b}_{k_+}}{\sqrt{2}} \frac{\partial}{\partial \bar{k}_x} \bar{c}_{k_-} \right) . \langle (\bar{X}' - i\bar{Y}') | \bar{Z}' \rangle \langle \uparrow' | \uparrow' \rangle \right] \right. \\
&\left. + \left[\left(\bar{c}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{c}_{k_-} \right) . \langle \bar{Z}' | \bar{Z}' \rangle \langle \downarrow' | \uparrow' \rangle \right] \right\}
\end{aligned} \tag{10.3}
$$

Therefore, we can write,

$$
\bar{X}_{12} = i \left\{ - \left(\bar{a}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{a}_{k_-} \right) \langle \downarrow' | \uparrow' \rangle + \left(\bar{c}_{k_+} \frac{\partial}{\partial \bar{k}_x} \bar{c}_{k_-} \right) \langle \downarrow' | \uparrow' \rangle \right\} \tag{10.4}
$$

We can prove that

$$\langle \downarrow' | \uparrow' \rangle = \frac{1}{2}(\hat{r}_1 + i\hat{r}_2) \tag{10.5}$$

Therefore, by (10.4) and (10.5), we get

$$\begin{aligned} \bar{X}_{12} &= i\left\{ -\left(\bar{a}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{a}_{k-}\right) + \left(\bar{c}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{c}_{k-}\right)\right\}\langle \downarrow' | \uparrow' \rangle \\ &= -i\left\{ -\left(\bar{a}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{a}_{k-}\right) + \left(\bar{c}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{c}_{k-}\right)\right\}.\frac{1}{2}(\hat{r}_1 + i\hat{r}_2) \\ &= \frac{-iA(\bar{k})}{2}(\hat{r}_1 + i\hat{r}_2) \end{aligned} \tag{10.6}$$

where

$$\bar{A}(\bar{k}) = \left(\bar{a}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{a}_{k-}\right) - \left(\bar{c}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{c}_{k-}\right) \tag{10.7}$$

From (10.6), we find,

$$|\bar{X}_{12}|^2 = \frac{1}{4}\bar{A}^2(\bar{k})(1+1) = \frac{1}{2}\bar{A}^2(\bar{k})[since, |\hat{r}_1| = |\hat{r}_2| = 1] \tag{10.8}$$

considering spin-up and spin-down, we have to multiply by 2

$$|\bar{X}_{12}|^2 = 2 \times \frac{1}{2}\bar{A}^2(\bar{k}) = \bar{A}^2(\bar{k}) \tag{10.9}$$

We can evaluate $\bar{X}_{11}$ *and* $\bar{X}_{22}$ in the following way:

$$\begin{aligned} \bar{X}_{11} &= i\int \bar{u}^*_{\bar{k}1}(\bar{r}).\frac{\partial}{\partial \bar{k}_x}\bar{u}_{\bar{k}1}(\bar{r}).\bar{d}^3\bar{r} \\ &= i\int \bar{d}^3\bar{r}\left\{\left(\bar{a}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{a}_{k-}\right) + \left(\bar{b}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{b}_{k-}\right) + \left(\bar{c}_{k+}\frac{\partial}{\partial \bar{k}_x}\bar{c}_{k-}\right)\right\} \\ &= \frac{1}{2}i\int \bar{d}^3\bar{r}\left\{\frac{\partial}{\partial \bar{k}_x}(\bar{a}_k^2 + \bar{b}_k^2 + \bar{c}_k^2)\right\} = \frac{1}{2}\bar{i}\int \bar{d}^3\bar{r}\left\{\frac{\partial}{\partial \bar{k}_x}(1)\right\} = 0, \ since\ \bar{a}^2_{k+} + \bar{b}^2_{k+} + \bar{c}^2_{k+} = 1. \end{aligned}$$

Therefore, $\bar{X}_{11} = 0$, and similarly we can prove $\bar{X}_{22} = 0$. Thus, we conclude that intra-band momentum matrix element due to external electric field ($\bar{X}_{cc}$) is zero. From the expression of $\bar{a}_{k\pm}$ we can write

$$\bar{a}^2{}_{k_+} = \bar{r}_0{}^2\left[\frac{\bar{E}_{g_0} - \gamma^2_{k_+}(\bar{E}_g - \delta')}{\bar{E}_{g_0} + \delta'}\right]^2 \text{ and } \bar{a}^2_{k-} = \bar{r}_0{}^2\left[\frac{\bar{E}_{g_0} - \gamma^2_{k_-}(\bar{E}_{g_0} - \delta')}{\bar{E}_{g_0} + \delta'}\right]^2.$$

Therefore, $2\bar{a}_{k-}\frac{\partial}{\partial k_x}\bar{a}_{k-} = \bar{r}_0{}^2\left[-\left(\frac{\bar{E}_{g_0}-\delta'}{\bar{E}_{g_0}+\delta'}\right)\right]\frac{\partial\gamma_{k-}^2}{\partial k_x}$ and $\frac{\partial\bar{a}_{k-}}{\partial k_x} = -\frac{\bar{r}_0{}^2}{2}\left(\frac{\bar{E}_{g_0}-\delta'}{\bar{E}_{g_0}+\delta'}\right)\frac{1}{\bar{a}_{k-}}\frac{\partial\gamma_{k-}^2}{\partial k_x}$.

Combining the above, we can write $\bar{a}_{k+}\frac{\partial\bar{a}_{k-}}{\partial k_x} = -\frac{\bar{r}_0{}^2}{2}\left(\frac{\bar{E}_{g_0}-\delta'}{\bar{E}_{g_0}+\delta'}\right)\frac{\bar{a}_{k+}}{\bar{a}_{k-}}\frac{\partial\gamma_{k-}^2}{\partial k_x}$.
Similarly, $\bar{c}_{k+} = \bar{t}\gamma_{k+}$ and $\bar{c}_{k-} = \bar{t}\gamma_{k-}$.
Therefore,

$$\bar{c}_{k+}\frac{\partial}{\partial\bar{k}_x}\bar{c}_{k-} = \frac{\bar{t}^2}{2}\frac{\bar{c}_{k+}}{c_{k-}}\frac{\partial\gamma_{k-}^2}{\partial\bar{k}_x}$$

$$\bar{A}(\bar{k}) = \left\{-\frac{\bar{r}_0{}^2}{2}\left[\frac{\bar{E}_{g_0}-\delta'}{\bar{E}_{g_0}+\delta'}\right]\frac{\bar{a}_{k+}}{\bar{a}_{k-}} - \frac{\bar{t}^2}{2}\frac{\bar{c}_{k+}}{\bar{c}_{k-}}\right\}\frac{\partial\gamma_{k-}^2}{\partial\bar{k}_x}$$

Now,

$$\left(\frac{\bar{a}_{k+}}{\bar{a}_{k-}}\right)^2 = \frac{\bar{E}_{g_0}-\gamma_{k+}^2(\bar{E}_{g_0}-\delta')}{\bar{E}_{g_0}-\gamma_{k-}^2(\bar{E}_{g_0}-\delta')} = \frac{\bar{E}_{g_0}-\frac{\eta-\bar{E}_{g_0}}{2(\eta+\delta')}(\bar{E}_{g_0}-\delta')}{\bar{E}_{g_0}-\frac{\eta+\bar{E}_g}{2(\eta+\delta')}(\bar{E}_g-\delta')}$$

$$= \frac{2\bar{E}_g-(\eta+\delta')-(\eta-\bar{E}_{g_0}(\bar{E}_{g_0}-\delta')}{2\bar{E}_g(\eta+\delta')-(\eta+\bar{E}_{g_0})(\bar{E}_{g_0}-\delta')} = \frac{\eta(\bar{E}_{g_0}+\delta')+\bar{E}_{g_0}(\bar{E}_{g_0}+\delta')}{\eta(\bar{E}_{g_0}+\delta')-\bar{E}_{g_0}(\bar{E}_{g_0}-3\delta')}$$

Therefore,

$$\left(\frac{\bar{a}_{k+}}{\bar{a}_{k-}}\right)^{22} = \frac{\eta+\bar{E}_{g_0}}{\eta-\bar{E}_{g_0}\left(\frac{\bar{E}_{g_0}-3\delta'}{\bar{E}_{g_0}+\delta'}\right)} = \frac{\eta+\bar{E}_{g_0}}{\eta-\bar{E}'_{g_0}}$$

where

$$\bar{E}_{g_0} = \frac{\bar{E}_{g_0}(\bar{E}_{g_0}-3\delta')}{\bar{E}_{g_0}+\delta'}$$

Thus, $\frac{\bar{a}_{k+}}{\bar{a}_{k-}} = \sqrt{\frac{\eta+\bar{E}_{g_0}}{\eta-\bar{E}_{g_0}}}$ Similarly, $\frac{\bar{c}_{k+}}{\bar{c}_{k-}} = \frac{\gamma_{k+}}{\gamma_{k-}} = \sqrt{\frac{\eta-\bar{E}_{g_0}}{\eta+\bar{E}_{g_0}}}$ and thus,

$$\bar{A}(\bar{k}) = -\left\{\bar{P}\left(\frac{\eta+\bar{E}_{g_0}}{\eta-\bar{E}'_{g_0}}\right)^{1/2} + \bar{Q}\left(\frac{\eta-\bar{E}_{g_0}}{\eta+\bar{E}'_{g_0}}\right)^{1/2}\right\}\frac{\partial\gamma_{k-}^2}{\partial\bar{k}_x} \tag{10.10}$$

where

$$\bar{P} = \frac{\bar{r}_0{}^2}{2}\left(\frac{\bar{E}_{g_0}-\delta'}{\bar{E}_{g_0}+\delta'}\right) \text{ and } \bar{Q} = \bar{t}^2/\,2.$$

Now, $\gamma_{k-}^2 = \frac{\eta + \bar{E}_{g_0}}{2(\eta + \delta')}$, so that $\frac{\partial \gamma_{k-}^2}{\partial \bar{k}_x} = \frac{1}{2}\left[\frac{\partial \eta / \partial k_x}{(\eta + \delta')} - \frac{\eta + \bar{E}_{g_0}}{(\eta + \delta')^2}\frac{\partial \eta}{\partial k_x}\right]$

Thus,

$$\frac{\partial \gamma_{k-}^2}{\partial \bar{k}_x} = \frac{1}{2}\left[\frac{\eta + \delta' - \eta - \bar{E}_{g_0}}{(\eta + \delta')}\right]\frac{\partial \eta}{\partial \bar{k}_x} = -\frac{1}{2}\frac{(\bar{E}_g - \delta')}{(\eta + \delta')^2}\cdot\frac{\partial \eta}{\partial \bar{k}_x} \tag{10.11}$$

From (10.10) and (10.11), we get

$$\bar{A}(\bar{k}) = \frac{1}{2}\frac{(\bar{E}_{g_0} - \delta')}{(\eta + \delta')^2}\cdot\frac{\partial \eta}{\partial \bar{k}_u}\cdot\left\{\bar{P}\left(\frac{\eta + \bar{E}_{g_0}}{\eta - \bar{E}'_{g_0}}\right)^{1/2} + \bar{Q}\left(\frac{\eta - \bar{E}_{g_0}}{\eta + \bar{E}'_{g_0}}\right)^{1/2}\right\} \tag{10.12}$$

This implies

$$\frac{\partial \eta}{\partial \bar{k}_x} = \frac{\bar{E}_{g_0}\hbar^2}{\bar{m}_r}\cdot\frac{\bar{k}_x}{\eta} \tag{10.13}$$

From (10.12) and (10.13), we can write

$$\bar{A}(\bar{k}) = \frac{\bar{E}_{g_0}\hbar^2}{2\bar{m}_r}\cdot\frac{\bar{k}_u}{\eta}\cdot\frac{(\bar{E}_{g_0} - \delta')}{(\eta + \delta')^2}\cdot\left\{\bar{P}\left(\frac{\eta + \bar{E}_{g_0}}{\eta - \bar{E}'_{g_0}}\right)^{1/2} + \bar{Q}\left(\frac{\eta - \bar{E}_{g_0}}{\eta + \bar{E}'_{g_0}}\right)^{1/2}\right\} \tag{10.14}$$

Thus,

$$|\bar{A}(k)|^2 = \frac{\bar{E}_{g_0}^2(\bar{E}_{g_0} - \delta')\hbar^2}{4\bar{m}_r}\frac{\hbar^2\bar{k}_x^2}{\bar{m}_r}\frac{1}{\eta^2}\frac{1}{(\eta + \delta')^4}\cdot\left\{\bar{P}\left(\frac{\eta + \bar{E}_{g_0}}{\eta - \bar{E}'_{g_0}}\right)^{1/2} + \bar{Q}\left(\frac{\eta - \bar{E}_{g_0}}{\eta + \bar{E}'_{g_0}}\right)^{1/2}\right\}^2 \tag{10.15}$$

and

$$\left|\bar{X}_{12}\right|^2 = \left|\bar{A}(`\bar{k})\right|^2 \tag{10.16}$$

From (10.15) and (10.16), we can write the square of the magnitude of the inter-band transition matrix element due to external electric field ($|X_{CV}|^2$)

It is well known that the energy Eigen value, $\bar{E}_n^{(2)}(\bar{k})$, in the presence of a perturbed Hamiltonian, $\overline{H'}$, is given by [1]

$$\bar{E}_n^{(2)}(\bar{k}) = \bar{E}_n(\bar{k}) + \langle n\bar{k}\left|\overline{H'}\right|n\bar{k}\rangle + \left\{|\langle n\bar{k}|H'|n\bar{k}\rangle|^2/[\bar{E}_n(\bar{k}) - \bar{E}_m(\bar{k})]\right\} \tag{10.17}$$

where

$$\bar{H}\psi_n(\bar{k},\bar{r}) = \bar{E}\psi(\bar{k},\bar{r}) \tag{10.18}$$

$$\bar{H} = \bar{H}_0 + \overline{H'} \tag{10.19}$$

$$\bar{H}_0\bar{u}_n(\bar{k},\bar{r}) = \bar{E}_n(\bar{k})\bar{u}_n(\bar{k},\bar{r}) \tag{10.20}$$

where $\bar{H}$ is the total Hamiltonian, $\psi(\bar{k},\bar{r})$ is the wave function, $\bar{u}_n(\bar{k},\bar{r})$ is the periodic function of it, H_O is the unperturbed Hamiltonian, n is the band index, and $\bar{E}_n(\bar{k})$ is the energy of an electron in the periodic lattice.

For an external electric field ($\bar{F}_S$) applied along the x-axis, the perturbed Hamiltonian ($\overline{H'}$)can be written as

$$\overline{H'} = -\bar{F}.\bar{x} \tag{10.21}$$

where

$$\bar{F} = (e\bar{F}_S)$$

Therefore, we get

$$\bar{E}_n^{(2)}(\bar{k}) = \bar{E}_n(\bar{k}) - \bar{F}\langle n\bar{k}\left|\overline{H'}\right|n\bar{k}\rangle + \bar{F}^2\left\{|\langle n\bar{k}\left|\overline{H'}\right|n\bar{k}\rangle|^2/\left[\bar{E}_n(\bar{k}) - \bar{E}_m(\bar{k})\right]\right. \tag{10.22}$$

In (10.22), the second and the third terms are due to the perturbation factor.

For

$$\bar{X}_{nm}(\bar{k}) = \langle n\bar{k}|x|m\bar{k}\rangle \tag{10.23}$$

we find

$$\bar{X}_{nm}(\bar{k}) = i\int \bar{u}_n^*(\bar{k},\bar{r})(\partial/\partial\bar{u})[\bar{u}_m(\bar{k},\bar{r})]\bar{d}^3\bar{r} \tag{10.24}$$

where $\bar{k}_x$ is the x component of the $\bar{k}$ and the integration in (10.24) extends over the unit cell. From (10.22), (10.23) and (10.24), with the $\bar{n}$ corresponds to the conduction band (C) and $\bar{m}$ corresponds to the valance band (V), we get

$$\bar{E}_n^{(2)}(\bar{k}) = \bar{E}_n(\bar{k}) - \bar{F}\bar{X}_{cc} + \{\bar{F}^2|\bar{X}_{CV}|^2[\bar{E}_C(\bar{k}) - \bar{E}_V(\bar{k})] \tag{10.25}$$

Thus, combining the appropriate equations, the dispersion relation of the conduction electrons in the presence of electric field along x-axis can be written as

$$\begin{aligned}\bar{I}_{11}(\bar{E}) &= \frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c} + \frac{\hbar^2\bar{k}_y^2}{2\bar{m}_c} + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c} + \frac{\bar{F}^2|\bar{X}_{12}|^2}{\eta} \\ &= \left[\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c} + \frac{\hbar^2\bar{k}_y^2}{2\bar{m}_c} + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c}\right. \\ &\quad + \left\{\frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c}\cdot\frac{2\bar{m}_c}{\bar{m}_r}\cdot\frac{\bar{F}^2\hbar^2\bar{E}_g^2(\bar{E}_{g_0}-\delta')^2}{4\bar{m}_r}\frac{1}{\eta^3}\frac{1}{(\eta+\delta')^4}\left[\bar{P}\left(\frac{\eta+E_{g_0}}{\eta-E'_{g_0}}\right)^{1/2}\right.\right. \\ &\quad \left.\left.\left. + \bar{Q}\left(\frac{\eta-E_g}{\eta+E_{g_0}}\right)^{1/2}\right]^2\right\}\right]\end{aligned} \tag{10.26}$$

when $\bar{F}\to 0$, we have from (10.26), $\bar{k}^2 \to \frac{2\bar{m}_c}{\hbar^2}\bar{I}_{11}(\bar{E})$and $\eta_1{}^2 = [\bar{E}_{g_0}^2 + \bar{E}_{g_0}\frac{2\bar{m}_c}{\bar{m}_r}\bar{I}_{11}(\bar{E})]$.

Using the method of successive approximation, we can write

$$1 = \frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c\bar{I}_{11}(\bar{E})} + \frac{\hbar^2\bar{k}_y^2}{2\bar{m}_c\bar{I}_{11}(\bar{E})} + \frac{\hbar^2\bar{k}_z^2}{2\bar{m}_c\bar{I}_{11}(\bar{E})} + \frac{\hbar^2\bar{k}_x^2}{2\bar{m}_c\bar{I}_{11}(\bar{E})}.\Phi(\bar{E},\bar{F}) \tag{10.27}$$

where,

$$\Phi(\bar{E},\bar{F}) = \frac{2\bar{m}_c}{\bar{m}_r}\frac{\bar{F}^2\hbar^2\bar{E}_g^2(\bar{E}_{g_0}-\delta')^2}{4\bar{m}_r}\frac{1}{\eta_1^3}\frac{1}{(\eta_1+\delta')^4}\left[\bar{P}\left(\frac{\eta_1+\bar{E}_{g_0}}{\eta_1-\bar{E}'_{g_0}}\right)^{1/2} + \bar{Q}\left(\frac{\eta_1-\bar{E}_{g_0}}{\eta_1+\bar{E}'_{g_0}}\right)^{1/2}\right]^2$$

Therefore, the $\bar{E}-\bar{k}$ dispersion relation in the presence of an external electric field for III–V, ternary, and quaternary materials whose unperturbed energy band structures are defined by the three-band model of Kane can be expressed as

$$\frac{\bar{k}_x^2}{\frac{2\bar{m}_c}{\hbar^2}\left[\frac{\bar{I}_{11}(\bar{E})}{1+\Phi(\bar{E},\bar{F})}\right]} + \frac{\bar{k}_y^2}{\frac{2\bar{m}_c}{\hbar^2}\bar{I}_{11}(\bar{E})} + \frac{\bar{k}_z^2}{\frac{2\bar{m}_c}{\hbar^2}\bar{I}_{11}(\bar{E})} = 1 \tag{10.28}$$

In (10.28), the coefficients of $\bar{k}_y$, and $\bar{k}_z$ are not same and, for this reason, this basic equation is "anisotropic" in nature, together with the fact that the anisotropic dispersion relation is the ellipsoid of revolution in the k-space.

From (10.28), the expressions of the effective electron masses along x, y, and z directions can, respectively, be written as

$$\bar{m}_x^*(\bar{E},\bar{F}) = \hbar^2\bar{k}_x\frac{\partial\bar{k}_x}{\partial\bar{E}}|_{\bar{k}_y=0,\bar{k}_z=0} = \bar{m}_c[1+\Phi(\bar{E},\bar{F})]^{-2}[[1+\Phi(\bar{E},\bar{F})]\overline{I'}_{11}(\bar{E}) - \bar{I}_{11}(\bar{E})\Phi'(\bar{E},\bar{F})] \tag{10.29}$$

$$\bar{m}_y^*(\bar{E},\bar{F}) = \hbar^2\bar{k}_y\frac{\partial\bar{k}_y}{\partial\bar{E}}|_{\bar{k}_x=0,\bar{k}_z=0} = \bar{m}_0\overline{I'}_{11}(\bar{E}) \tag{10.30}$$

$$\bar{m}_z^*(\bar{E},\bar{F}) = \hbar^2\bar{k}_z\frac{\partial\bar{k}_z}{\partial\bar{E}}|_{\bar{k}_X=0,\bar{k}_y=0} = \bar{m}_0\overline{I'}_{11}(\bar{E}) \tag{10.31}$$

where $\overline{I'}_{11}(\bar{E}) = \frac{\partial}{\partial\bar{E}}(\bar{I}_{11}(\bar{E}))$ and $\Phi'(\bar{E},\bar{F}) = \frac{\partial}{\partial\bar{E}}[\Phi(\bar{E},\bar{F})]$

It may be noted from (10.29) that the effective mass along *x*-direction is a function of both electron energy and electric field, respectively, whereas from (10.30) and (10.31), we can infer the expressions of the effective masses along *y* and *z* directions are same and they depend on the electron energy only. Thus, in the presence of an electric field, the mass anisotropy for Kane-type materials depends both on electron energy and electric field, respectively.

The use of the usual approximation [2]

$$\bar{k}_x^2 \approx \frac{1}{3}\bar{k}^2 \tag{10.32}$$

in (10.28) leads to the simplified expression of the electron energy spectrum in the present case as

$$\begin{aligned}\bar{I}_{11}(E) = {} & \frac{\hbar^2\bar{k}^2}{2\bar{m}_c} \\ & + \frac{\bar{F}^2\hbar^2\bar{E}_g^2(\bar{E}_{g_0}-\delta')^2}{12\bar{m}_r}\frac{2\bar{m}_c}{\bar{m}_r}\bar{I}_{11}(\bar{E})\frac{1}{\eta_1} \\ & \frac{1}{(\eta_1+\delta')^4}\left\{\bar{P}\left(\frac{\eta_1+\bar{E}_{g_0}}{\eta_1-\bar{E}'_{g_0}}\right)^{1/2} + \bar{Q}\left(\frac{\eta_1-\bar{E}_{g_0}}{\eta_1+\bar{E}'_{g_0}}\right)^{1/2}\right\}^2\end{aligned} \tag{10.33}$$

The (10.33) can approximately be written as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c} = \left[e_1\bar{E}^4 + e_2\bar{E}^3 + e_3\bar{E}^2 + e_4\bar{E} + e_5 - \frac{e_6}{1+\bar{C}\bar{E}} + e_7(1+\bar{C}\bar{E})^{-2}\right] \tag{10.34}$$

where

$$e_1 = \bar{Q}_f.\omega_1,\quad \bar{Q}_f = \frac{\bar{m}_c}{\bar{m}_r}\bar{E}_g^{-4}[5e_f\bar{E}_{g_0}^{-2} - 6\bar{G}_f + 7\bar{h}_f\bar{E}_{g_0}^{-4}],$$

$$e_f = \bar{A}_f\bar{P}_f,\quad \bar{A}_f = [\bar{F}\hbar\bar{E}_{g_0}(\bar{E}_{g_0}-\delta')]^2\bar{m}_c(6\bar{m}_r^2(\delta')^4)^{-1},$$

$$\bar{F} = e\bar{F}_s,\quad \bar{G}_f = e_f(4\delta' + \bar{C}_f),\quad \bar{C}_f = (2\bar{E}_{g_0}\bar{Q}^2 + \bar{P}\bar{Q}(\bar{E}_{g_0} - \overline{E'}_{g_0}) - 2\bar{P}^2\bar{E}_{g_0}),$$

$$\bar{E}'_{g_0} = \frac{\bar{E}'_{g_0}(\bar{E}'_{g_0}-3\delta')}{\bar{E}'_{g_0}+\delta'},\quad \bar{P} = \frac{\bar{r}_0^2}{2}\left(\frac{\bar{E}'_{g_0}-\delta'}{\bar{E}'_{g_0}+\delta'}\right),\ \bar{r}_0 = \left[\frac{6}{\chi}(\bar{E}'_{g_0}+\Delta)\left(\bar{E}'_{g_0}+\frac{2}{3}\Delta\right)\right]^{1/2},\ \bar{Q} = \frac{t^2}{2},$$

$$\bar{t}=\left[\frac{6}{\chi}\left(\overline{E'}_{g_0}+\frac{2}{3}\Delta\right)\right]^{1/2},\quad \bar{h}_f=(4\delta'\bar{e}_f\bar{C}_f)(\bar{B}_f)^{-1},\quad \bar{B}_f=(\bar{P}+\bar{Q})^2$$

$$\bar{P}_f=\bar{E}'^{-3}_{g_0}(e_f\bar{E}'^{-2}_{g_0}-\bar{G}_f+\bar{h}_f\bar{E}^{-4}_{g_0}),\quad \omega_1=\bar{a}_1^2,\quad \bar{a}_1=\frac{\bar{a}\bar{b}}{\bar{c}},\quad \bar{a}=\frac{1}{\bar{E}_{g_0}},$$

$$\bar{b}=\frac{1}{\bar{E}_{g_0}+\Delta},\quad \bar{c}=\left(\bar{E}'_{g_0}+\frac{2}{3}\Delta\right)^{-1},$$

$$e_2=\bar{Q}_f.\omega_2,\quad \omega_2=2\bar{a}_1\bar{b}_1,\quad \bar{b}_1=(\bar{c})^{-2}(\bar{a}\bar{c}+\bar{b}\bar{c}-\bar{a}\bar{b}),$$

$$\bar{e}_3=(1-\bar{P}_f)\bar{a}_1+\bar{Q}_f.\omega_3,\quad \omega_3=(\bar{b}_1^2+2\bar{a}_1\bar{c}_1),$$

$$\bar{c}_1=\left[\frac{1}{\bar{c}}\left(1-\frac{\bar{a}}{\bar{c}}\right)\left(1-\frac{\bar{b}}{\bar{c}}\right)\right],\ e_4=[(1-\bar{P}_f)\bar{b}_1+\bar{Q}_f\omega_4],\quad \omega_4=2\bar{b}_1\bar{c}_1,\ e_5=[(1-\bar{P}_f)\bar{c}_1+\omega_5\bar{Q}_f]$$

$$\omega_5=(\bar{c}_1^2-2\bar{c}_1\bar{b}_1),\ e_7=\bar{Q}_f\omega_7,\ \omega_7=\bar{c}_1^2,\ e_6=\left[(1-\bar{P}_f)\bar{c}_1-\bar{Q}_f\omega_6\right]\ and\ \omega_6=\frac{2\bar{c}_1\bar{b}_1}{\bar{c}}\left(1-\frac{\bar{c}\bar{c}_1}{\bar{b}_1}\right)\Bigg]$$

Using (10.26b) and (10.34), we get

$$\frac{\bar{h}^2\bar{k}^2}{2\bar{m}_c}\int_{-\infty}^{\bar{E}}\bar{F}(\bar{V})d\bar{V}=e_1\int_{-\infty}^{\bar{E}}(\bar{E}-\bar{V})^4\bar{F}(\bar{V})d\bar{V}+e_2\int_{-\infty}^{\bar{E}}(\bar{E}-\bar{V})^3\bar{F}(\bar{V})d\bar{V}+e_3\int_{-\infty}^{\bar{E}}(\bar{E}-\bar{V})^2\bar{F}(\bar{V})d\bar{V}$$
$$+\bar{e}_4\int_{-\infty}^{\bar{E}}(\bar{E}-\bar{V})\bar{F}(\bar{V})d\bar{V}+e_5\int_{-\infty}^{\bar{E}}\bar{F}(\bar{V})\bar{d}\bar{V}-e_6\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})\bar{d}\bar{V}}{[1+\bar{c}(\bar{E}-\bar{V})]}+e_7\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})d\bar{V}}{[1+\bar{c}(\bar{E}-\bar{V})]^2} \tag{10.35}$$

We can prove that

$$\int_{-\infty}^{\bar{E}}(\bar{E}-\bar{V})^4\bar{F}(\bar{V})d\bar{V}=\frac{\bar{E}^4}{2}[1+Erf(\bar{E}/\eta_g)]+\frac{3\eta_g^4}{8\pi}\left[1+Erf(\bar{E}/\eta_g)-\frac{2\eta_g}{3\bar{E}}\exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)\right]$$
$$+\frac{3}{2}(\bar{E},\eta_g)^2[1+Erf(\bar{E}/\eta_g)]+\frac{\bar{E}^3\eta_g}{\sqrt{\pi}}\exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)+\frac{2}{\sqrt{\pi}}\bar{E}\eta_g^3\exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)\left[1+\frac{\bar{E}^2}{\eta_g^2}\right]$$
$$=\psi_0(\bar{E},\eta_g) \tag{10.36}$$

From Chapter 2, we know that

$$\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})d\bar{V}}{[1+\bar{c}(\bar{E}-\bar{V})]}=\bar{c}_1(\bar{c},\bar{E},\eta_g)-i\bar{c}_2(\bar{c},\bar{E},\eta_g) \tag{10.37}$$

where

$$\bar{c}_1(\bar{c},\bar{E},\eta_g)=\left[\frac{2}{\bar{c}\eta_g\sqrt{\pi}}\exp(-\bar{u}^2)\left[\sum_{\bar{p}=1}^{\infty}\exp\left(\frac{-\bar{p}^2}{4}\right)(\bar{p})^{-1}Sinh(\bar{p}\bar{u})\right]\right],$$

$$\bar{c}_2(\bar{c},\bar{E},\eta_g)=\frac{\sqrt{\pi}}{\bar{c}\eta_g}\exp(-\bar{u}^2)$$

and $\bar{u}=\frac{1+\bar{c}\bar{E}}{\bar{c}\eta_g}$

We know that

$$\frac{\partial}{\partial\bar{x}}\int_{\bar{A}(\bar{x})}^{\bar{B}(\bar{x})}\bar{F}(\bar{x},\zeta)d\zeta=\int_{\bar{A}(\bar{x})}^{\bar{B}(\bar{x})}\frac{\partial}{\partial\bar{x}}[\bar{F}(\bar{x},\zeta)]\bar{d}\zeta+\bar{F}(\bar{x},B(\bar{x}))\frac{\partial\bar{B}(\bar{x})}{\partial\bar{x}}-\bar{F}(\bar{x},\bar{A}(\bar{x}))\frac{\partial\bar{A}(\bar{x})}{\partial\bar{x}}\tag{10.38}$$

Using (10.37) and (10.38), we get

$$\int_{-\infty}^{\bar{E}}\frac{\bar{F}(\bar{V})d\bar{V}}{[1+\bar{c}(\bar{E}-\bar{V})]}=\bar{c}_3(\bar{c},\bar{E},\eta_g)-i\bar{c}_4(\bar{c},\bar{E},\eta_g)\tag{10.39}$$

where

$$\bar{c}_3(\bar{c},\bar{E},\eta_g)=\left[\frac{-4\bar{u}\exp(-\bar{u}^2)}{\bar{c}^2\eta_g^2\sqrt{\pi}}\left[\sum_{\bar{p}=1}^{\infty}\exp\left(\frac{-\bar{p}^2}{4}\right)(\bar{p})^{-1}Sinh(\bar{p}\,\bar{u})\right]+\frac{1}{\pi\bar{c}\eta_g}\exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)\right.$$

$$\left.-\frac{2\exp(-\bar{u}^2)}{\bar{c}^2\eta_g^2\sqrt{\pi}}\sum_{\bar{p}=1}^{\infty}\exp\left(\frac{-\bar{p}^2}{4}\right)Cosh(\bar{p}\bar{u})\right]\ and\ \bar{D}_3(\bar{c},\bar{E},\eta_g)=\frac{2u}{\bar{c}^2\eta_g^2}\exp(-\bar{u}^2)$$

Therefore, the DR in HD Kane-type materials can be written using (10.35), (10.36), (10.37), and (10.39) as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c}=\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})\tag{10.40}$$

where,

$$\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})=2[1+Erf(\bar{E}/\eta_g)]^{-1}[e_1\psi_0(\bar{E},\eta_g)+e_2\psi_1(\bar{E},\eta_g)+e_3\theta_0(\bar{E},\eta_g)+e_4\gamma_0(\bar{E},\eta_g)$$

$$+e_5\frac{1}{2}[1+Erf(\bar{E}/\eta_g)]-e_6\bar{c}_1(\bar{E},\bar{c},\eta_g)+e_7\bar{c}_3(\bar{E},\bar{c},\eta_g)],\ \psi_1(\bar{E},\eta_g)$$

$$=\left[\frac{\bar{E}}{2}[1+Erf(\bar{E}/\eta_g)]\left[\bar{E}^2+\frac{3}{2}\eta_g^2\right]+\frac{\eta_g}{2\sqrt{\pi}}\exp\left(\frac{-\bar{E}^2}{\eta_g^2}\right)(4\bar{E}^2+\eta_g^2)\right]$$

and

$$\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F}) = 2[1+Erf(\bar{E}/\eta_g)]^{-1}[e_6\bar{c}_2(\bar{E},\bar{c},\eta_g)+e_7\bar{D}_3((\bar{E},\bar{c},\eta_g)]$$

The DOS function is given by

$$\bar{N}_F(\bar{E}) = 4\pi\bar{g}_v\left(\frac{2\bar{m}_c}{\bar{h}^2}\right)^{\frac{3}{2}}\left[\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}'_2(\bar{E},\bar{c},\eta_g,\bar{F})\right]\sqrt{\left[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})\right]} \tag{10.41}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E},\eta_g,\bar{F}) = \bar{m}_c\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) \tag{10.42a}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{1}{3\pi^2}\left(\frac{2\bar{m}_c}{\bar{h}^2}\right)^{\frac{3}{2}}\text{Re}\,al\;\;part\;\;of[\Theta_{20,1}(\bar{E}_{f20,1},\eta_g,\bar{F})+\Theta_{20,2}(\bar{E}_{f20,1},\eta_g,\bar{F})] \tag{10.42b}$$

where

$$\Theta_{20,1}(\bar{E}_{f20,1},\eta_g,\bar{F}) = [\bar{J}_1(\bar{E}_{f20,1},\bar{c},\eta_g,\bar{F})+j\bar{J}_2(\bar{E}_{f20,1},\bar{c},\eta_g,\bar{F})]^{\frac{3}{2}},$$

$$\Theta_{20,2}(\bar{E}_{f20,1},\eta_g,\bar{F}) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\Theta_{20,1}(\bar{E}_{f20,1},\eta_g,\bar{F})]$$

and $\bar{E}_{f20,1}$ is the Fermi energy in this case.

Using (1.31f) and (10.42b) we can study the entropy in this case.

10.2.2 The entropy under magnetic quantization in HD Kane-type materials in the presence of intense electric field

The DR of the conduction electrons in HD optoelectronic materials under electric field can be written in presence of quantizing magnetic field B along x-direction whose unperturbed electron energy spectra are defined by the three band of Kane as

$$\left(\bar{n}+\frac{1}{2}\right)\hbar\bar{w}_0+\frac{\bar{\hbar}^2\bar{k}_x{}^2}{2\bar{m}_c} = [\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})]\omega_0 = \frac{e\bar{B}}{\bar{m}_c} \tag{10.43}$$

From (10.43) we get,

$$\bar{k}_x{}^2 = \bar{w}_{11}(\bar{E},\bar{F},\bar{n},\eta_g) \tag{10.44}$$

where,

$$\bar{w}_{11}(\bar{E},\bar{F},\bar{n},\eta_g)=\frac{2\bar{m}_c}{\hbar^2}\left[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})-\left(\bar{n}+\frac{1}{2}\right)\hbar\omega_0\right]$$

The density-of-states function for both the cases can, respectively, be expressed as

$$\bar{N}(\bar{E},\bar{c},\eta_g,\bar{F})=\frac{\bar{g}_v e\bar{B}\sqrt{2\bar{m}_c}}{2\pi^2\hbar^2}\sum_{\bar{n}=0}^{\bar{n}\max}\frac{[\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}'_2(\bar{E},\bar{c},\eta_g,\bar{F})]\bar{H}(\bar{E}-\bar{E}_{n1HD})}{\sqrt{[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})]-(\bar{n}+\frac{1}{2})\hbar\omega_o}} \tag{10.45}$$

where $\bar{E}_{n1HD}$ is the Landau level in this case and can be expressed a

$$\left(\bar{n}+\frac{1}{2}\right)\hbar w_0=[\bar{J}_1(\bar{E}_{n1HD},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E}_{n1HD},\bar{c},\eta_g,\bar{F})] \tag{10.46}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E},\eta_g,\bar{F})=\bar{m}_c\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) \tag{10.47a}$$

The electron concentration can be written as

$$\bar{n}_0=\frac{e\bar{B}}{\pi^2\hbar}\,Real\ \ part\ of\sum_{\bar{n}=0}^{\bar{n}\max}[\Theta_{20,3}(\bar{E}_{f20,2},\eta_g,\bar{n},\bar{F})+\Theta_{20,4}(\bar{E}_{f20,2},\eta_g,\bar{n},\bar{F})] \tag{10.47b}$$

where

$$\Theta_{20,3}(\bar{E}_{f20,2},\eta_g,\bar{n},\bar{F})=[\bar{w}_{11}(\bar{E}_{f20,2},\bar{F},\bar{n},\eta_g)]^{\frac{1}{2}},$$

$$\Theta_{20,4}(\bar{E}_{f20,2},\bar{F},\bar{n},\eta_g)=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\Theta_{20,3}(\bar{E}_{f20,2},\bar{F},\bar{n},\eta_g)]$$

and $\bar{E}_{f20,2}$ is the Fermi energy in this case

Using (1.31f) and (10.47b), we can study the entropy in this case.

10.2.3 Entropy in QWs in HD Kane-type materials in the presence of intense electric field

The DR in this case is given by

$$\frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\frac{\hbar^2\bar{k}_s^{\,2}}{2\bar{m}_c}=[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})] \tag{10.48}$$

The DOS function in this case is given by

$$\bar{N}_{2D}(\bar{E},\bar{c},\eta_g,\bar{F}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}'_2(\bar{E},\bar{c},\eta_g,\bar{F})]\bar{H}(\bar{E}-\bar{E}_{n_{z18,1HD}}) \tag{10.49}$$

where $\bar{E}_{n_{z18,1HD}}$ is the sub-band energy in this case and can be expressed as

$$\frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = [\bar{J}_1(\bar{E}_{n_{z18,1HD}},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E}_{n_{z18,1HD}},\bar{c},\eta_g,\bar{F})] \tag{10.50}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E},\eta_g,\bar{F}) = \bar{m}_c\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) \tag{10.51a}$$

$$\bar{n}_0 = \frac{\bar{g}_v\bar{m}_c}{\pi\hbar^2}Real\ \ part\ of\ \sum_{\bar{n}=0}^{\bar{n}_{\max}}[\Theta_{20,5}(\bar{E}_{f20,3},\eta_g,\bar{F}) + \Theta_{20,6}(\bar{E}_{f20,3},\eta_g,\bar{F})] \tag{10.51b}$$

where

$$\Theta_{20,5}(\bar{E}_{f20,3},\eta_g,\bar{F}) = \left[\bar{J}_1(\bar{E}_{f20,3},\bar{c},\eta_g,\bar{F}) + j\bar{J}_2(\bar{E}_{f20,3},\bar{c},\eta_g,\bar{F}) - \left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2\right]$$

$$\Theta_{20,6}(\bar{E}_{f20,3},\eta_g,\bar{F}) = \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\Theta_{20,5}(\bar{E}_{f20,3},\eta_g,\bar{F})]$$

and $\bar{E}_{f20,3}$ is the Fermi energy in this case.

Using (1.31f) and (10.51b), we can study the entropy in this case.

10.2.4 Entropy in NWs in HD Kane-type materials in the presence of intense electric field

The DR in this case is given by

$$\frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 + \frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_y\pi}{\bar{d}_y}\right)^2 + \frac{\hbar^2\bar{k}_x{}^2}{2\bar{m}_c} = [\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})] \tag{10.52}$$

The DOS function in this case is given by

$$\bar{N}_{1D}(\bar{E},\bar{c},\eta_g,\bar{F}) = \frac{\bar{g}_v\sqrt{2\bar{m}_c}}{\pi\hbar}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\frac{[\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}'_2(\bar{E},\bar{c},\eta_g,\bar{F})]\bar{H}(\bar{E}-\bar{E}_{n_{z18,2HD}})}{\sqrt{[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})] - \bar{G}_2(\bar{n}_y,\bar{n}_z)}} \tag{10.53}$$

where $\bar{E}_{n_{z18,2HD}}$ is the sub-band energy in this case and can be expressed as

$$\frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2=[\bar{J}_1(\bar{E}_{n_{z18,\,2HD}},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E}_{n_{z18,\,2HD}},\bar{c},\eta_g,\bar{F})] \quad (10.54)$$

and $\bar{G}_2(\bar{n}_y,\bar{n}_z)$, is defined in (10.13) of chapter 3.

The EEM in this case is given by

$$\bar{m}^*(\bar{E},\eta_g,\bar{F})=\bar{m}_c\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) \quad (10.55a)$$

The electron concentration can be given as

$$\bar{n}_0=\frac{2\bar{g}_v\sqrt{2\bar{m}_c}}{\pi\hbar}\,Real\ \ part\ of\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}[\Theta_{20,7}(\bar{E}_{f20,4},\eta_g,\bar{F})+\Theta_{20,8}(\bar{E}_{f20,4},\eta_g,\bar{F})] \quad (10.55b)$$

where

$$\Theta_{20,7}(\bar{E}_{f20,4},\eta_g,\bar{F})=\left[\bar{J}_1(\bar{E}_{f20,4},\bar{c},\eta_g,\bar{F})+\bar{j}\bar{J}_2(\bar{E}_{f20,4},\bar{c},\eta_g,\bar{F})-\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2-\left(\frac{\pi\bar{n}_y}{\bar{d}_y}\right)^2\right]^{\frac{1}{2}},$$

$$\Theta_{20,8}(\bar{E}_{f20,4},\eta_g,\bar{F})=\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\Theta_{20,7}(\bar{E}_{f20,4},\eta_g,\bar{F})]$$

and $\bar{E}_{f20,4}$ is the Fermi energy in this case.

Using (1.31f) and (10.55b) we can study the entropy in this case.

10.2.5 Magneto entropy in QWs of HD Kane-type materials in the presence of intense electric field

The DR in this case is given by

$$\frac{\hbar^2}{2\bar{m}_c}\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2+\left(\bar{n}+\frac{1}{2}\right)\hbar\omega_0=[\bar{J}_1(\bar{E}_{n_{z18,\,4HD}},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E}_{n_{z18,\,4HD}},\bar{c},\eta_g,\bar{F})] \quad (10.56)$$

where, $\bar{E}_{n_{z18,\,4HD}}$ is the totally quantized energy in this case

The DOS function in this case is given by

$$\bar{N}_{QWBHD}(\bar{E},\eta_g,\bar{F})=\frac{\bar{g}_v eB}{\pi\hbar}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}=0}^{\bar{n}\max}\delta'\ (\bar{E}-\bar{E}_{n_{z18,\,4HD}}) \quad (10.57a)$$

The electron concentration be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\, Real\ Part\ of \sum_{\bar{n}_x=1}^{\bar{n}_{x\max}} \sum_{\bar{n}=0}^{\bar{n}_{\max}} \bar{F}_{-1}(\eta_{20,7}) \tag{10.57b}$$

where $\eta_{20,7} = \frac{\bar{E}_{f20,7} - \bar{E}_{n_{z18,4HD}}}{k_B\bar{T}}$

and $\bar{E}_{f20,7}$ is the Fermi energy in this case

Using (1.31f) and (10.57b), we can study the entropy in this case.

10.2.6 Entropy in accumulation and inversion layers of Kane-type materials in the presence of intense electric field

(a) The 2D DR in accumulation layers of HD III–V, ternary and quaternary materials, in this case can be expressed as

$$[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})] = \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_c} + \frac{\hbar|e|\bar{F}_s}{\sqrt{2\bar{m}_c}}\left(\frac{2\sqrt{2\bar{S}_i}^{3/2}}{3}\right)[\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}'_2(\bar{E},\bar{c},\eta_g,\bar{F})]' \tag{10.58}$$

Since the DR in accordance with the HD three-band model of Kane is complex in nature, (10.60) will also be complex. The both complexities occur due to the presence of poles in the finite complex plane of the dispersion relation of the materials in the absence of band tails.

The EEM can be expressed as

$$\bar{m}^*(\bar{E},\bar{c},\eta_g,\bar{F},i) = \bar{m}_c\, \mathrm{Re}\, al\ part\ of\ [\bar{P}_{3HDL1}(\bar{E},\bar{c},\eta_g,\bar{F},i)]' \tag{10.59}$$

where,

$$\bar{P}_{3HDL1}(\bar{E},\bar{c},\eta_g,\bar{F},i) = [\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})] - \frac{\hbar|e|\bar{F}_s}{\sqrt{2\bar{m}_c}}\left(\frac{2\sqrt{2\bar{S}_i}^{3/2}}{3}\right)[\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}'_2(\bar{E},\bar{c},\eta_g,\bar{F})]']$$

Thus, one can observe that the EEM is a function of electric field, scattering potential, the sub-band index, surface electric field, the Fermi energy, and the other spectrum constants due to the combined influence of $\bar{E}_{g_0}$ and Δ.

The sub-band energy $\bar{E}_{400HD}$ is given by

$$[\bar{J}_1(\bar{E}_{400HD},\bar{c},\eta_g,\bar{F})+\bar{i}\bar{J}_2(\bar{E}_{400HD},\bar{c},\eta_g,\bar{F})]=\frac{\hbar|e|\bar{F}_s}{\sqrt{2\bar{m}_c}}\left(\frac{2\sqrt{2\bar{S}_i}^{3/2}}{3}\right)[\bar{J}'_1(\bar{E}_{400HD},\bar{c},\eta_g,\bar{F})+\bar{i}\bar{J}'_2(\bar{E}_{400HD},\bar{c},\eta_g,\bar{F})]' \tag{10.60}$$

The DOS function can be written as

$$\bar{N}_{2D}(\bar{E},\bar{c},\eta_g,\bar{F})=\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}[\bar{P}_{3HDL1}(\bar{E},\bar{c},\eta_g,\bar{F},i)]'\,\bar{H}(\bar{E}-\bar{E}_{400HD}) \tag{10.61a}$$

Thus, the DOS function is complex in nature.

The electron concentration can be expressed as

$$\bar{n}_s=\frac{\bar{g}_v\bar{m}_c}{\pi\hbar^2}\,Real\ Part\ of\sum_{i=0}^{i_{\max}}[\bar{P}_{3HDL1}(\bar{E}'_{f20,8},\bar{c},\eta_g,\bar{F})+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{P}_{3HDL1}(\bar{E}'_{f20,8},\bar{c},\eta_g,\bar{F})]+\frac{\bar{t}_i}{3\pi^2}\left(\frac{2\bar{m}_c}{\hbar^2}\right)^{\frac{3}{2}}[\Theta_{20,1}(\bar{E}'_{f20,1},\eta_g,\bar{F})+\Theta_{20,2}(\bar{E}'_{f20,1},\eta_g,\bar{F})] \tag{10.61b}$$

where $\bar{t}_i=\frac{\bar{E}_{i\max}}{e\bar{F}_s(1+i_{\max})}$,

$\bar{E}_{i\max}$ is root of the Real Part of (10.62) when $\bar{k}_s=0$ and $\bar{E}'_{f20,8}=eV_g-\frac{e^2\bar{n}_s\bar{d}_{ox}}{\varepsilon_{ox}}+\bar{E}_{f20,1}$

Using (1.31f) and (10.61b) we can study the entropy in this case.

(b) In the absence of bandtails, the DR in this case assumes the form

$$[\bar{J}_{11}(\bar{E},\bar{F})]=\frac{\hbar^2k_s^2}{2\bar{m}_c}+\frac{\hbar|e|\bar{F}_s}{\sqrt{2\bar{m}_c}}\left(\frac{2\sqrt{2\bar{S}_i}^{3/2}}{3}\right)[\bar{J}_{11}(\bar{E},\bar{F})]' \tag{10.62}$$

where $\bar{J}_{11}(\bar{E},\bar{F})=[e_1\bar{E}^4+e_2\bar{E}^3+e_3\bar{E}^2+e_4\bar{E}+e_5-\frac{e_6}{1+\bar{C}\bar{E}}+e_7(1+\bar{C}\bar{E})^{-2}]$(10.63) represents the DR of the 2D electrons in inversion layers of III–V, ternary, and quaternary materials under the intense electric field limit whose bulk electrons in the absence of any perturbation obey the three band model of Kane.

The EEM can be expressed as

$$\bar{m}^*(\bar{E},\bar{F},i)=\bar{m}_c\,[\bar{P}_{31}(\bar{E},\bar{F},i)]' \tag{10.63}$$

where,

$$\bar{P}_{31}(\bar{E},\bar{F},i) = [[\bar{J}_{11}(\bar{E},\bar{F})] - \frac{\hbar|e|\bar{F}_s}{\sqrt{2\bar{m}_c}}\left(\frac{2\sqrt{2\bar{S}_i}^{3/2}}{3}\right)[\bar{J}_{11}(\bar{E},\bar{F})]']$$

Thus, one can observe that the EEM is a function of the sub-band index, the light intensity, surface electric field, the Fermi energy, and the other spectrum constants due to the combined influence of $\bar{E}_{g_0}$ and Δ.

The sub-band energy $\bar{E}_{401}$ in this case can be obtained from the (10.64) as

$$0 = \left[[\bar{J}_{11}(\bar{E}_{401},\bar{F})] - \frac{\hbar|e|\bar{F}_s}{\sqrt{2\bar{m}_c}}\left(\frac{2\sqrt{2\bar{S}_i}^{3/2}}{3}\right)[\bar{J}_{11}^{'}(\bar{E}_{401},\bar{F})]'\right] \tag{10.64}$$

Thus, the 2D total DOS function in weak electric field limit can be expressed as

$$\bar{N}_{2D}(\bar{E},\bar{F}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}[\bar{P}_{31}(\bar{E},\bar{F},i)]' \ \bar{H}(\bar{E}-\bar{E}_{401}) \tag{10.65a}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v\bar{m}_c}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}\left[\bar{P}_{31}(\bar{E}_{f20,9},\bar{F},i) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{P}_{31}(\bar{E}_{f20,9},\bar{F},\bar{i}\right]\right] \tag{10.65b}$$

where $\bar{E}_{f20,9}$ is the Fermi energy in this case

Using (1.31f) and (10.65b), we can study the entropy in this case.

10.2.7 Entropy in doping superlattices of HD Kane-type materials in the presence of intense electric field

The DR in doping superlatticesof HD III–V, ternary and quaternary materials in the presence of intense electric field whose unperturbed electrons are defined by the three-band model of Kane can be expressed as

$$[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})] = \left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{91HD1}(\bar{E},\bar{c},\eta_g,\bar{F}) + \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_c} \tag{10.66}$$

where

$$\omega_{91HD1}(\bar{E},\bar{c},\eta_g,\bar{F}) = \left(\frac{n_s|e|^2}{d_0\varepsilon_{sc}[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})]'\bar{m}_c}\right)^{\frac{1}{2}}$$

The sub-band energies $\bar{E}_{452}$ can be written as

$$[\bar{J}_1(\bar{E}_{452},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E}_{452},\bar{c},\eta_g,\bar{F})]=\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{91HD1}(\bar{E}_{452},\bar{c},\eta_g,\bar{F}) \tag{10.67}$$

The EEM in this case is given by

$$\bar{m}^*(\bar{E},\bar{c},\eta_g,\bar{F},\bar{n}_i)=\bar{m}_c\,\mathrm{Re}al\ part\ of\ [\bar{P}_{3HDL3}(\bar{E},\bar{c},\eta_g,\bar{F},\bar{n}_i)]' \tag{10.68}$$

where

$$[\bar{P}_{3HDL3}(\bar{E},\bar{c},\eta_g,\bar{F},\bar{n}_i)]=[[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})]-(\bar{n}_i+\frac{1}{2})\hbar\omega_{91HD1}(\bar{E},\bar{c},\eta_g,\bar{F})]$$

The DOS function in this case is given by

$$\bar{N}_{2DDSL}(\bar{E},\bar{c},\eta_g,\bar{F})=\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}$$
$$\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\frac{[\bar{J}'_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}'_2(\bar{E},\bar{c},\eta_g,\bar{F})-(\bar{n}_i+\frac{1}{2})\hbar\omega'_{91HD1}(\bar{E},\bar{c},\eta_g,\bar{F})]\bar{H}(\bar{E}-\bar{E}_{452})}{\sqrt{[\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F})+i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F})]-(\bar{n}_i+\frac{1}{2})\hbar\omega_{91HD1}(\bar{E},\bar{c},\eta_g,\bar{F})}} \tag{10.69a}$$

The electron concentration can be written as

$$\bar{n}_s=\frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_i=1}^{\bar{n}_{i_{max}}}\left[\bar{P}_{3HDL3}(\bar{E}_{f20,20},\bar{c},\eta_g,\bar{F},\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{P}_{3HDL3}(\bar{E}_{f20,20},\bar{c},\eta_g,\bar{F},\bar{n}_i)]\right] \tag{10.69b}$$

where $\bar{E}_{f20,20}$ is the Fermi energy in this case.

Using (1.31f) and (10.69b) we can study the entropy in this case.

10.2.8 Entropy in QWHD effective mass superlattices of Kane-type materials in the presence of intense electric field

Following Sasaki [3], the electron dispersion law in HD III–V effective mass superlattices (EMSLs) in the presence of light waves, the dispersion relations of whose constituent materials in the absence of any perturbation are defined by the three band model of Kane can be written as

$$\bar{k}_x^2=\left[\frac{1}{\bar{L}_0^2}\left\{\cos^{-1}(\bar{f}_{18HD1}(\bar{E},\bar{k}_y,\bar{k}_z,\bar{F}))\right\}^2-\bar{k}_\perp^2\right] \tag{10.70}$$

In which,

$$\bar{f}_{18HD1}(\bar{E},\bar{k}_y,\bar{k}_z,\bar{F}) = \bar{a}_{1HD1,18}\cos[\bar{a}_0\bar{C}_{1HD1,18}(\bar{E},\bar{k}_\perp,\bar{F}) + \bar{b}_0\bar{D}_{1HD1,18}(\bar{E},\bar{k}_\perp,\bar{F})]$$

$$-\bar{a}_{2HD1,18}\cos[\bar{a}_0\bar{C}_{1HD1,18}(\bar{E},\bar{k}_\perp,\bar{F}) + \bar{b}_0\bar{D}_{1HD1,18}(\bar{E},\bar{k}_\perp,\bar{F})]$$

$$\bar{a}_{1HD1,18} = \left[\sqrt{\frac{\bar{m}_{c2}\,\mathrm{Re}\,al\,part\,of\,[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\,\mathrm{Re}\,al\,part\,of\,[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}}+1\right]^2 \left[4\left(\frac{\bar{m}_{c2}\,\mathrm{Re}\,al\,part\,of\,[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\,\mathrm{Re}\,al\,part\,of\,[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}\right)^{\frac{1}{2}}\right]^{-1},$$

$$\bar{a}_{2HD1,18} = \left[\sqrt{\frac{\bar{m}_{c2}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}}-1\right]^2 \left[4\left(\frac{\bar{m}_{c2}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}\right)^{\frac{1}{2}}\right]^{-1}$$

$$\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F}) = \bar{J}_3(\bar{E},\bar{c},\eta_g,\bar{F}),$$

$$\bar{C}_{1HD1,18}(\bar{E},\bar{k}_\perp,\bar{F}) \equiv \left[\left(\frac{2\bar{m}_{c1}}{\hbar^2}\right)\bar{J}_3(\bar{E},\bar{c},\eta_{g1},\bar{F}) - \bar{k}_\perp^2\right]^{\frac{1}{2}}$$

and

$$\bar{D}_{1HD1,18}(\bar{E},\bar{k}_\perp,\bar{F}) \equiv \left[\left(\frac{2\bar{m}_{c1}}{\hbar^2}\right)\bar{J}_3(\bar{E},\bar{c},\eta_{g2},\bar{F}) - \bar{k}_\perp^2\right]^{\frac{1}{2}}$$

The DR in QWHD effective mass superlattices of Kane type materials in the presence of intense electric field, the dispersion relations of whose constituent materials in the absence of any perturbation are defined by the three-band model of Kane can be written as

$$\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 = \left[\frac{1}{\bar{L}_0^2}\left\{\cos^{-1}(\bar{f}_{18HD1}(\bar{E},\bar{k}_y,\bar{k}_z,\bar{F}))\right\}^2 - \bar{k}_\perp^2\right] \tag{10.71}$$

The EEM in this case assumes the form

$$\bar{m}^*(\bar{k}_\perp,\bar{E},\bar{F}) = \frac{\hbar^2}{\bar{L}_0^2}\left|\left[\frac{\cos^{-1}[\bar{f}_{18HD1}(\bar{E},\bar{k}_y,\bar{k}_z,\bar{F})]\overline{f'}_{18HD1}(\bar{E},\bar{k}_y,\bar{k}_z,\bar{F})}{\sqrt{1-\bar{f}_{18HD1}^2(\bar{E},\bar{k}_y,\bar{k}_z,\bar{F})}}\right]\right| \tag{10.72}$$

The subband energies $\bar{E}_{600}$ can be written as

$$\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right) = \left[\frac{1}{\bar{L}}\left\{\cos^{-1}(\bar{f}_{18HD1}(\bar{E}_{600}, \bar{k}_y, \bar{k}_{z,}\bar{F}))\right\}\right] \tag{10.73}$$

The density of states function, the electron concentration and the entropy have to be evaluated numerically.

10.2.9 Entropy in NWHD effective mass superlattices of Kane-type materials in the presence of intense electric field

Following Sasaki [3], the magneto entropy in HD III–V effective mass superlattices (entropySLs) in the presence of intense electric field, the dispersion relations of whose constituent materials in the absence of any perturbation are defined by the three-band model of Kane can be written as

$$\bar{k}_x^2 = \left[\frac{1}{\bar{L}_0^2}\left\{\cos^{-1}(\bar{f}_{18HD2}(\bar{E}, \bar{n}, \bar{F}))\right\}^2 - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right] \tag{10.74}$$

In which,

$$\bar{f}_{18HD2}(\bar{E},\ \bar{n}, \bar{F}) = \bar{a}_{1HD1,18}\cos[\bar{a}_0\bar{C}_{1HD2,18}(\bar{E},\ \bar{n}, \bar{F}) + \bar{b}_0\bar{D}_{1HD2,18}(\bar{E},\ \bar{n}, \bar{F})]$$

$$-\bar{a}_{2HD1,18}\cos[\bar{a}_0\bar{C}_{1HD2,18}(\bar{E},\ \bar{n}, \bar{F}) + \bar{b}_0\bar{D}_{1HD2,18}(\bar{E},\ \bar{n}, \bar{F})]$$

$$\bar{a}_{1HD1,18} = \left[\sqrt{\frac{\bar{m}_{c2}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}}+1\right]^2 \left[4\left(\frac{\bar{m}_{c2}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}\right)^{\frac{1}{2}}\right]^{-1},$$

$$\bar{a}_{2HD1,18} = \left[\sqrt{\frac{\bar{m}_{c2}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}}-1\right]^2 \left[4\left(\frac{\bar{m}_{c2}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g2},\bar{F})]}{\bar{m}_{c1}\mathrm{Re}\,al\,part\,of[\bar{J}_3(0,\bar{c},\eta_{g1},\bar{F})]}\right)^{\frac{1}{2}}\right]^{-1}$$

$$\bar{J}_1(\bar{E},\bar{c},\eta_g,\bar{F}) + i\bar{J}_2(\bar{E},\bar{c},\eta_g,\bar{F}) = \bar{J}_3(\bar{E},\bar{c},\eta_g,\bar{F}),$$

$$\bar{C}_{1HD2,18}(\bar{E},\ \bar{n}, \bar{F}) \equiv \left[\left(\frac{2\bar{m}_{c1}}{\hbar^2}\right)\bar{J}_3(\bar{E},\bar{c},\eta_{g1},\bar{F}) - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{\frac{1}{2}}$$

and

$$\bar{D}_{1HD2,18}(\bar{E},\ \bar{n},\bar{F}) \equiv \left[\left(\frac{2\bar{m}_{c1}}{\hbar^2}\right)\bar{J}_3(\bar{E},\bar{c},\eta_{g2},\bar{F}) - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right]^{\frac{1}{2}}$$

The DOS function in this case is given by

$$\bar{N}_{100}(\bar{E},\bar{F}) = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}}[\omega_{100}(\bar{E},\bar{n},\bar{F})]' \tag{10.75}$$

where

$$\omega_{100}(\bar{E},\bar{n},\bar{F}) = \left[\left[\frac{1}{\bar{L}_0^2}\left\{\cos^{-1}(\bar{f}_{18HD2}(\bar{E},\bar{n},\bar{F}))\right\}^2 - \frac{2e\bar{B}}{\hbar}(\bar{n}+\frac{1}{2})\right]\right]^{\frac{1}{2}}$$

The EEM in this case assumes therefore

$$\bar{m}^*(\bar{n},\bar{E},\bar{F}) = \frac{\hbar^2}{\bar{L}_0^2}\left|\left[\frac{\cos^{-1}[\bar{f}_{18HD2}(\bar{E},\bar{n},\bar{F})]\overline{f'}_{18HD2}(\bar{E},\bar{n},\bar{F})}{\sqrt{1-\bar{f}_{18HD2}^2(\bar{E},\bar{n},\bar{F})}}\right]\right| \tag{10.76}$$

The Landau sub-band energies E_{602} can be written as

$$0 = \left[\frac{1}{\bar{L}_0^2}\left\{\cos^{-1}(\bar{f}_{18HD2}(\bar{E}_{602},\bar{n},\bar{F}))\right\}^2 - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right] \tag{10.77a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi^2\hbar}\ Real\ Part\ of \sum_{\bar{n}=0}^{\bar{n}_{\max}}[[\omega_{100}(\bar{E}_{f20,23},\bar{n},\bar{F})] + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\ [\omega_{100}(\bar{E}_{f20,23},\bar{n},\bar{F})]] \tag{10.77b}$$

Using (1.31f) and (10.77b), we can study the entropy in this case.

10.2.10 Magneto entropy in QWHD effective mass superlattices of Kane-type materials in the presence of intense electric field

Following Sasaki [3], the electron dispersion law in HD III-V effective mass superlattices in the presence of light waves, the dispersion relations of whose constituentmaterials in the absence of any perturbation are defined by the three-band model of Kane can be written as

$$\left(\frac{\bar{n}_x\pi}{\bar{d}_x}\right)^2 = \left[\frac{1}{\bar{L}_0^2}\left\{\cos^{-1}(\bar{f}_{18HD2}(\bar{E}_{601},\bar{n},\bar{F}))\right\}^2 - \frac{2e\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right)\right] \tag{10.78}$$

where, $\bar{E}_{601}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{601}(\bar{E},\bar{F},\eta_g)=\frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\delta'(\bar{E}-\bar{E}_{601}) \tag{10.79a}$$

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v e\bar{B}}{\pi\hbar}Real\ Part\ of\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{20,25}) \tag{10.79b}$$

where $\eta_{20,25}=\frac{\bar{E}_{f20,25}-\bar{E}_{601}}{k_B T}$

and $\bar{E}_{f20,25}$ is the Fermi energy in this case.

Using (1.31f) and (20.89b) we can study the entropy in this case.

10.2.11 Entropy in QWHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field

The DR in bulk specimens of the HD constituent materials of III–V SLs in the presence of intense electric field can be expressed as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_{cj}}=\bar{J}_{1j}(\bar{E},\Delta_j,\bar{E}_{g0j},\eta_j,\bar{F})+i\bar{J}_{2j}(\bar{E},\Delta_j,\bar{E}_{g0j},\eta_j,\bar{F}) \tag{10.80}$$

where $\bar{j}=1,2,$

$$\begin{aligned}\bar{J}_{1j}(\bar{E},\Delta_j,\bar{E}_{g0j},\eta_j,\bar{F})&=2[1+Erf(\bar{E}/\eta_{g_j})]^{-1}[e_{1j}\psi_{0j}(\bar{E},\eta_{g_j})+e_{2j}\psi_{1j}(\bar{E},\eta_{g_j})\\&+e_{3j}\theta_{0j}(\bar{E},\eta_{g_j})+e_{4j}\gamma_0(\bar{E}\eta_{g_j})+e_{5j}\frac{1}{2}[1+Erf(\bar{E}/\eta_{g_j})]\\&-e_{6j}\bar{c}_{1j}(\bar{E},\bar{c},\eta_{g_j})+e_{7j}\bar{c}_{3j}(\bar{E},\bar{c},\eta_{g_j})],\ \psi_{1j}(\bar{E},\eta_{g_j})\\&=\left[\frac{\bar{E}}{2}[1+Erf(\bar{E}/\eta_{g_j})]\left[\bar{E}^2+\frac{3}{2}\eta_{g_j}^2\right]\right.\\&\left.+\frac{\eta_{g_j}}{2\sqrt{\pi}}\exp\left(\frac{-\bar{E}^2}{\eta_{g_j}^2}\right)(4\bar{E}^2+\eta_{g_j}^2)\right],\end{aligned}$$

$$\bar{J}_{2j}(\bar{E},\Delta_j,\bar{E}_{g0j},\eta_j,\bar{F})=2[1+Erf(\bar{E}/\eta_{g_j})]^{-1}[e_{6j}\bar{c}_{2j}(\bar{E},\bar{c},\eta_{g_j})+e_{7j}\bar{D}_{3j}(\bar{E},\bar{c},\eta_{g_j})],$$

$$e_{fj}=\bar{A}_{fj}\bar{P}_{fj},\quad \bar{A}_{fj}=[\bar{F}\hbar\bar{E}_{g_j}(\bar{E}_{g_j}-\delta'_j)]^2\bar{m}_{cj}(6\bar{m}_{rj}^2(\delta'_j)^4)^{-1},$$

$$\bar{F} = e\bar{F}_s, \quad \bar{G}_{fj} = e_{fj}(4\delta'_j + \bar{C}_{fj}), \quad \bar{C}_{fj} = (2\bar{E}_{g_j}Q_j^2 + P_jQ_j(\bar{E}_{g_j} - \bar{E}'_{g_j}) - 2P_j^2\bar{E}_{g_j}),$$

$$\bar{E}'_{g_j} = \frac{\bar{E}_{g_j}(\bar{E}_{g_j} - 3\delta'_j)}{\bar{E}_{g_j} + \delta'_j}, \ \bar{P}_j = \frac{\bar{r}_{0j}^2}{2}\left(\frac{\bar{E}_{g_j} - \delta'_j}{\bar{E}_{g_j} + \delta'_j}\right), \ \bar{r}_{0j} = \left[\frac{6}{\chi_j}(\bar{E}_{g_j} + \Delta_j)\left(\bar{E}_{g_j} + \frac{2}{3}\Delta_j\right)\right]^{1/2}, \ \bar{Q}_j = \frac{t_j^2}{2},$$

$$\bar{t}_j = \left[\frac{6}{\chi_j}\left(\bar{E}_{g_j} + \frac{2}{3}\Delta_j\right)\right]^{1/2}, \quad \bar{h}_{fj} = (4\delta'_j e_{fj}\bar{C}_{fj})(\bar{B}_{fj})^{-1}, \quad \bar{B}_{fj} = (\bar{P}_j + \bar{Q}_j)^2$$

$$\bar{P}_{fj} = \bar{E}_{g_j}^{-3}(\bar{e}_{fj}\bar{E}_{g_j}^{-2} - \bar{G}_{fj} + \bar{h}_{fj}\bar{E}_{g_j}^{-4}), \quad \omega_{1j} = \bar{a}_{1j}^2, \quad \bar{a}_{1j} = \frac{a_jb_j}{c_j},$$

$$\bar{a}_j = \frac{1}{\bar{E}_{g_j}}, \quad \bar{b}_j = \frac{1}{\bar{E}_{g_j} + \Delta_j}, \quad \bar{c}_j = \left(\bar{E}_{g_j} + \frac{2}{3}\Delta_j\right)^{-1},$$

$$e_{2j} = \bar{Q}_{fj}.\omega_{2j}, \quad \omega_{2j} = 2\bar{a}_{1j}\bar{b}_{1j}, \quad \bar{b}_{1j} = (\bar{c}_j)^{-2}(\bar{a}_j\bar{c}_j + \bar{b}_j\bar{c}_j - \bar{a}_j\bar{b}_{j_j}),$$

$$e_{3j} = (1 - \bar{P}_{fj})\bar{a}_{1j} + \bar{Q}_{fj}.\omega_{3j}, \quad \omega_{3j} = (\bar{b}_{1j}^2 + 2\bar{a}_{1j}\bar{c}_{1j}),$$

$$\bar{c}_{1j} = \left[\frac{1}{\bar{c}_j}\left(1 - \frac{a_j}{\bar{c}_j}\right)\left(1 - \frac{b_j}{\bar{c}_j}\right)\right], \quad e_{4j} = [(1 - \bar{P}_{fj})\bar{b}_{1j} + \bar{Q}_{fj}\omega_{4j}],$$

$$\omega_{4j} = 2\bar{b}_{1j}\bar{c}_{1j}, \quad e_{5j} = [(1 - \bar{P}_{fj})\bar{c}_{1j} + \omega_{5j}\bar{Q}_{fj}]$$

$$\omega_{5j} = (\bar{c}_{1j}^2 - 2\bar{c}_{1j}\bar{b}_{1j}), \ \bar{e}_{7j} = \bar{Q}_{fj}\omega_{7j}, \ \omega_{7j} = \bar{c}_{1j}^2, \quad \bar{e}_{6j} = [(1 - \bar{P}_{fj})\bar{c}_{1j} - \bar{Q}_{fj}\omega_{6j}]$$

and $\omega_{6j} = \dfrac{2\bar{c}_{1j}\bar{b}_{1j}}{\bar{c}_j}\left(1 - \dfrac{\bar{c}_j\bar{c}_{1j}}{\bar{b}_{1j}}\right)\Bigg]$

Therefore, the DR in HD III–V SLs with graded interfaces in the presence of intense electric field can be expressed as [4]

$$\bar{k}_z^2 = \bar{G}_{8,19} + i\bar{H}_{8,19} \tag{10.81}$$

where

$$\bar{G}_{8,19} = \left[\frac{\bar{C}_{7,19}^2 - \bar{D}_{7,19}^2}{\bar{L}_0^2} - k_s^2\right], \ \bar{C}_{7,19} = \cos^{-1}(\omega_{7,19}),$$

$$\omega_{7,19} = (2)^{\frac{-1}{2}}\left[(1 - \bar{G}_{7,19}^2 - \bar{H}_{7,19}^2) - \sqrt{(1 - \bar{G}_{7,19}^2 - \bar{H}_{7,19}^2)^2 + 4\bar{G}_{7,19}^2}\right]^{\frac{1}{2}}$$

$$\rho_{11,19}\bar{H}_{5,19} - \rho_{12,19}\bar{H}_{5,19} + (1/12)(\rho_{12,19}\bar{G}_{6,19} - \rho_{14,19}\bar{H}_{6,19})\}],$$

$$\bar{G}_{1,19} = [(\cos(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))$$
$$+ (\sin(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\sinh(g_{1,19}))(\sin(\bar{g}_{2,19}))], \bar{h}_{1,19}$$

$$= e_{1,19}(\bar{b}_0 - \Delta_0), e_{1,19} = 2^{-\frac{1}{2}}\left(\sqrt{\bar{t}_{1,19}^2 + \bar{t}_{2,19}^2} + \bar{t}_{1,19}\right)^{\frac{1}{2}},$$

$$\bar{h}_{2,19} = e_{2,19}(\bar{b}_0 - \Delta_0),\ e_{2,19} = 2^{-\frac{1}{2}}\left(\sqrt{\bar{t}_{1,19}^2 + \bar{t}_{2,19}^2} - \bar{t}_{1,19}\right)^{\frac{1}{2}},$$

$$\bar{g}_{1,19} = \bar{d}_{1,19}(\bar{a}_0 - \Delta_0),\ \bar{d}_{1,19} = 2^{\frac{-1}{2}}\left(\sqrt{\bar{x}_{1,19}^2 + \bar{y}_{1,19}^2} + \bar{x}_{1,19}\right)^{\frac{1}{2}},$$

$$\bar{x}_{1,19} = [-(2\bar{m}_{c2}/\hbar^2).\bar{J}_{11}(\bar{E} - \bar{V}_0, \bar{E}_{g2}, \Delta_2, \eta_{g2}, \bar{F}) + \bar{k}_s^2],$$
$$y_1 = [(2\bar{m}_{c2}/\hbar^2).\bar{J}_{22}(\bar{E} - \bar{V}_0, \bar{E}_{g2}, \Delta_2, \eta_{g2}, \bar{F})],$$

$$\bar{g}_{2,19} = \bar{d}_{2,19}(\bar{a}_0 - \Delta_0),\ \bar{d}_{2,19} = 2^{-\frac{1}{2}}\left(\sqrt{\bar{x}_{1,19}^2 + \bar{y}_{1,19}^2} - \bar{x}_{1,19}\right)^{\frac{1}{2}},$$

$$\rho_{5,19} = (\rho_{3,19}^2 + \rho_{4,19}^2)^{-1}[\rho_{1,19}\rho_{3,19} - \rho_{2,19}\rho_{4,19}],$$

$$\rho_{1,19} = [\bar{d}_{1,19}^2 + e_{2,19}^2 - \bar{d}_{2,19}^2 - e_{1,19}^2],\ \rho_{3,19} = [\bar{d}_{1,19}e_{1,19} + \bar{d}_{2,19}e_{2,19}],$$

$$\rho_{2,19} = 2[\bar{d}_{1,19}\bar{d}_{2,19} + e_{1,19}e_{2,19}],$$

$$\rho_{4,19} = [\bar{d}_{1,19}e_{2,19} - e_{1,19}\bar{d}_{2,19}],$$

$$\bar{G}_{2,19} = [(\sin(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))$$
$$+ (\cos(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19}))],$$

$$\rho_{6,19} = (\rho_{3,19}^2 + \rho_{4,19}^2)^{-1}[\rho_{1,19}\rho_{4,19} + \rho_{2,19}\rho_{3,19}],$$

$$\bar{H}_{2,19} = [(\sin(\bar{h}_{1,19}))(\cos(\bar{h}_{2,19}))(\sin(\bar{g}_{2,19}))(\cosh(\bar{g}_{1,19}))$$
$$- (\cos(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(sinh(\bar{g}_{1,19}))(cos(\bar{g}_{2,19}))],$$

$$\rho_{7,19} = [(e_{1,19}^2 + e_{2,19}^2)^{-1}[e_{1,19}(\bar{d}_{1,19}^2 - \bar{d}_{2,19}^2) - 2\bar{d}_{1,19}\bar{d}_{2,19}e_{2,19}] - 3e_{1,19}],$$

$$\bar{G}_{3,19} = [(\sin(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))$$
$$+ (\cos(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19}))],$$

$$\rho_{8,19} = [(e_{1,19}^2 + e_{2,19}^2)^{-1}[e_{2,19}(\bar{d}_{1,19}^2 - \bar{d}_{2,19}^2) + 2\bar{d}_{1,19}\bar{d}_{2,19}e_{1,19}] + 3e_{2,19}],$$

$$\bar{H}_{3,19} = [(\sin(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\sin(\bar{g}_{2,19}))(\sinh(\bar{g}_{1,19}))$$
$$- (\cos(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))],$$

$$\rho_{9,19} = [(\bar{d}_{1,19}^2 + \bar{d}_{2,19}^2)^{-1}[\bar{d}_{1,19}(e_{2,19}^2 - e_{1,19}^2) + 2e_{2,19}\bar{d}_{2,19}e_{1,19}] + 3\bar{d}_{1,19}],$$

$$\bar{G}_{4,19} = [(\cos(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\cos(\bar{g}_{2,19}))(\sinh(\bar{g}_{1,19})) - (\sin(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19}))],$$

$$\rho_{10,19} = [(\bar{d}_{1,19}^2 + \bar{d}_{2,19}^2)^{-1}[\bar{d}_{2,19}(e_{2,19}^2 - e_{1,19}^2) + 2e_{2,19}\bar{d}_{2,19}e_{1,19}] + 3\bar{d}_{1,19}],$$

$$\bar{H}_{4,19} = [(\cos(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19})) + (\sin(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))],$$

$$\rho_{11,19} = 2[\bar{d}_{1,19}^2 + e_{2,19}^2 - \bar{d}_{2,19}^2 - e_{1,19}^2],$$

$$\bar{G}_{5,19} = [(\cos(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\cos(\bar{g}_{2,19}))(\cosh(\bar{g}_{1,19})) - (\sin(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19}))],$$

$$\rho_{12,19} = 4[\bar{d}_{1,19}\bar{d}_{2,19} + e_{1,19}e_{2,19}],$$

$$H_{5,19} = [(\cos(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19})) + (\sin(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))],$$

$$\rho_{13,19} = [\{5(\bar{d}_{1,19}e_{1,19}^3 - 3e_{1,19}e_{2,19}^2\bar{d}_{1,19}) + 5\bar{d}_{2,19}(e_{1,19}^3 - 3e_{1,19}^2e_{2,19})\}(\bar{d}_{1,19}^2 + \bar{d}_{2,19}^2)^{-1} + (e_{1,19}^2 + e_{2,19}^2)^{-1}\{5(e_{1,19}\bar{d}_{1,19}^3 - 3\bar{d}_{2,19}e_{1,19}^2\bar{d}_{1,19}) + 5(\bar{d}_{2,19}^3e_{2,19} - 3\bar{d}_{1,19}^2\bar{d}_{2,19}\bar{e}_{2,19})\} - 34(\bar{d}_{1,19}e_{1,19} + \bar{d}_{2,19}e_{2,19})],$$

$$\bar{G}_{6,19} = [(\sin(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19})) + (\cos(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19}))],$$

$$\rho_{14,19} = [\{5(\bar{d}_{1,19}e_{2,19}^3 - 3e_{2,19}e_{1,19}^2\bar{d}_{1,19}) + 5\bar{d}_{2,19}(-e_{1,19}^3 + 3e_{2,19}^2e_{1,19})\}(\bar{d}_{1,19}^2 + \bar{d}_{2,19}^2)^{-1} + (e_{1,19}^2 + e_{2,19}^2)^{-1}\{5(-e_{1,19}\bar{d}_{2,19}^3 + 3\bar{d}_{1,19}^2\bar{d}_{2,19}e_{1,19}) + 5(-\bar{d}_{1,19}^3e_{2,19} + 3\bar{d}_{2,19}^2\bar{d}_{1,19}e_{2,19})\} + 34(\bar{d}_{1,19}e_{2,19} - \bar{d}_{2,19}e_{1,19})],$$

$$\bar{H}_{6,19} = [(\sin(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19})) - (\cos(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))],$$

$$\bar{H}_{7,19} = [\bar{H}_{1,19} + (\rho_{5,19}\bar{H}_{2,19}/2) + (\rho_{6,19}\bar{G}_{2,19}/2) + (\Delta_0/2) \{\rho_{8,19}\bar{G}_{3,19} + \rho_{7,19}\bar{H}_{3,19} + \rho_{10,19}\bar{G}_{4,19} + \rho_{9,19}\bar{H}_{4,19} + \rho_{12,19}\bar{G}_{5,19} + \rho_{11,19}\bar{H}_{5,19} + (1/12)(\rho_{14,19}\bar{G}_{6,19} + \rho_{13,19}\bar{H}_{6,19})\}],$$

$$\bar{H}_{1,19} = [(\sin(\bar{h}_{1,19}))(\cosh(\bar{h}_{2,19}))(\cosh(\bar{g}_{1,19}))(\sin(\bar{g}_{2,19})) + (\cos(\bar{h}_{1,19}))(\sinh(\bar{h}_{2,19}))(\sinh(\bar{g}_{1,19}))(\cos(\bar{g}_{2,19}))],$$

$$\bar{D}_{7,19} = \sin^{-1}(\bar{\omega}_{7,19}), \bar{H}_{8,19} = (2\bar{C}_{7,19}\bar{D}_{7,19}/\bar{L}_0^2)$$

The simplified DR of HD QWs of III–V superlattices with graded interfaces can be expressed as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{G}_{8,19} + i\bar{H}_{8,19} \tag{10.82}$$

The sub-band equation in this case can be expressed as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \left|\bar{G}_{8,19} + i\bar{H}_{8,19}\right|_{\bar{k}_s = 0 \text{ and } \bar{E} = \bar{E}_{700}} \tag{10.83}$$

where $\bar{E}_{700}$ is the sub-band energy in this case.

The EEM and the DOS function should be obtained numerically in this case.

10.2.12 Entropy in NWHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field

Entropy in NWHD III–V SLs with graded interfaces in the presence of intense electric fieldcan be expressed as [4]

$$\bar{k}_z^2 = \bar{G}_{8,20} + i\bar{H}_{8,20} \tag{10.84}$$

where,

$$\bar{G}_{8,20} = \left[\frac{\bar{C}_{7,20}^2 - \bar{D}_{7,20}^2}{\bar{L}_0^2} - \bar{k}_s^2\right],\ \bar{C}_{7,20} = \cos^{-1}(\bar{\omega}_{7,20}),$$

$$\bar{\omega}_{7,20} = (2)^{-1/2}\left[(1 - \bar{G}_{7,20}^2 - \bar{H}_{7,20}^2) - \sqrt{(1 - \bar{G}_{7,20}^2 - \bar{H}_{7,20}^2)^2 + 4\bar{G}_{7,20}^2}\right]^{1/2}$$

$$\begin{aligned}\bar{G}_{7,20} = [&\bar{G}_{1,20} + (\rho_{5,20}\bar{G}_{2,20}/2) - (\rho_{6,20}\bar{H}_{2,20}/2) + (\Delta_0/2)\\ &\{\rho_{6,20}\bar{H}_{2,20} - \rho_{8,20}\bar{H}_{3,20} + \rho_{9,20}\bar{H}_{4,20} - \rho_{10,20}\bar{H}_{4,20}\\ &+ \rho_{11,20}\bar{H}_{5,20} - \rho_{12,20}\bar{H}_{5,20} + (1/12)(\rho_{12,20}\bar{G}_{6,20} - \rho_{14,20}\bar{H}_{6,20})\}]\end{aligned}$$

$$\begin{aligned}G_{1,20} = &[(\cos(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(cosh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20}))\\ &+ (\sin(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(sin(\bar{g}_{2,20}))],\end{aligned}$$

$$\bar{h}_{1,20} = e_{1,20}(\bar{b}_0 - \Delta_0),\ e_{1,20} = 2^{-1/2}\left(\sqrt{\bar{t}_{1,20}^2 + \bar{t}_{2,20}^2} + \bar{t}_{1,20}\right)^{1/2},$$

$$\bar{t}_{1,20} = [(2\bar{m}_{c1}/\hbar^2).\bar{J}_{11}(\bar{E}, \Delta_1, \bar{E}_{g_{01}}, \bar{F}) - \bar{G}_2(\bar{n}_y, \bar{n}_z)], \bar{t}_{2,20} = [(2\bar{m}_{c1}/\hbar^2)\bar{J}_{21}(\bar{E}, \Delta_1, \bar{E}_{g_{01}}, \bar{F})],$$

$$\bar{h}_{2,20} = e_{2,20}(\bar{b}_0 - \Delta_0), e_{2,20} = 2^{-1/2}\left(\sqrt{\bar{t}_{1,20}^2 + \bar{t}_{2,20}^2} + \bar{t}_{1,20}\right)^{1/2},$$

$$\bar{g}_{1,20} = d_{1,20}(\bar{a}_0 - \Delta_0), d_{1,20} = 2^{-1/2}\left(\sqrt{\bar{x}_{1,20}^2 + \bar{y}_{1,20}^2} + \bar{x}_{1,20}\right)^{1/2},$$

$$\bar{x}_{1,20} = [-(2\bar{m}_{c2}/\hbar^2).\bar{J}_{11}(\bar{E} - V_0, \bar{E}_{g2}, \Delta_2, \eta_{g2}, \bar{F}) + \bar{G}_2(\bar{n}_y, \bar{n})],$$

$$\bar{y}_1 = [(2\bar{m}_{c2}/\hbar^2).\bar{J}_{22}((\bar{E} - V_0, \bar{E}_{g2}, \Delta_2, \eta_{g2}, \bar{F})],$$

$$\bar{g}_{2,20} = d_{2,20}(\bar{a}_0 - \Delta_0), \bar{d}_{2,20} = 2^{-1/2}\left(\sqrt{\bar{x}_{1,20}^2 + \bar{y}_{1,20}^2} - \bar{x}_{1,20}\right)^{1/2},$$

$$\rho_{5,20} = (\rho_{3,20}^2 + \rho_{4,20}^2)^{-1}[\rho_{1,20}\rho_{3,20} - \rho_{2,20}\rho_{4,20}],$$

$$\rho_{1,20} = [d_{1,20}^2 + e_{2,20}^2 - d_{2,20}^2 - e_{1,20}^2], \rho_{3,20} = [d_{1,20}e_{1,20} + d_{2,20}e_{2,20}],$$

$$\rho_{2,20} = 2[d_{1,20}d_{2,20} + e_{1,20}e_{2,20}], \rho_{4,20} = [d_{1,20}\bar{e}_{2,20} - e_{1,20}d_{2,20}],$$

$$\bar{G}_{2,20} = [(\sin(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20})) + (\cos(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20}))],$$

$$\rho_{6,20} = (\rho_{3,20}^2 + \rho_{4,20}^2)^{-1}[\rho_{1,20}\rho_{4,20} + \rho_{2,20}\rho_{3,20}],$$

$$\bar{H}_{2,20} = [(\sin(\bar{h}_{1,20}))(\cos(\bar{h}_{2,20}))(\sin(g_{1,20}))(\cosh(g_{1,20})) - (\cos(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20}))],$$

$$\rho_{7,20} = (e_{1,20}^2 + e_{2,20}^2)^{-1}[e_{1,20}(d_{1,20}^2 - d_{2,20}^2) - 2d_{1,20}d_{2,20}e_{2,20}] - 3e_{1,20}],$$

$$\bar{G}_{3,20} = [(\sin(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20})) + (\cos(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20}))],$$

$$\rho_{8,20} = (e_{1,20}^2 + e_{2,20}^2)^{-1}[e_{2,20}(d_{1,20}^2 - d_{2,20}^2) + 2d_{1,20}d_{2,20}e_{1,20}] + 3e_{2,20}],$$

$$\bar{H}_{3,20} = [(\sin(\bar{h}_{1,20}))(\cos(\bar{h}_{2,20}))(\sin(\bar{g}_{2,20}))(\sinh(\bar{g}_{1,20})) - (\cos(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20}))],$$

$$\rho_{9,20} = (d_{1,20}^2 + d_{2,20}^2)^{-1}[d_{1,20}(e_{2,20}^2 - e_{1,20}^2) + 2e_{2,20}d_{2,20}e_{1,20}] + 3d_{1,20}],$$

$$\bar{G}_{4,20} = [(\cos(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\cos(g_{2,20}))(\sinh(g_{1,20})) - (\sin(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20}))],$$

$$\rho_{10,20} = [-(d_{1,20}^2 + d_{2,20}^2)^{-1}[d_{2,20}(-e_{2,20}^2 + e_{1,20}^2) + 2e_{2,20}d_{2,20}e_{1,20}] + 3d_{2,20}],$$

$$\bar{H}_{4,20} = [(\cos(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20})) + (\sin(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20}))],$$

$$\rho_{11,20} = 2[d_{1,20}^2 + e_{2,20}^2 - d_{2,20}^2 - e_{1,20}^2],$$

$$\bar{G}_{5,20} = [(\cos(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\cos(\bar{g}_{2,20}))(\cosh(\bar{g}_{1,20})) - (\sin(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20}))],$$

$$\rho_{12,20} = 4[d_{1,20}d_{2,20} + e_{1,20}e_{2,20}],$$

$$\bar{H}_{5,20} = [(\cos(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20})) + (\sin(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20}))],$$

$$\rho_{13,20} = [\{5[d_{1,20}e_{1,20}^3 - 3e_{1,20}e_{2,20}^2d_{1,20}) + 5d_{2,20}(e_{1,20}^3 - 3e_{1,20}^2e_{2,20})\}(d_{1,20}^2 + d_{2,20}^2)^{-1} + (e_{1,20}^2 + e_{2,20}^2)^{-1}\{5(e_{1,20}d_{1,20}^3 - 3d_{2,20}e_{1,20}^2d_{1,20}) + 5(d_{2,20}^3e_{2,20} - 3d_{1,20}^2d_{2,20}e_{2,20})\} - 34(d_{1,20}e_{1,20} + d_{2,20}e_{2,20})],$$

$$\bar{G}_{6,20} = [(\sin(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20})) + (\cos(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20}))],$$

$$\rho_{14,20} = [\{5[d_{1,20}e_{1,20}^3 - 3e_{1,20}e_{1,20}^2d_{1,20}) + 5d_{2,20}(-e_{1,20}^3 + 3e_{2,20}^2e_{1,20})\}(d_{1,20}^2 + d_{2,20}^2)^{-1} + (e_{1,20}^2 + e_{2,20}^2)^{-1}\{5(-e_{1,20}d_{1,20}^3 + 3d_{1,20}^2d_{2,20}e_{1,20}) + 5(-d_{1,20}^3e_{2,20} + 3d_{2,20}^2d_{1,20}e_{2,20})\} + 34(d_{1,20}e_{2,20} - d_{2,20}e_{1,20})],$$

$$\bar{H}_{6,20} = [(\sin(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20})) - (\cos(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20}))],$$

$$\bar{H}_{7,20} = [\bar{H}_{1,20} + (\rho_{5,20}\bar{H}_{2,20}/2) + (\rho_{6,20}\bar{G}_{2,20}/2) + (\Delta_0/2)\{\rho_{8,20}\bar{G}_{3,20} + \rho_{7,20}\bar{H}_{3,20} + \rho_{10,20,}\bar{G}_{4,20} + \rho_{9,20}\bar{H}_{4,20} + \rho_{12,20}\bar{G}_{5,20} + \rho_{11,20}\bar{H}_{5,20} + (1/12)(\rho_{14,20}\bar{G}_{6,20} + \rho_{13,20}\bar{H}_{6,20})\}],$$

$$\bar{H}_{1,20} = [(\sin(\bar{h}_{1,20}))(\sinh(\bar{h}_{2,20}))(\cosh(\bar{g}_{1,20}))(\cos(\bar{g}_{2,20})) + (\cos(\bar{h}_{1,20}))(\cosh(\bar{h}_{2,20}))(\sinh(\bar{g}_{1,20}))(\sin(\bar{g}_{2,20}))],$$

$$\bar{D}_{7,20} = \sinh^{-1}(\omega_{7,20}), \bar{H}_{8,20} = (2\bar{C}_{7,19}\bar{D}_{7,20}/\bar{L}_0^2)$$

The sub-band equation in this case can be expressed as

$$0 = [\bar{G}_{8,20} + i\bar{H}_{8,20}]|_{\bar{E}=\bar{E}_{610}} \tag{10.85}$$

where $\bar{E}_{610}$ is the sub-band energy in this case.

At low temperatures where the quantum effects become prominent, the DOS function for the lowest SL mini-band is given by

$$\bar{N}_{HDSL}(\bar{E},\eta_g,\bar{F}) = \frac{\bar{g}_v}{\pi}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\frac{[\overline{G'}_{8,20}+i\overline{H'}_{8,20}]}{\sqrt{\bar{G}_{8,20}+i\bar{H}_{8,20}}}\bar{H}(\bar{E}-\bar{E}_{601}) \tag{10.86}$$

The EEM can be written as

$$\bar{m}^*(\bar{E},\bar{n}_y,\bar{n}_z\eta_g,\bar{F}) = \frac{\hbar^2}{2}(\overline{G'}_{8,20}) \tag{10.87}$$

The electron concentration is given by

$$\bar{n}_0 = \frac{2\bar{g}_v}{\pi}Real\ Part\ of\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}[[\bar{G}'_{8,20}+i\bar{H}'_{8,20}]+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{G}'_{8,20}+i\bar{H}'_{8,20}]]|_{\bar{E}=\bar{E}_{f20,26}} \tag{10.88}$$

where $\bar{E}_{f20,26}$ is the Fermi energy in this case.

10.2.13 Entropy in QDHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field

The DR in QDHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field can be expressed as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = [\bar{G}_{8,20}+i\bar{H}_{8,20}]|_{\bar{E}=\bar{E}_{620}} \tag{10.89}$$

where $\bar{E}_{620}$ is the sub – band energy in this case.

The DOS function is given by

$$\bar{N}_{QDHDSL}(\bar{E},\eta_g,\bar{F}) = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\delta'(\bar{E}-\bar{E}_{620}) \tag{10.90a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{2\bar{g}_v}{\bar{d}_x\bar{d}_y\bar{d}_z}Real\ Part\ of\sum_{\bar{n}_x=1}^{\bar{n}_{x\max}}\sum_{\bar{n}_y=1}^{\bar{n}_{y\max}}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\bar{F}_{-1}(\eta_{20,620}) \tag{10.90b}$$

where $\eta_{20,620} = \frac{\bar{E}_{f20,620}-\bar{E}_{620}}{k_BT}$

and $\bar{E}_{f20,620}$ is the Fermi energy in this case

Using (1.31f) and (10.90b) we can study the entropy in this case.

10.2.14 Magneto entropy in HD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field

Magnetoentropy in HD III–V SLs with graded interfaces in the presence of intense electric field can be expressed as

$$\bar{k}_z^2 = \bar{G}_{8,19n} + i\bar{H}_{8,19n} \tag{10.91}$$

where

$$\bar{G}_{8,19n} = \left[\frac{\bar{C}_{7,19n}^2 - \bar{D}_{7,19n}^2}{\bar{L}_0^2} = \frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right], \bar{C}_{7,19n} = \cos^{-1}(\omega_{7,19n}),$$

$$\omega_{7,19n} = (2)^{-1/2}\left[(1 - \bar{G}_{7,19n}^2 - \bar{H}_{7,19n}^2) - \sqrt{(1 - \bar{G}_{7,19n}^2 - \bar{H}_{7,19n}^2)^2 + 4\bar{G}_{7,19n}^2}\right]^{1/2},$$

$$\begin{aligned}\bar{G}_{7,19n} = [&\bar{G}_{7,19n} + (\rho_{5,19n}\bar{G}_{2,19n}/2) - (\rho_{6,19n}\bar{H}_{2,19n}/2) + (\Delta_0/2)\{\rho_{7,19n}\bar{H}_{2,19n} - \rho_{2,19n}\bar{H}_{3,19n} \\ &+ \rho_{9,19n}\bar{H}_{4,19n} - \rho_{10,19n}\bar{H}_{4,19n} + \rho_{11,19n}\bar{H}_{5,19n} - \rho_{12,19n}\bar{H}_{5,19n} \\ &+ (1/12)(\rho_{12,19n}\bar{G}_{6,19n} - \rho_{14,19n}\bar{H}_{6,19})\}],\end{aligned}$$

$$\begin{aligned}\bar{G}_{1,19n} = [&(\cos(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(\cosh(\bar{g}_{1,19n}))(\cos(\bar{g}_{2,19n})) \\ &+ (\sin(\bar{h}_{1,19n}))(sinh(\bar{h}_{2,19n}))(\sinh(\bar{g}_{1,9n}))(\sin(\bar{g}_{2,19n}))]\end{aligned}$$

$$\bar{h}_{1,19n} = e_{1,19n}(\bar{b}_0 - \Delta_0), e_{1,19n} = 2^{-1/2}{}^{1/2}, \left(\sqrt{\bar{t}_{1,19n}^2 + \bar{t}_{2,19n}^2} + \bar{t}_{1,19n}\right)$$

$$\bar{t}_{1,19n} = [(2\bar{m}_{c1} + \hbar^2).\bar{J}_{11}(\bar{E}, \Delta_1, \bar{E}_{g01}, \bar{F}) - \frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\bar{t}_{2,19n} = [(2\bar{m}_{c1}/\hbar^2)\bar{J}_{21}(\bar{E}, \Delta_1, \bar{E}_{g01}, \bar{F})],$$

$$\bar{h}_{2,19n} = e_{2,19n}(\bar{b}_0 - \Delta_0), e_{2,19n} = 2^{-1/2}\left(\sqrt{\bar{t}_{1,19n}^2 + \bar{t}_{2,19n}^2} - \bar{t}_{1,19n}\right)^{1/2},$$

$$\bar{g}_{1,19n} = d_{1,19n}(\bar{a}_0 - \Delta_0), d_{1,19n} = 2^{-1/2}\left(\sqrt{\bar{x}_{1,19n}^2 + \bar{y}_{1,19n}^2} + \bar{x}_{1,19n}\right)^{1/2},$$

$$\bar{x}_{1,19n} = \left[-(2\bar{m}_{c2} + \hbar^2).\bar{J}_{11}(\bar{E} - \bar{V}_0, \bar{E}_{g2}, \Delta_2, \eta_{g2}, \bar{F}) + \frac{2e\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right)\right],$$

$$y_1 = [(2\bar{m}_{c2}/\hbar^2)\bar{J}_{22}(\bar{E} - \bar{V}_0, \bar{E}_{g2}, \Delta_2, \eta_{g2}, \bar{F})],$$

$$\bar{g}_{2,19n} = d_{2,19n}(\bar{a}_0 - \Delta_0), d_{2,19n} = 2^{-1/2}\left(\sqrt{\bar{x}_{1,19n}^2 + \bar{y}_{1,19n}^2} - \bar{x}_{1,19n}\right)^{1/2},$$

$$\rho_{5,19n} = (\rho_{3,19n}^2 + \rho_{4,19n}^2)^{-1}[\rho_{1,19n}\rho_{3,19n}^2 - \rho_{2,19n}\rho_{4,19n}],$$

$$\rho_{1,19n} = [d_{1,19n}^2 + e_{2,19n}^2 - d_{2,19n}^2 - e_{1,19n}^2], \rho_{3,19n} = [d_{1,19n}e_{1,19n} + d_{2,19n}e_{2,19n}],$$

$$\rho_{2,19n} = 2[d_{1,19n}d_{2,19n} + e_{1,19n}e_{2,19n}], \rho_{4,19n} = [d_{1,19n}e_{2,19n} - e_{1,19n}d_{2,19n}],$$

$$\begin{aligned}\bar{G}_{2,19n} = [&(\sin(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(\sinh(\bar{g}_{1,19n}))(\cos(\bar{g}_{2,19n}))\\ &+ (\cos(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(\cosh(\bar{g}_{1,19n}))(\sin(\bar{g}_{2,19n}))]\end{aligned}$$

$$\rho_{6,19n} = (\rho_{3,19n}^2 + \rho_{4,19n}^2)^{-1}[\rho_{1,19n}\rho_{4,19n} + \rho_{2,19n}\rho_{3,19n}],$$

$$\begin{aligned}\bar{H}_{2,19n} = [&(\sin(\bar{h}_{1,19n}))(\cos(\bar{h}_{2,19n}))(\sin(\bar{g}_{2,19n}))(\cosh(\bar{g}_{1,19n}))\\ &- (\cos(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(\sinh(\bar{g}_{1,19n}))(\cos(\bar{g}_{2,19n}))]\end{aligned}$$

$$\rho_{7,19n} = [(e_{1,19n}^2 + e_{2,19n}^2)^{-1}[e_{1,19n}(d_{1,19n}^2 - d_{2,19n}^2] - 2d_{1,19n}d_{2,19n}e_{2,19n}] - 3e_{1,19n}],$$

$$\begin{aligned}G_{3,19n} = [&(\sin(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(cosh(\bar{g}_{1,19n}))(\cos(\bar{g}_{2,19n}))\\ &+ (\cos(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(sinh(\bar{g}_{1,19n}))(\sin(\bar{g}_{2,19n}))],\end{aligned}$$

$$\rho_{8,19n} = [(e_{1,19n}^2 + e_{2,19n}^2)^{-1}[e_{2,19n}(d_{1,19n}^2 - d_{2,19n}^2] + 2d_{1,19n}d_{2,19n}e_{1,19n}] + 3e_{2,19n}],$$

$$\begin{aligned}\bar{H}_{3,19n} = [&(\sin(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(\sin(\bar{g}_{2,19n}))(sinh(\bar{g}_{1,19n}))\\ &- (\cos(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(cosh(\bar{g}_{1,19n}))(\cos(\bar{g}_{2,19n}))],\end{aligned}$$

$$\rho_{9,19n} = [(d_{1,19n}^2 + d_{2,19n}^2)^{-1}[d_{1,19n}(e_{2,19n}^2 - e_{1,19n}^2] + 2e_{2,19n}d_{2,19n}e_{1,19n}] + 3d_{1,19n}],$$

$$\begin{aligned}\bar{G}_{4,19n} = [&(cos(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(cos(\bar{g}_{2,19n}))(sinh(\bar{g}_{1,19n}))\\ &- (sin(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(cosh(\bar{g}_{1,19n}))(\sin(\bar{g}_{2,19n}))],\end{aligned}$$

$$\rho_{10,19n} = [(d_{1,19n}^2 + d_{2,19n}^2)^{-1}[d_{2,19n}(e_{2,19n}^2 - e_{1,19n}^2] + 2e_{2,19n}d_{2,19n}e_{1,19n}] + 3d_{1,19n}],$$

$$\begin{aligned}\bar{H}_{4,19n} = [&(cos(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(cosh(\bar{g}_{1,19n}))(sin(\bar{g}_{2,19n}))\\ &- (sin(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(\sinh(\bar{g}_{1,19n}))(cos(\bar{g}_{2,19n}))],\end{aligned}$$

$$\rho_{11,19n} = 2[(d_{1,19n}^2 + e_{2,19n}^2 - d_{2,19n}^2 - e_{1,19n}^2],$$

$$\begin{aligned}\bar{G}_{5,19n} = [&(cos(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(cos(\bar{g}_{2,19n}))(cosh(\bar{g}_{1,19n}))(sinh(\bar{g}_{1,19n}))\\ &- (sin(\bar{h}_{2,19n}))(\sinh(\bar{g}_{1,19n}))(\sin(\bar{g}_{2,19n}))],\end{aligned}$$

$$\rho_{12,19n} = 4[(d_{1,19n}d_{2,19n} + e_{1,19n}e_{2,19n}],$$

$$\bar{H}_{5,19n} = [(cos(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(sin(\bar{g}_{1,19n}))(\sin(\bar{g}_{2,19n})) + (sin(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(\cosh(\bar{g}_{1,19n}))(cos(\bar{g}_{2,19n}))],$$

$$\begin{aligned}\rho_{13,19n} = [&\{5(d_{1,19n}e_{1,19n}^3 - 3e_{1,19n}e_{2,19n}^2 d_{1,19n}) \\ &+ 5d_{2,19n}(e_{1,19n}^3 - 3e_{1,19n}^2 e_{2,19n})\}(d_{1,19n}^2 + d_{2,19n}^2)^{-1} \\ &+ (e_{1,19n}^2 + e_{2,19n}^2)^{-1}\{5(e_{1,19n}d_{1,19n}^3 - 3d_{2,19n}e_{1,19n}^2 d_{1,19n}) \\ &+ 5(d_{2,19n}^3 e_{2,19n} - 3d_{1,19n}^2 d_{2,19n}e_{2,19n})\} \\ &- 34(d_{1,19n}e_{1,19n} + d_{2,19n}e_{2,19n})]\end{aligned}$$

$$\bar{G}_{6,19n} = [(sin(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(sinh(\bar{g}_{1,19n}))(\cos(\bar{g}_{2,19n})) + (cos(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(cosh(\bar{g}_{1,19n}))(\sin(\bar{g}_{2,19n}))],$$

$$\begin{aligned}\rho_{14,19n} = [&\{5(\bar{d}_{1,19n}e_{2,19n}^3 - 3e_{2,19n}e_{1,19n}^2 d_{1,19n}) \\ &+ 5d_{2,19n}(-e_{1,19n}^3 + 3e_{2,19n}^2 e_{1,19n})\}(d_{1,19n}^2 + d_{2,19n}^2)^{-1} \\ &+ (e_{1,19n}^2 + e_{2,19n}^2)^{-1}\{5(-e_{1,19n}d_{2,19n}^3 + 3d_{1,19n}^2 d_{1,19n}e_{1,19n}) \\ &+ 5(-d_{1,19n}^3 e_{2,19n} + 3d_{2,19n}^2 d_{1,19n}e_{2,19n})\} \\ &+ 34(d_{1,19n}e_{2,19n} - d_{2,19n}e_{1,19n})]\end{aligned}$$

$$\bar{H}_{6,19n} = [(\sin(\bar{h}_{1,19n}))(\cosh(\bar{h}_{2,19n}))(\cosh(\bar{g}_{1,19n}))(\sin(\bar{g}_{2,19n})) - (\cos(\bar{h}_{1,19n}))(\sinh(\bar{h}_{2,19n}))(\sinh(\bar{g}_{1,19n}))(\cos(\bar{g}_{2,19n}))],$$

$$\begin{aligned}\bar{H}_{7,19n} = [&\bar{H}_{7,19n} + (\rho_{5,19n}\bar{H}_{2,19n}/2) + (\rho_{6,19n}\bar{G}_{2,19n}/2) + (\Delta_0/2)\{\rho_{8,19n}\bar{G}_{3,19n} + \rho_{7,19n}\bar{H}_{3,19n} \\ &+ \rho_{10,19n}\bar{G}_{4,19n} + \rho_{9,19n}\bar{H}_{4,19n} + \rho_{12,19n}\bar{G}_{5,19n} + \rho_{11,19n}\bar{H}_{5,19n} \\ &+ (1/12)(\rho_{14,19n}\bar{G}_{6,19n} + \rho_{13,19n}\bar{H}_{6,19n})\}],\end{aligned}$$

$$\bar{H}_{1,19n} = [(\sin(\bar{h}_{1,19n}))(sinh(\bar{h}_{2,19n}))(\cosh(\bar{g}_{1,19n}))(cos(\bar{g}_{2,19n})) + (\cos(\bar{h}_{1,19n}))(cosh(\bar{h}_{2,19n}))(\sinh(\bar{g}_{1,19n}))(sin(\bar{g}_{2,19n}))],$$

$$D_{7,19n} = \sinh^{-1}(\omega_{7,19n}), \bar{H}_{8,19n} = (2\bar{C}_{7,19n}\bar{D}_{7,19n}/\bar{L}_0^2)$$

The sub-band equation in this case can be expressed as

$$0 = [\bar{G}_{8,19} + i\bar{H}_{8,19n}]|_{\bar{E}=\bar{E}_{630}} \tag{10.92}$$

where $\bar{E}_{630}$ is the Landau sub-band energy in this case.

At low temperatures where the quantum effects become prominent, the DOS function for the lowest SL mini-band is given by

$$\bar{N}_{HDSL}(\bar{E},\eta_g,\bar{F}) = \frac{\bar{g}_v e\bar{B}}{2\pi^2\hbar}\sum_{\bar{n}=0}^{\bar{n}_{\max}} \frac{[\overline{G'}_{8,19n} + i\overline{H'}_{8,19n}]}{\sqrt{\bar{G}_{8,19n} + i\bar{H}_{8,10n}}}\bar{H}(\bar{E}-\bar{E}_{630}) \tag{10.93}$$

The EEM can be written as

$$\bar{m}^*(\bar{E},\bar{n},\eta_g) = \frac{\hbar^2}{2}(\overline{G'}_{8,19n}) \tag{10.94a}$$

The electron concentration is given by

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{2\pi^2\hbar} Real\ Part\ of[\sum_{\bar{n}=0}^{\bar{n}_{\max}}[[\bar{G}_{8,19n} + i\bar{H}_{8,19n}] + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{G}_{8,19n} + i\bar{H}_{8,19n}]]|_{\bar{E}=\bar{E}_{f630}}] \tag{10.94b}$$

where E_{f630} is the Fermi energy in this case.

Using (1.31f) and (10.94b), we can study the entropy in this case.

10.2.15 Magneto entropy in QWHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field

The magneto DR in QWHD superlattices of Kane-type materials with graded interfaces in the presence of intense electric field can be expressed as

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = [\bar{G}_{8,19n} + i\bar{H}_{8,19n}]|_{\bar{E}=\bar{E}_{650}} \tag{10.95}$$

where $\bar{E}_{650}$ is the totally quantized energy in this case.

The DOS function is given by

$$\bar{N}_{QWHDSLB}(\bar{E},\eta_g,\bar{F}) = \frac{\bar{g}_v}{\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\delta'(\bar{E}-\bar{E}_{650}) \tag{10.96a}$$

The electron concentration can be expressed as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\ Real\ Part\ of\ \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{20,650}) \tag{10.96b}$$

where $\eta_{20,650} = \frac{\bar{E}_{f20,650}-\bar{E}_{650}}{k_B T}$

and $\bar{E}_{f20,650}$ is the Fermi energy in this case

Using (1.31f) and (10.96b) we can study the entropy in this case.

10.3 Open research problems

(R.10.1) Investigate the entropy in the presence of intense external non-uniform electric field for all the HD superlattices whose respective dispersion relations of the carriers are given in this chapter.

(R.10.2) Investigate the entropy for the HD materials in SLs the presences of Gaussian, exponential, Kane, Halperian, Lax and Bonch-Burevich types of band tails [16] for all SL systems as discussed in this chapter in the presence of external oscillatory and non-uniform electric field.

(R.10.3) Investigate the entropy in the presence of external non-uniform electric field for short period, strained layer, random and Fibonacci HD superlattices in the presence of an arbitrarily oriented alternating electric field.

(R.10.4) Investigate all the appropriate problems of this chapter for a Dirac electron.

(R.10.5) Investigate all the appropriate problems of this chapter by including the many body, broadening and hot carrier effects respectively.

(R.10.6) Investigate all the appropriate problems of this chapter by removing all the mathematical approximations and establishing the respective appropriate uniqueness conditions.

References

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11 Appendix B: Entropy in doping superlattices of HD nanomaterials

Change is the only unchangeable law of nature.

11.1 Introduction

The technological importance of superlattices in general, and specifically doping superlattices has already been stated in the preface and also in the references [1–20] of this chapter. In Section 11.1.1, of the theoretical background, the entropy in doping superlattices of HD nonlinear optical materials has been investigated. Section 11.2.2 contains the results for doping superlattices of HD III–V, ternary and quaternary materials in accordance with the three- and the two-band models of Kane together with parabolic energy bands and they form the special cases of Section 11.11.1. Sections 11.2.3, 11.2.4, and 11.2.5 contain the study of the entropy for doping superlattices of HD II–VI, IV–VI, stressed and Kane type materials, respectively. Section 11.3 contains five open research problems for this chapter.

11.2 Theoretical background

11.2.1 Entropy in doping superlattices of HD nonlinear optical materials

DR of the conduction electrons in doping superlattices of HD nonlinear optical materials can be expressed by using (1.26) and following the method as given in [19, 20] as

$$\frac{(\bar{n}_i + \frac{1}{2})}{\hbar \bar{T}_{21}(\bar{E}, \eta_g)} \omega_{8HD}(\bar{E}, \eta_g) + \frac{\hbar^2 \bar{k}_s^2}{2\bar{m}^*_{\perp} \bar{T}_{21}(\bar{E}, \eta_g)} = 1 \tag{11.1}$$

Where

$$\omega_{8HD}(\bar{E}, \eta_g) \equiv Real\, party\, of \left(\frac{\bar{n}_0 |e|^2}{d_0 \varepsilon_{sc} [\bar{m}^*_{||} \bar{T}'_{21}(\bar{E}, \eta_g)]} \right)^{1/2}$$

$\bar{n}_i (= 0, 1, 2...)$ is the mini-band index for nipi structures and d_0 is the superlattice period.

EEM in this case assumes the form

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$$\bar{m}^{*}(\bar{E}_{FnHD},\bar{n}_i,\eta_g) = Real\ part\ of\left(\frac{\hbar^2}{2}\right)\bar{G}'_{21HD}(\bar{E}_{FnHD},\bar{n}_i,\eta_g) \tag{11.2}$$

where,

$$\bar{G}_{21HD}(\bar{E},\eta_g,\bar{n}_i) = \frac{2\bar{m}^{*}_{\perp}\bar{T}_{22}(\bar{E},\eta_g)}{\hbar^2}\left[\frac{(\bar{n}_i+\frac{1}{2})}{\hbar\bar{T}_{21}(\bar{E},\eta_g)}\omega_{8HD}(\bar{E},\eta_g)\right]$$

and $\bar{E}_{FnHD}$ is the Fermi energy in the present case as measured from the edge of the conduction band in vertically upward direction in the absence of any quantization.

From (11.2), we observe that the EEM is a function of the Fermi energy, nipisubband index, scattering potential and the other material constants, which is the characteristic feature of doping superlattices of HD nonlinear optical materials.

The subband energy $\bar{E}_{1n_iHD}$ can be written as

$$\frac{(\bar{n}_i+\frac{1}{2})}{\hbar\bar{T}_{21}(\bar{E},\eta_g)}\omega_{8HD}(\bar{E}_{1n_iHD},\eta_g) = 1 \tag{11.3}$$

The DOS function for doping superlattices of HD nonlinear optical materials can be expressed as

$$\bar{N}_{nipiHD}(\bar{E},\eta_g) = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\bar{G}'_{21HD}(\bar{E},\eta_g,\bar{n}_i)\bar{H}-(\bar{E}-\bar{E}_{1n_iHD}) \tag{11.4}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\mathrm{Re}\,al\ Part\ of\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{G}_{21HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{G}_{21HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)\right]\right]\right] \tag{11.4b}$$

Using (1.31f) and (11.4b), we can study the entropy in this case.

DR of the conduction electrons in doping superlattices of nonlinear optical materials in the absence of band tails assumes the following form

$$\psi_1(\bar{E}) = \psi_2(\bar{E})k_s^2+\psi_3(\bar{E})\left(\bar{n}_i+\frac{1}{2}\right)\frac{2\bar{m}^{*}_{||}}{\hbar}\omega_8(\bar{E}) \tag{11.5}$$

where

$$\omega_8(\bar{E}) \equiv \left(\frac{\bar{n}_0|e|^2}{\bar{d}_0\varepsilon_{sc}[\theta_1(\bar{E})]}\right)^{1/2} and\ \theta_1(\bar{E}) \equiv \frac{\hbar^2}{2}\left\{\frac{\psi_3(\bar{E})[\psi_1(\bar{E})]'-\psi_1(\bar{E})[\psi_3(\bar{E})]'}{[\psi_3(\bar{E})]^2}\right\}$$

The EEM in this case can be written as

$$\bar{m}^{*}(\bar{E}_{Fn},\bar{n}_i)=\left(\frac{\hbar^2}{2}\right)R_{81}(\bar{E},n_i)|_{\bar{E}-\bar{E}_{Fn}} \tag{11.6}$$

where,

$$\bar{R}_{81}(\bar{E},n_i)\equiv[\psi_2(\bar{E})]^{-2}\left\{[\psi_2(\bar{E})]'-\left(\frac{2\bar{m}^{*}_{||}}{\hbar^2}\right)[\psi_3(\bar{E})]'\left(\bar{n}_i+\frac{1}{2}\right)[\omega_8(\bar{E})]\right.$$
$$\left.-\left(\frac{2\bar{m}^{*}_{||}}{\hbar}\right)[\psi_3(\bar{E})]\left(\bar{n}_i+\frac{1}{2}\right)[\omega_8(\bar{E})]'\right\}$$
$$-\left\{[\psi_1(\bar{E})]'-\left(\frac{2\bar{m}^{*}_{||}}{\hbar^2}[\psi_3(\bar{E})]''\bar{n}_i+\frac{1}{2}\right)[\omega_8(\bar{E})]\right\}[\psi_2(\bar{E})]']$$

and $\bar{E}_{Fn}$ is the Fermi energy in the present case as measured from the edge of the conduction band in vertically upward direction in the absence of any quantization.

The subband energy $(\bar{E}_{1ni})$ can be written as

$$\psi_1(\bar{E}_{1ni})=\psi_3(\bar{E}_{1ni})\left(\bar{n}_i+\frac{1}{2}\right)\frac{2\bar{m}^{*}_{||}}{\hbar}\omega_8(\bar{E}_{1ni}) \tag{11.7}$$

The DOS function for doping superlattices of nonlinear optical materials can be expressed as

$$\bar{N}_{nipi}(\bar{E})=\frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\bar{R}_{81}(\bar{E},\bar{n}_i)\bar{H}-(\bar{E}-\bar{E}_{1n_i}) \tag{11.8}$$

The electron concentration in this case can be written as

$$\bar{n}_0=\frac{\bar{g}_v}{2\pi}\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{R}_{81}(\bar{E}_{Fn},\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{R}_{81}(\bar{E}_{Fn},\bar{n}_i)]\right]\right] \tag{11.8b}$$

Using (1.44) and (11.8b), we can study the entropy in this case.

11.2.2 Entropy in doping superlattices of HD III–V, ternary, and quaternary materials

(a) The electron energy spectrum in doping superlattices of HD III–V, ternary, and quaternary materials can be expressed from (11.1) under the conditions $\Delta_{||}=\Delta_{\perp}=\Delta$, $\delta=0$ and $\bar{m}_{||}^{*}=\bar{m}_{\perp}^{*}=\bar{m}_c$, as

$$\frac{\hbar^2\bar{k}^2}{2\bar{m}_c}=\left[\bar{T}_{31}(\bar{E},\eta_g)+i\bar{T}_{32}(\bar{E},\eta_g)-\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{9HD}(\bar{E},\eta_g)\right] \tag{11.9}$$

where

$$\omega_{9HD}(\bar{E},\eta_g) \equiv \left(\frac{\bar{n}_0|e|^2}{d_0\varepsilon_{sc}\overline{T}'_{31}(\bar{E},\eta_g)\bar{m}_c}\right)^{1/2}$$

The EEM in this case assumes the form

$$\bar{m}^*(\bar{E}_{FnHD},\bar{n}_i,\eta_g) = Re\,al\ part\ of\left(\frac{\hbar^2}{2}\right)\overline{G'}_{23HD}(\bar{E}_{FnHD},\bar{n}_i,\eta_g) \tag{11.10}$$

where

$$\bar{G}_{23HD}(\bar{E}_{FnHD},\bar{n}_i,\eta_g) = \frac{2\bar{m}}{\hbar^2}\left[\bar{T}_{31}(\bar{E}_{FnHD},\eta_g) + i\bar{T}_{32}(\bar{E}_{FnHD},\eta_g) - \left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{9HD}(\bar{E}_{FnHD},\eta_g)\right]$$

The subband energy $\bar{E}_{2n_1HD}$ can be written as

$$[\bar{T}_{31}(\bar{E}_{2n_iHD},\eta_g) + i\bar{T}_{32}(\bar{E}_{2n_iHD},\eta_g) - \left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{9HD}(\bar{E}_{2n_iHD},\eta_g)] = 0 \tag{11.11}$$

The DOS function for doping superlattics of HD III–V, ternary, and quaternary materials can be expressed as

$$\bar{N}_{nipiHD}(\bar{E},\eta_g) = \frac{\bar{g}_v\bar{m}_c}{\pi\hbar^2}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\overline{G'}_{23HD}(\bar{E},\eta_g,\bar{n}_i)\bar{H}-(\bar{E}-\bar{E}_{2n_iHD}) \tag{11.12a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\mathrm{Re}\,al\ Part\ of\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{G}_{23HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{G}_{23HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)\right]\right]\right] \tag{11.12b}$$

Using (1.31f) and (11.12b), we can study the entropy in this case.

In the absence of band tails, the DR in this case assumes the form

$$\bar{I}_{11}(\bar{E}) = \left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{19}(\bar{E}) + \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_c} \tag{11.13}$$

where

$$\omega_{19}(\bar{E}) \equiv \left[\frac{\bar{n}_0|e|^2}{d_0\varepsilon_{sc}\overline{I'}_{11}(\bar{E})\bar{m}_c}\right]^{1/2}$$

The EEM in this case can be written as

$$\bar{m}^{*}(\bar{E}_{Fn}, \bar{n}_i) = \bar{m}_c \bar{R}_{82}(\bar{E}, \bar{n}_i)|_{\bar{E}=\bar{E}_{Fn}} \tag{11.14}$$

in which

$$\bar{R}_{82}(\bar{E}, \bar{n}_i) \equiv \left\{ [\bar{I}_{11}(\bar{E})]' - \left(\bar{n}_i + \frac{1}{2}\right)\hbar[\omega_{19}(\bar{E})]' \right\}$$

From (11.14), we observe that EEM in this case is a function of the Fermi energy, nipisubband index and other material constants which form the characteristic feature of doping superlattices of III–V, ternary, and quaternary compounds whose bulk DR is defined by the three-band model of Kane.

The subband energies $(\bar{E}_{2ni})$ can be written as

$$\bar{I}_{11}(\bar{E}_{2ni}) = \left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{19}(\bar{E}_{2ni}) \tag{11.15}$$

The DOS function in this case can be expressed as

$$\bar{N}_{nipi}(\bar{E}) = \frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2} \sum_{\bar{n}_i=0}^{\bar{n}_{i\max}} \bar{R}_{82}(\bar{E}, \bar{n}_i)\bar{H} - (\bar{E} - \bar{E}_{2n_i}) \tag{11.16a}$$

The electron concentration in this case can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{R}_{82}(\bar{E}_{Fn}, \bar{n}_i) + \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r})\left[\bar{R}_{82}(\bar{E}_{Fn}, \bar{n}_i)\right]\right]\right] \tag{11.16b}$$

Using (1.44) and (11.16b), we can study the entropy in this case.

(b) The electron energy spectrum in doping superlattices of HD III–V, ternary and quaternary materials whose energy band structures in the absence of band tails are described by the two-band model of Kane can be expressed from (11.13) under the conditions $\Delta >> E_g$ or $\Delta << E_g$, as

$$\frac{\hbar^2 \bar{k}_s^2}{2\bar{m}_c} = \left[\gamma_2(\bar{E}, \eta_g) - \left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{10HD}(\bar{E}, \eta_g)\right] \tag{11.17}$$

where

$$\omega_{10HD}(\bar{E}) \equiv \left(\frac{\bar{n}_0|e|^2}{d_0\varepsilon_{sc}\gamma'_2(\bar{E}, \eta_g)\bar{m}_c}\right)^{1/2}$$

The EEM in this case assumes the form

$$\bar{m}^{*}(\bar{E}_{FnHD}, \bar{n}_i, \eta_g) = \left(\frac{\hbar^2}{2}\right)\overline{G'}_{25HD}(\bar{E}_{FnHD}, \eta_g, \bar{n}_i) \tag{11.18}$$

where,

$$\bar{G}_{25HD}(\bar{E}_{FnHD},\eta_g,\bar{n}_i)=\frac{2\bar{m}_c}{\hbar^2}\left[\gamma_2(\bar{E}_{FnHD},\eta_g)-\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{10HD}(\bar{E}_{FnHD},\eta_g)\right]$$

The subband energy $\bar{E}_{3n_iHD}$ can be written as

$$\left[\gamma_2(\bar{E}_{3n_iHD},\eta_g)-\left(\bar{n}_i+\frac{1}{2}\right)\hbar^2\omega_{9HD}(\bar{E}_{3n_iHD},\eta_g)\right]=0 \tag{11.19}$$

The DOS function in this case is given by

$$\bar{N}_{nipiHD}(\bar{E},\eta_g)=\frac{\bar{g}_v\bar{m}_c}{\pi\hbar^2}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\overline{G'}_{25HD}(\bar{E},\eta_g,\bar{n}_i)\bar{H}(\bar{E}-\bar{E}_{3n_iHD}) \tag{11.20}$$

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v}{2\pi}\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{G}_{25HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{G}_{25HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)\right]\right]\right] \tag{11.20b}$$

Using (1.31f) and (11.20b), we can study the entropy in this case.

In the absence of band tails, the DR in this case assumes the form

$$\bar{E}(1+\alpha\bar{E})=\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{20}(\bar{E})+\frac{\hbar^2\bar{k}_s^2}{2\bar{m}_c} \tag{11.21}$$

where

$$\omega_{20}(\bar{E})\equiv\left(\frac{\bar{n}_0|e|^2}{d_0\varepsilon_{sc}(1+2\alpha\bar{E})\bar{m}_c}\right)^{1/2}$$

The EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{Fn},\bar{n}_i)=\bar{m}_c\bar{R}_{182}(\bar{E},\bar{n}_i)|_{\bar{E}=\bar{E}_{Fn}} \tag{11.22}$$

in which $\bar{R}_{182}(\bar{E},\bar{n}_i)\equiv\{[1+2\alpha\bar{E}]-\left(\bar{n}_i+\frac{1}{2}\right)\hbar[\omega_{19}(\bar{E})]'\}$.

From (11.22), we observe that the EEM in this case is a function of the Fermi energy, nipi subband index and the other material constants which form the characteristic feature of doping superlattices of III–V, ternary, and quaternary compounds whose bulk DRs is defined by the three-band model of Kane.

The subband energies $(\bar{E}_{3n_i})$ can be written as

$$\bar{E}_{3n_i}(1+\alpha\bar{E}_{3n_i})=\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{20}(\bar{E}_{3n_i}) \tag{11.23}$$

The DOS function in this case can be expressed as

$$\bar{N}_{nipi}(\bar{E}) = \frac{\bar{m}_c \bar{g}_v}{\pi\hbar^2} \sum_{\bar{n}_i=0}^{\bar{n}_{i\max}} \bar{R}_{182}(\bar{E}, \bar{n}_i)\bar{H} - (\bar{E} - \bar{E}_{3n_i}) \tag{11.24a}$$

The electron concentration in this case can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi} \left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}} \left[\bar{R}_{182}(\bar{E}_{Fn}, \bar{n}_i) + \sum_{\bar{r}=1}^{\bar{s}} \bar{L}(\bar{r}) \left[\bar{R}_{182}(\bar{E}_{Fn}, \bar{n}_i) \right] \right] \right] \tag{11.24b}$$

Using (1.44) and (11.24b), we can study the entropy in this case.

(c) The electron energy spectrum in nipi structures of HD III–V, ternary, and quaternary materials whose energy band structures in the absence of band tails are described by the parabolic energy bands can be expressed as

$$\frac{\hbar^2 \bar{k}_s^2}{2\bar{m}_c} = \left[\gamma_3(\bar{E}, \eta_g) - \left(\bar{n}_i + \frac{1}{2} \right) \hbar\omega_{11HD}(\bar{E}, \eta_g) \right] \tag{11.25}$$

where

$$\omega_{11HD}(\bar{E}) \equiv \left(\frac{\bar{n}_0 |e|^2}{d_0 \varepsilon_{sc} \gamma_2'(\bar{E}, \eta_g) \bar{m}_c} \right)^{1/2}$$

The EEM in this case assumes the form

$$\bar{m}^*(\bar{E}_{FnHD}, \bar{n}_i, \eta_g) = \left(\frac{\hbar^2}{2} \right) \overline{G'}_{27HD}(\bar{E}_{FnHD}, \bar{n}_i, \eta_g) \tag{11.26}$$

where

$$\bar{G}_{27HD}(\bar{E}_{FnHD}, \bar{n}_i, \eta_g) = \frac{2\bar{m}_c}{\hbar^2} \left[\gamma_3(\bar{E}_{FnHD}, \eta_g) - \left(\bar{n}_i + \frac{1}{2} \right) \hbar\omega_{11HD}(\bar{E}_{FnHD}, \eta_g) \right]$$

The subband energy $\bar{E}_{4n_iHD}$ can be expressed as

$$\left[\gamma_3(\bar{E}_{4n_iHD}, \eta_g) - \left(\bar{n}_i + \frac{1}{2} \right) \hbar^2 \omega_{11HD}(\bar{E}_{4n_iHD}, \eta_g) \right] = 0 \tag{11.27}$$

The DOS function in this case is given by

$$\bar{N}_{nipiHD}(\bar{E}, \eta_g) = \frac{\bar{g}_v \bar{m}_c}{\pi\hbar^2} \sum_{\bar{n}_i=0}^{\bar{n}_{i\max}} \overline{G'}_{27HD}(\bar{E}, \eta_g, n_i)\bar{H}(\bar{E} - \bar{E}_{4n_iHD}) \tag{11.28a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{G}_{27HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{G}_{27HD}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)\right]\right]\right] \tag{11.28b}$$

Using (1.31f) and (11.28b), we can study the entropy in this case.

In the absence of band tails, the DR in this case assumes the form

$$\bar{E} = \left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{21} + \frac{\hbar^2\bar{k}_s^2}{2\bar{m}_c} \tag{11.29}$$

where

$$\omega_{21}(\bar{E}) \equiv \left(\frac{\bar{n}_0|e|^2}{d_0\varepsilon_{sc}\bar{m}_c}\right)^{1/2}$$

The EEM in this case can be written as

$$\bar{m}^*(\bar{E}_{Fn},\bar{n}_i) = \bar{m}_c \tag{11.30}$$

Thus the EEM in this case is a constant quantity.

The subband energies $(\bar{E}_{4ni})$ can be written as

$$\bar{E}_{4n_i} = \left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{21} \tag{11.31}$$

The DOS function in this case can be expressed as

$$\bar{N}_{nipi}(\bar{E}) = \frac{\bar{m}_c\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\bar{H} - (\bar{E}-\bar{E}_{4n_i}) \tag{11.32a}$$

The electron concentration in this case can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{R}_{1821}(\bar{E}_{Fn},\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{R}_{1821}(\bar{E}_{Fn},\bar{n}_i)\right]\right]\right] \tag{11.32b}$$

where,

$$\bar{R}_{1821}(\bar{E},\bar{n}_i) \equiv \left\{\bar{E}_{Fn} - \left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{21}\right\}$$

Using (1.44) and (11.32b), we can study the entropy in this case.

11.2.3 Entropy in doping superlattices of HD II–VI materials

The 2D electron dispersion law in doping superlattices of HD II–VI materials can be expressed as

$$\gamma_3(\bar{E},\eta_g)=\overline{a'}_0\bar{k}_s^2+\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{30}(\bar{E},\eta_g)\pm\bar{\lambda}_0\bar{k}_s,\omega_{30}(\bar{E},\eta_g)\equiv\left(\frac{\bar{n}_0|d|^2}{d_0\gamma'_3(\bar{E},\eta_g)\varepsilon_{sc}\bar{m}^*_{||}}\right)^{1/2} \tag{11.33}$$

EEM in this case assumes the form as

$$\bar{m}^*(\bar{E}_{FnHD},\bar{n}_i,\eta_g)=\bar{m}^*_{\perp}\left\{1-\bar{\lambda}_0\left[(\bar{\lambda}_0)^2+4\overline{a'}_0\gamma_3(\bar{E}_{FnHD},\eta_g)\right.\right.$$
$$\left.\left.-4\overline{a'}_0\left(\bar{n}_i+\frac{1}{2}\right)\hbar^2\omega_{30}(\bar{E}_{FnHD},\eta_g)\right]^{-1/2}\right\}\gamma'_3(\bar{E}_{FnHD},\eta_g) \tag{11.34}$$

The subband energy can be written as

$$\left[\gamma_3(\bar{E}_{6n_iHD},\eta_g)=\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{30}(\bar{E}_{6n_iHD},\eta_g)\right] \tag{11.35}$$

The DOS function in this case is given by

$$\bar{N}_{nipiHD}(\bar{E})=\frac{\bar{g}_v}{4\pi(\overline{a'}_0)^2}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{G}_{30HD}(\bar{E},\eta_g,\bar{n}_i)\right]'\bar{H}(\bar{E}-\bar{E}_{6n_iHD}) \tag{11.36a}$$

where

$$\bar{G}_{30HD}(\bar{E},\eta_g,\bar{n}_i)=\left[(\bar{\lambda}_0)-2d_0\left\{\left(\bar{n}_i+\frac{1}{2}\right)\hbar\omega_{30}(\bar{E},\eta_g,\bar{n}_i)-\gamma_3(\bar{E},\eta_g,\bar{n}_i)\right\}\right]$$

The electron concentration can be written as

$$\bar{n}_0=\frac{\bar{g}_v}{4\pi(\bar{a}'_0)^2}\left[\sum_{n_i=0}^{\bar{n}_{i\max}}\left[G_{30HD}(\bar{E}_{FNHD},\bar{n}_g,\bar{n}_i)+\sum_{\overline{r=1}}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{G}_{30HD}(\bar{E}_{FNHD},\bar{n}_g,\bar{n}_i)\right]\right]\right] \tag{11.36b}$$

Using (1.31f) and (11.36b), we can study the entropy in this case.

In the absence of bandtails, the carrier dispersion law in doping superlattices of II–VI compounds can be expressed as

$$\bar{E}=\overline{a'}_0\bar{k}_s^{\,2}+\left(\bar{n}_i+\frac{1}{2}\right)\hbar\bar{\omega}_{10}\pm\overline{\lambda_0 k_s},\bar{\omega}_{10}=\left(\frac{\bar{n}_0\,\|\bar{e}\|}{d_0\varepsilon_{sc}\bar{m}^*_{||}}\right)^{1/2} \tag{11.37}$$

Using (11.37), EEM in this case can be written as

$$\bar{m}^*(\bar{F}_{Fn},\bar{n}_i)=\bar{m}^*_{\perp}\left\{1-\bar{\lambda}_0\left[(\bar{\lambda}_0)^2+4\overline{a'}_0\bar{E}_{Fn}-4\overline{a'}_0\left(\bar{n}_i+\frac{1}{2}\right)\hbar^2\bar{\omega}_{10}\right]^{-1/2}\right\} \tag{11.38}$$

Thus, the EEM in this case is a function of the Fermi energy, the nipi subband index number and the energy spectrum constants due to the presence of $\bar{\lambda}_0$.

The subband energies $(\bar{E}_{8n_i})$ assume the form as

$$\bar{E}_{8n_i} = \left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{10} \tag{11.39}$$

The DOS function in this case can be expressed as

$$\bar{N}_{nipi}(\bar{E}) = \frac{\bar{m}^*_{\perp}\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[1 - \frac{\bar{a}_{81}}{\sqrt{\bar{E} + \bar{b}_{81}(n_i)}}\right]H - (\bar{E} - \bar{E}_{8n_i}) \tag{11.40a}$$

in which $\bar{a}_{81} = \frac{\bar{\lambda}_0}{2\sqrt{\bar{a}'_0}}$ and $\bar{b}_{81}(\bar{n}_i) \equiv \left[\frac{1}{4\bar{a}'_0}\left[(\bar{\lambda}_0)^2 - 4\overline{a'}_0\left(\bar{n}_i + \frac{1}{2}\right)\hbar\omega_{10}\right]\right]$.

The use of Equation (8.22) leads to the electron concentration as

$$\bar{n}_0 = \frac{\bar{m}^*_{\perp}\bar{g}_v\bar{k}_B\bar{T}}{\pi\hbar^2 d_0}\sum_{\bar{n}_i=0}^{\bar{n}_i\max}\left[\bar{F}_0(\bar{\eta}_{81}) - \left(\frac{\bar{a}_{81}}{\sqrt{\bar{k}_B\bar{T}}}\left[2\left(\sqrt{\bar{\eta}_{81} + \bar{c}_{81}(\bar{n}_i)} - \sqrt{\bar{c}_{81}(\bar{n}_i)}\right)\right]\right) + \sum_{\bar{r}=1}^{\bar{s}} 2(1 - 2^{1-2\bar{r}})\zeta(2\bar{r})\frac{(-1)^{2\bar{r}-1}(2\bar{r}-1)!}{(\bar{\eta}_{81} + \bar{c}_{81}(\bar{n}_i))^{2\bar{r}}}\right] \tag{11.40b}$$

where, $\bar{\eta}_{81} \equiv \frac{\bar{E}_{Fn} - \bar{E}_{3ni}}{k_B T}$ and $\bar{c}_{81}(\bar{n}_i) \equiv \frac{\bar{b}_{81}(\bar{n}_i) + \bar{E}_{3ni}}{k_B T}$

Using (1.44) and (11.40b), we can study the entropy in this case.

11.2.4 Entropy in doping superlattices of HD IV–VI materials

The 2D electron dispersion law in this case is given by

$$\bar{k}_s^2 = \delta_{15}(\bar{E}, \eta_g, \bar{n}_i) \tag{11.41}$$

where

$$\delta_{15}(\bar{E}, \eta_g, \bar{n}_i) = [2\delta_{12}(\bar{E}, \eta_g)]^{-1}\left[-\delta_{13}(\bar{E}, \eta_g, \bar{n}_i) + \sqrt{\delta_{13}^2(\bar{E}, \eta_g, \bar{n}_i) - 4\delta_{12}(\bar{E}, \eta_g)\delta_{14}(\bar{E}, \eta_g, \bar{n}_i)}\right],$$

$$\delta_{12}(\bar{E}, \eta_g) = \frac{\alpha\hbar^4\bar{Z}_0(\bar{E}, \eta_g)}{4\bar{m}_t^+\bar{m}_l^-}, \delta_{13}(\bar{E}, \eta_g, \bar{n}_i) = \hbar^2[\lambda_{71}(\bar{E}, \eta_g)\delta_{11}(\bar{E}, \eta_g, \bar{n}_i) + \lambda_{12}(\bar{E}, \eta_g)],$$

and

$$m^{*}_{HD}(\bar{E},\eta_g) = \frac{\hbar^2}{4\lambda^2_{76}(\bar{E},\eta_g)}\left[2\lambda_{74}(\bar{E},\eta_g) - \left\{ -\lambda'_{73}(\bar{E},\eta_g) + \frac{\lambda_3(\bar{E},\eta_g)\lambda'_{73}(\bar{E},\eta_g) + 2\lambda'_{74}(\bar{E},\eta_g)\lambda_{75}(\bar{E},\eta_g) + 2\lambda_{74}(\bar{E},\eta_g)\lambda'_{75}(\bar{E},\eta_g)}{\sqrt{\lambda^2_{73}(\bar{E},\eta_g) + 4\lambda_{74}(\bar{E},\eta_g)\lambda_{75}(\bar{E},\eta_g)}} \right\} - 2\lambda'_{74}(\bar{E},\eta_g)\left\{ -\lambda_{73}(\bar{E},\eta_g) + \sqrt{\lambda^2_{73}(\bar{E},\eta_g) + 4\lambda_{74}(\bar{E},\eta_g)\lambda_{75}(\bar{E},\eta_g)} \right\}\right]\right]$$

EEM in this case assumes the form

$$\bar{m}^{*}(\bar{F}_{FnHD},\bar{n}_i,\eta_g) = \left(\frac{\hbar^2}{2}\right)\delta'_{15}(\bar{E}_{FnHD},\eta_g,\bar{n}_i) \tag{11.42}$$

The subband energy $\bar{E}_{9n_iHD}$ can be expressed as in this case as

$$0 = \delta_{15}(\bar{E}_{9n_iHD},\eta_g,\bar{n}_i) \tag{11.43}$$

The DOS function in this case is given by

$$\bar{N}_{nipiHD}(\bar{E}) \equiv \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}[\delta_{15}(\bar{E},\eta_g,\bar{n}_i)]'\bar{H}(\bar{E}-\bar{E}_{9n_iHD}) \tag{11.44a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\delta_{15}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\delta_{15}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)\right]\right]\right] \tag{11.44b}$$

Using (1.31f) and (11.44b), we can study the entropy in this case.

The carrier energy spectrum in doping superlatticesof IV–VI compounds in the absence of band tails can be written as

$$\bar{k}^2_s = (\hbar^2\bar{S}_{19})^{-1}\left[-\bar{S}_{20}(\bar{E},n_i) + \sqrt{\bar{S}^2_{20}(\bar{E},n_i) + 4\bar{S}_{19}\bar{S}_{21}(\bar{E},n_i)}\right] \tag{11.45}$$

In which,

$$\bar{S}_{19} \equiv \left[\frac{\alpha}{\bar{m}^{+}_t\bar{m}^{-}_t}\right],$$

$$\bar{S}_{20}(\bar{E},n_i) = \left\{\frac{1}{\bar{m}^{*}_t} - \left(\frac{\alpha\bar{E}}{\bar{m}^{+}_t}\right) + \frac{1+\alpha\bar{E}}{\bar{m}^{-}_t} + \frac{\alpha\hbar^2}{2\bar{m}^{+}_l\bar{m}^{-}_t}\left(\bar{n}_i+\frac{1}{2}\right)\bar{T}(\bar{E})\frac{\alpha\hbar^2}{2\bar{m}^{-}_l\bar{m}^{+}_t}\left(\bar{n}_i+\frac{1}{2}\right)\bar{T}(\bar{E})\right\}$$

$$\bar{T}(\bar{E}) \equiv \frac{2\bar{m}^{*}(0)}{\hbar}\omega_{11}(\bar{E}), \bar{m}^{*}(0) \equiv \left(\frac{\bar{m}_l^{*}\bar{m}_l^{-}}{\bar{m}_l^{*}+\bar{m}_l^{-}}\right), \omega_{11}(\bar{E}) \equiv \left(\frac{\bar{n}_0|e|^2}{d_0\varepsilon_{sc}\bar{m}^{*}(\bar{E})}\right)^{1/2},$$

$$\bar{m}^{*}(\bar{E}) \equiv \frac{1}{4\bar{t}_1}\left[-(\bar{t}_2(\bar{E}))' + \frac{\bar{t}_2(\bar{E})(\bar{t}_2(\bar{E}))' + 2\bar{t}_1(1+2\alpha\bar{E})}{\sqrt{\bar{t}_2^2(\bar{E}) + 4\bar{E}\bar{t}_1(1+\alpha\bar{E})}}\right],$$

$$\bar{t}_1 \equiv \left(\frac{\alpha}{4\bar{m}_l^{-}\bar{m}_l^{+}}\right), \bar{t}_2(\bar{E}) \equiv \frac{1}{2}\left[\left(\frac{1}{\bar{m}_l^{*}}\right) - \left(\frac{\alpha\bar{E}}{\bar{m}_l^{+}}\right) + \left(\frac{1+\alpha\bar{E}}{\bar{m}_l^{-}}\right)\right], (\bar{t}_2(\bar{E}))' \equiv \frac{\alpha}{2}\left(\frac{1}{\bar{m}_l^{-}} - \left(\frac{1}{\bar{m}_l^{+}}\right)\right)$$

and

$$\bar{S}_{21}(\bar{E},\bar{n}_i) \equiv \left[\bar{E}(1+\alpha\bar{E}) + \frac{\alpha\bar{E}\hbar^2}{2\bar{m}_l^{+}}\left(\bar{n}_i+\frac{1}{2}\right)\bar{T}(\bar{E}) + \frac{\hbar^2}{2m_l^{-}}\left(\bar{n}_i+\frac{1}{2}\right)\bar{T}(\bar{E})(1+\alpha\bar{E})\right.$$
$$\left. + \frac{\hbar^4}{4\bar{m}_l^{-}\bar{m}_l^{+}}\left(\bar{n}_i+\frac{1}{2}\right)\bar{T}(\bar{E}) - \left(\frac{\hbar^2}{2\bar{m}_l^{*}}\right)\bar{T}(\bar{E})\left(\bar{n}_i+\frac{1}{2}\right)\right]$$

Using (11.45), EEM in this case can be written as

$$\bar{m}^{*}(\bar{E}_{Fn},\bar{n}_i) = \bar{R}_{84}(\bar{E},\bar{n}_i)|_{\bar{E}=\bar{E}_{Fn}} \tag{11.46}$$

where,

$$\bar{R}_{84}(\bar{E},\bar{n}_i) \equiv \left[-(\bar{S}_{20}(\bar{E},\bar{n}_i))' + \frac{\bar{S}_{20}(\bar{E},\bar{n}_i)[\bar{S}_{20}(\bar{E},\bar{n}_i)]' + 2\bar{S}_{19}[\bar{S}_{21}(\bar{E},\bar{n}_i)]'}{[\{[\bar{S}_{20}(\bar{E},\bar{n}_i)]\}^2 + 4\bar{S}_{19}\bar{S}_{21}(\bar{E},\bar{n}_i)]^{1/2}}\right],$$

Thus, one can observe that EEM in this case is a function of both the Fermi energy and the nipi subband index number together with the spectrum constants of the system due to the presence of band nonparabolicity.

The subband energies $(\bar{E}_{10n_i})$ can be written as

$$\left[\bar{E}_{10n_i} - \frac{\hbar^2}{2\bar{m}_l^{-}}\bar{T}(\bar{E}_{10n_i})\left(\bar{n}_i+\frac{1}{2}\right)\right]\left[1+\alpha\bar{E}_{10n_i} + \alpha\frac{\hbar^2}{2\bar{m}_l^{+}}\bar{T}(\bar{E}_{10n_i})\left(\bar{n}_i+\frac{1}{2}\right)\right]$$
$$= \left[\frac{\hbar^2}{2\bar{m}_l^{*}}\bar{T}(\bar{E}_{10n_i})\left(\bar{n}_i+\frac{1}{2}\right)\right] \tag{11.47}$$

The DOS function in this case assumes the form as

$$\bar{N}_{nipi}(\bar{E}) = \frac{g_v}{\pi\hbar^2}\sum_{\bar{n}_i=0}^{\bar{n}_{i_{\max}}}\bar{R}_{84}(\bar{E},n_i)\bar{H}(\bar{E}-\bar{E}_{10n_i}) \tag{11.48a}$$

The electron concentration in this case can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\left[\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{R}_{84}(\bar{E}_{Fn},\bar{n}_i) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})\left[\bar{R}_{84}(\bar{E}_{Fn},\bar{n}_i)\right]\right]\right] \tag{11.48b}$$

Using (1.44) and (11.48b) we can study the entropy in this case.

11.2.5 Entropy in doping superlattices of HD stressed Kane-type materials

The 2D DR in this case is given by

$$\bar{P}_{11}(\bar{E},\eta_g)\bar{k}_x^2 + Q_{11}(\bar{E},\eta_g)\bar{k}_y^2 + \bar{S}_{11}(\bar{E},\eta_g)\delta_{19}(\bar{E},\eta_g,\bar{n}_i) = 1 \tag{11.49}$$

where,

$$\delta_{19}(\bar{E},\eta_g,\bar{n}_i) = \frac{2}{\hbar}\bar{m}_{zz}^{*}(0,\eta_g)\left(\bar{n}_i + \frac{1}{2}\right)\left[\frac{\bar{n}_i e^2}{\bar{d}_0\varepsilon_{sc}\bar{m}_{zz}(\bar{E},\eta_g)}\right]^{1/2}$$

The EEM in this case assumes the form

$$\bar{m}^{*}(\bar{F}_{FnHD},\bar{n}_i,\eta_g) = \left(\frac{\hbar^2}{2}\right)\delta'_{20}(\bar{E}_{FnHD},\eta_g,\bar{n}_i) \tag{11.50}$$

where

$$\delta_{20}(\bar{E}_{FnHD},\eta_g,\bar{n}_i) = \frac{[1-\bar{S}_{11}(\bar{E}_{FnHD},\eta_g,\bar{n}_i)\delta_{19}(\bar{E}_{FnHD},\eta_g,\bar{n}_i)]}{\sqrt{\bar{P}_{11}(\bar{E}_{FnHD},\eta_g)\bar{Q}_{11}(\bar{E}_{FnHD},\eta_g)}}$$

The sub-band energy $\bar{E}_{15n_iHD}$ can be expressed in this case as

$$\bar{S}_{11}(\bar{E}_{15n_iHD},\eta_g)\delta_{19}(\bar{E}_{15n_iHD},\eta_g,\bar{n}_i) = 1 \tag{11.51}$$

The DOS function in this case is given by

$$\bar{N}_{nipiHD}(\bar{E}) = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}[\delta_{20}(\bar{E},\eta_g,\bar{n}_i)]'\bar{H}(\bar{E}-\bar{E}_{15n_iHD}) \tag{11.52a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\delta_{20}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i) + \sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\delta_{20}(\bar{E}_{FnHD},\bar{\eta}_g,\bar{n}_i)]\right] \tag{11.52b}$$

Using (1.31f) and (12.52b), we can study the entropy in this case

The electron dispersion law in the doping superlatticesof stressed Kane-type materials can be written as

$$\frac{\bar{k}_x^2}{\left[\bar{a}_0(\bar{E})\right]^2}+\frac{\bar{k}_y^2}{\left[\bar{b}_0(\bar{E})\right]^2}+\frac{1}{\left[\bar{c}_0(\bar{E})\right]^2}\frac{2\bar{m}_z^*(0)}{\hbar}\left(\bar{n}_i+\frac{1}{2}\right)\omega_{12}(\bar{E})=1 \tag{11.53}$$

where $\omega_{12}(\bar{E})\equiv\left(\frac{\bar{n}_0|e|^2}{d_0\varepsilon_{sc}\bar{m}_z^*(\bar{E})}\right)^{\frac{1}{2}}$ and $\bar{m}_z^*(\bar{E})\equiv\hbar^2\bar{c}_0(\bar{E})\frac{\partial}{\partial\bar{E}}\left[\bar{c}_0(\bar{E})\right]$

The use of (11.53) leads to the expression of EEM as

$$\bar{m}^*(\bar{E}_{Fn},\bar{n}_i)=\left(\frac{\hbar^2}{2}\right)\bar{R}_{85}(\bar{E},\bar{n}_i)|_{\bar{E}=\bar{E}_{Fn}} \tag{11.54}$$

where

$$\begin{aligned}\bar{R}_{85}(\bar{E},\bar{n}_i)\equiv&\left[\left(\bar{a}_0(\bar{E})\right)'\bar{b}_0(\bar{E})+\left(\bar{b}_0(\bar{E})\right)'\bar{a}_0(\bar{E})\right]\left[1-\frac{1}{\left[\bar{c}_0(\bar{E})\right]^2}\frac{2\bar{m}_z^*(0)}{\hbar}\left(\bar{n}_i+\frac{1}{2}\right)\omega_{12}((\bar{E}))\right]\\&-\left[\frac{\bar{a}_0(\bar{E})\bar{b}_0(\bar{E})}{\left[\bar{c}_0(\bar{E})\right]^2}\frac{2\bar{m}_z^*(0)}{\hbar}\left(\bar{n}_i+\frac{1}{2}\right)\left[\omega_{12}(\bar{E})\right]'\right]\\&+\left[\frac{\bar{a}_0(\bar{E})\bar{b}_0(E)\left[\bar{c}_0(\bar{E})\right]'}{\left[\bar{c}_0(\bar{E})\right]^3}\frac{4\bar{m}_z^*(0)}{\hbar}\left(\bar{n}_i+\frac{1}{2}\right)\left[\omega_{12}(\bar{E})\right]\right]\end{aligned} \tag{11.55}$$

Thus, EEM is a function of the Fermi energy and the nipisubband index due to the presence of stress and band nonparabolicity only.

The subband energies $(\bar{E}_{25n_i})$ can be written as

$$\frac{1}{\left[\bar{c}_0(\bar{E}_{25n_i})\right]^2}\frac{2\bar{m}_z^*(0)}{\hbar}\left(\bar{n}_i+\frac{1}{2}\right)\omega_{12}(\bar{E}_{25n_i})=1 \tag{11.56}$$

The DOS function can be written as

$$\bar{N}_{nipi}(\bar{E})=\frac{\bar{g}_v}{\pi\hbar^2}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\bar{R}_{85}(\bar{E},\bar{n}_i)\bar{H}(\bar{E}-\bar{E}_{25n_i}) \tag{11.57}$$

The electron concentration in this case can be written as

$$\bar{n}_0=\frac{\bar{g}_v}{2\pi}\sum_{\bar{n}_i=0}^{\bar{n}_{i\max}}\left[\bar{R}_{85}(\bar{E}_{Fn},\bar{n}_i)+\sum_{\bar{r}=1}^{\bar{s}}\bar{L}(\bar{r})[\bar{R}_{85}(\bar{E}_{Fn},\bar{n}_i)]\right] \tag{11.58}$$

Using (1.44) and (11.58), we can study the entropy in this case.

11.3 Open research problems

R.11.1 Investigate the entropy in the presence of an arbitrarily oriented nonquantizing magnetic field for nipi structures of HD nonlinear optical materials by including the electron spin. Study all the special cases for HD III–V, ternary, and quaternary materials in this context.

R.11.2 Investigate the entropy s in nipi structures of HD IV–VI, II–VI, and stressed Kane-type compounds in the presence of an arbitrarily oriented nonquantizing magnetic field by including the electron spin.

R.11.3 Investigate the entropy for HD nipi structures of all the materials as stated in this chapter in the presence of nonuniform strain.

R.11.4 Investigate the entropy for all the problems from R.11.1 to R.11.3 in the presence of an additional arbitrarily oriented electric field.

R.11.5 Investigate the entropy for all the problems from R.11.1 to R.11.5 in the presence of arbitrarily oriented crossed electric and magnetic fields.

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12 Appendix C: Entropy in QWHDSLs under magnetic quantization

The Smallest deeds always exceed the grandest of intentions.

12.1 Introduction

In this chapter, the magneto entropy in III–V, II–VI, IV–VI, HgTe/CdTe, and strained layer quantum well heavily doped superlattices (QWHDSLs) with graded interfaces [1–10] has been studied in Sections 12.2.1–12.2.5 From Sections 12.2.6–12.2.10, the magnetoentropy in III–V, II–VI, IV–VI, HgTe/CdTe, and strained layer quantum well HD effective mass superlattices, respectively, has been presented. This appendix presents four open research problems.

12.2 Theoretical background

12.2.1 Entropy in III–V QWHDSLs with graded interfaces under magnetic quantization

The entropy in HD quantum well III–V superlattices under magnetic quantization assumes the form

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{G}_{8E_{41,n}} + i\bar{H}_{8E_{41,n}} \tag{12.1}$$

where $\bar{E}_{41,n}$ is the totally quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\left(\frac{\bar{g}_v e\bar{B}}{\pi\hbar}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_z=0}^{\bar{n}_{\max}}\delta'(\bar{E}-\bar{E}_{41,n}) \tag{12.2a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\text{Re}al\ Part\ of\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{41,n}) \tag{12.2b}$$

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Where

$$\eta_{41,n} = \frac{\bar{E}_{F41,n} - \bar{E}_{41,n}}{\bar{k}_B \bar{T}}$$

and $\bar{E}_{F41,n}$ is the fermic energy in this case.

Using (1.31f) and (12.2b), we can study the entropy in this case.

12.2.2 Entropy in II–VI quantum well HD superlattices with graded interfaces under magnetic quantization

The entropy in quantum well HD II–VI superlattices under magnetic quantization assumes the form

$$\left(\frac{\bar{n}_z \pi}{\bar{d}_z}\right)^2 = \bar{G}_{19E_{42,n}} + i\bar{H}_{19E_{42,n}} \tag{12.3}$$

Where $\bar{E}_{42,n}$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\left(\frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\right)\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_z=0}^{\bar{n}_{\max}}\delta'(\bar{E} - \bar{E}_{42,n}) \tag{12.4a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{42,n}) \tag{12.4b}$$

where

$$\eta_{42,n} = \frac{\bar{E}_{F42,n} - \bar{E}_{42,n}}{\bar{k}_B \bar{T}}$$

and $\bar{E}_{F42,n}$ is the fermic energy in this case.

Using (1.31f) and (12.4b) we can study the entropy in this case.

12.2.3 Entropy in IV–VI quantum well HD superlattices with graded interfaces under magnetic quantization

The entropy in quantum well HD quantum well IV–VI superlattices under magnetic quantization assumes the form

$$\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\varphi_2(\bar{E}_{43,n}, n)\right\}\right]^2 - \frac{2|e|\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \tag{12.5}$$

where $\bar{E}_{42,n}$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_z=0}^{\bar{n}_{\max}}\delta'(\bar{E}-\bar{E}_{43,n}) \tag{12.6a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v eB}{\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{43,n}) \tag{12.6b}$$

where

$$\eta_{43,n} = \frac{\bar{E}_{F43,n} - \bar{E}_{43,n}}{\bar{k}_B\bar{T}}$$

and $\bar{E}_{F43,n}$ is the Fermi energy in this case.

Using (1.31f) and (12.6b) we can study the entropy in this case.

12.2.4 Entropy in HgTe/CdTe quantum well HD superlattices with graded interfaces under magnetic quantization

The entropy in quantum well HD HgTe/CdTe superlatices under magnetic quantization assumes the form

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \bar{G}_{192E_{44,n}} + i\bar{H}_{192E_{44,n}} \tag{12.7}$$

Where $\bar{E}_{44,n}$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_z=0}^{\bar{n}_{\max}}\delta'(\bar{E}-\bar{E}_{44,n}) \tag{12.8a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\text{Real Part of}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{44,n}) \tag{12.8b}$$

where

$$\eta_{44,n} = \frac{\bar{E}_{F44,n} - \bar{E}_{44,n}}{\bar{k}_B \bar{T}}$$

and $\bar{E}_{F44,n}$ is the fermic energy in this case.

Using (1.31f) and (12.8b), we can study the entropy in this case.

12.2.5 Entropy in strained layer quantum well HD superlattices with graded interfaces under magnetic quantization

The entropy of the conduction electrons in HD quantum well strained layer SLs with graded interfaces can be expressed as

$$\left(\frac{\pi \bar{n}_z}{\bar{d}_z}\right)^2 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\varphi_6(\bar{E}_{47,n}, n)\right\}\right]^2 - \frac{2|e|B}{\hbar}\left(\bar{n} + \frac{1}{2}\right) \tag{12.9}$$

where $\bar{E}_{47,n}$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E}) \frac{\bar{g}_v e\bar{B}}{2\pi\hbar} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \sum_{\bar{n}_z=0}^{\bar{n}_{\max}} \delta'(\bar{E} - \bar{E}_{47,n}) \tag{12.10a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \sum_{\bar{n}=1}^{\bar{n}_{\max}} \bar{F}_{-1}(\eta_{47,n}) \tag{12.10b}$$

where

$$\eta_{47,n} = \frac{\bar{E}_{F47,n} - \bar{E}_{47,n}}{\bar{k}_B \bar{T}}$$

and $\bar{E}_{F47,n}$ is the fermic energy in this case.

Using (1.31f) and (12.10b), we can study the entropy in this case.

12.2.6 Entropy in III–V quantum well HD effective mass super lattices under magnetic quantization

The dispersion relation in quantum well HD III–V superlattices under magnetic quantization assumes the form

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \delta_{7A1,n} + i\delta_{8A1,n} \tag{12.11}$$

where $\bar{A}1$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=0}^{\bar{n}_{\max}}\delta'(\bar{E}-A1) \tag{12.12a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v eB}{\pi\hbar}\text{Re}al\ Part\ of\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\bar{\eta}_{A1}) \tag{12.12b}$$

where

$$\bar{\eta}_{A1} = \frac{\bar{E}_{FA1}-\bar{E}_{A1}}{\bar{k}_B\bar{T}}$$

and $\bar{E}_{FA1}$ is the fermic energy in this case.

Using (1.31f) and (12.12b) we can study the entropy in this case.

12.2.7 Entropy in II–VI quantum well HD effective mass super lattices under magnetic quantization

The dispersion relation in quantum well HD III–V superlattices under magnetic quantization assumes the form

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \Delta_{13A2,n} + i\Delta_{13A2,n} \tag{12.13}$$

where $\bar{A}2$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_z=0}^{\bar{n}_{\max}}\delta'(\bar{E}-A2) \tag{12.14a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v eB}{\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{A2}) \tag{12.14b}$$

where

$$\eta_{A2} = \frac{\bar{E}_{FA2} - \bar{E}_{A2}}{\bar{k}_B \bar{T}}$$

and $\bar{E}_{FA2}$ is the fermic energy in this case.

Using (1.31f) and (12.14b), we can study the entropy in this case.

12.2.8 Entropy in IV–VI quantum well HD effective mass super lattices under magnetic quantization

The entropy of the conduction electrons in HD quantum well strained layer SLs with graded interfaces can be expressed as

$$\left(\frac{\pi \bar{n}_z}{\bar{d}_z}\right)^2 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2} f_{23}(A3, n)\right\}\right]^2 - \frac{2|e|\bar{B}}{\hbar}\left(\bar{n} + \frac{1}{2}\right) \tag{12.15}$$

where $\bar{A}3$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E}) \frac{\bar{g}_v e\bar{B}}{2\pi\hbar} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \sum_{\bar{n}_z=0}^{\bar{n}_{\max}} \delta'(\bar{E} - \bar{A}3) \tag{12.16a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar} \sum_{\bar{n}_z=1}^{\bar{n}_{z\max}} \sum_{\bar{n}=1}^{\bar{n}_{\max}} \bar{F}_{-1}(\eta_{A3}) \tag{12.16b}$$

where

$$\eta_{43,n} = \frac{\bar{E}_{F43,n} - \bar{E}_{43,n}}{\bar{k}_B \bar{T}}$$

and $\bar{E}_{FA3}$ is the fermic energy in this case.

Using (1.31f) and (12.16b), we can study the entropy in this case.

12.2.9 Entropy in HgTe/CdTe quantum well HD effective mass super lattices under magnetic quantization

The entropy in quantum well HD III–V superlattices under magnetic quantization assumes the form

$$\left(\frac{\bar{n}_z\pi}{\bar{d}_z}\right)^2 = \Delta_{13A4,n} + i\Delta_{13A4,n} \tag{12.17}$$

where $\bar{A}4$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_z=0}^{\bar{n}_{\max}}\delta'(\bar{E}-A4) \tag{12.18a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\text{Re}al\ Part\ of\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{A4}) \tag{12.18b}$$

where

$$\eta_{A4} = \frac{\bar{E}_{FA4}-\bar{E}_{A4}}{\bar{k}_B\bar{T}}$$

and $\bar{E}_{FA4}$ is the fermic energy in this case.

Using (1.31f) and (12.18b), we can study the entropy in this case.

12.2.10 Entropy in strained layer quantum well HD effective mass super lattices under magnetic quantization

Entropy of the conduction electrons in HD quantum well strained layer SLs with graded interfaces can be expressed as

$$\left(\frac{\pi\bar{n}_z}{\bar{d}_z}\right)^2 = \frac{1}{\bar{L}_0^2}\left[\cos^{-1}\left\{\frac{1}{2}\bar{f}_{40}(\bar{A}8,\bar{n})\right\}\right]^2 - \frac{2|e|\bar{B}}{\hbar}\left(\bar{n}+\frac{1}{2}\right) \tag{12.19}$$

where $\bar{A}8$ is the totlly quantized energy in this case.

The DOS function in this case can be expressed as

$$\bar{N}_{MQWSL}(\bar{E})\frac{\bar{g}_v e\bar{B}}{2\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}_z=0}^{\bar{n}_{\max}}\delta'(\bar{E}-A8) \tag{12.20a}$$

The electron concentration can be written as

$$\bar{n}_0 = \frac{\bar{g}_v e\bar{B}}{\pi\hbar}\sum_{\bar{n}_z=1}^{\bar{n}_{z\max}}\sum_{\bar{n}=1}^{\bar{n}_{\max}}\bar{F}_{-1}(\eta_{A8}) \tag{12.20b}$$

where

$$\eta_{A8} = \frac{\bar{E}_{FA8} - \bar{E}_{A8}}{\bar{k}_B \bar{T}}$$

and $\bar{E}_{FA8}$ is the fermic energy in this case.

Using (1.31f) and (12.20b), we can study the entropy in this case.

12.3 Open research problems

R.12.1 Investigate the magneto entropy in the presence of an arbitrarily oriented nonquantizing magnetic field in III–V, II–VI, IV–VI, HgTe/CdTe, and strained layerHD quantum well superlattices with graded interfacesby including the electron spin.

R.12.2 Investigate the magneto entropy in III–V, II–VI, IV–VI, HgTe/CdTe, and strained layer HD effective mass quantum well superlattices in the presence of an arbitrarily oriented nonquantizing magnetic field by including the electron spin.

R.12.3 Investigate the entropy for all the problems from R.12.1 to R.12.2 in the presence of an additional arbitrarily oriented electric field.

R.12.4 Investigate the entropy for all the problems from R.12.1 to R.12.3 in the presence of arbitrarily oriented crossed electric and magnetic fields.

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13 Appendix D: Entropy in accumulation and inversion layers of non-parabolic materials

Excellence is nothing but an attitude of mind.

13.1 Introduction

It is well known that the electrons in bulk materials in general, have three dimensional freedom of motion. When, these electrons are confined in a one dimensional potential well whose width is of the order of the carrier wavelength, the motion in that particular direction gets quantized while that along the other two directions remains as free. Thus, the energy spectrum appears in the shape of discrete levels for the one dimensional quantization, each of which has a continuum for the two dimensional free motion. The transport phenomena of such one dimensional confined carriers have recently studied [1–30] with great interest. For the metal-oxide-materials (MOS) structures, the work functions of the metal and the materials substrate are different and the application of an external voltage at the metal-gate causes the change in the charge density at the oxide materials interface leading to a bending of the energy bands of the materials near the surface. As a result, a one dimensional potential well is formed at the materials interface. The spatial variation of the potential profile is so sharp that for considerable large values of the electric field, the width of the potential well becomes of the order of the de Broglie wavelength of the carriers. The Fermi energy, which is near the edge of the conduction band in the bulk, becomes nearer to the edge of the valance band at the surface creating accumulation layers. The energy levels of the carriers bound within the potential well get quantized and form electric subbands. Each of the subband corresponds to a quantized level in a plane perpendicular to the surface leading to a quasi two dimensional electron gas. Thus, the extreme band bending at low temperature allows us to observe the quantum effects at the surface. Though considerable work has already been done, nevertheless it appears from the literature that the entropy in accumulation layers of non-parabolic Materials has yet to be investigated in details. For the purpose of comparison we shall also study the entropy for inversion layers of non-parabolic compounds.

In what follows in Section 13.2.1, of the theoretical background, the entropy in accumulation and Inversion layers of nonlinear optical materials has been studied under weak electric field limit. Section 13.2.2 contains the results for accumulation and Inversion layers of III-V, ternary and quaternary materials for the weak electric field limit whose bulk electrons obey the three and the two band models of Kane together with parabolic energy bands and they form the special cases of Section 13.2.1. Section 13.2.3 contains the study of the entropy for accumulation and Inversion layers of II-VI Materials, which is valid for all values of electric field. Sections 13.2.4 and

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13.2.5 contain the study of the entropy in accumulation and inversion layers of IV–VI and stressed materials respectively. Section 13.2.6 contains the study of the entropy in accumulation and inversion layers of Ge. This appendix contains 12 open research problems.

13.2 Theoretical background

13.2.1 The entropy in accumulation and inversion layers of non-linear optical materials

In the presence of a surface electric field $\overline{F}_s$ along $\overline{z}$ direction and perpendicular to the surface, (1.26) assumes the form

$$\frac{\hbar^2\overline{k}_z^2}{2\overline{m}_{||}^*}+\frac{\hbar^2\overline{k}_s^2}{2\overline{m}_{\perp}^*}\frac{\overline{T}_{21}(\overline{E}-|e|\overline{F}_s\overline{z},\eta_g)}{\overline{T}_{22}(\overline{E}-|e|\overline{F}_s\overline{z},\eta_g)}=\overline{T}_{21}(\overline{E}-|e|\overline{F}_s\overline{z},\eta_g) \tag{13.1}$$

where, for this chapter, $\overline{E}$ represents the electron energy as measured from the edge of the conduction band at the surface in the vertically upward direction.

The quantization rule for 2D carriers in this case, is given by [5]

$$\int_0^{\overline{z}_t}\overline{k}_z\overline{dz}=\frac{2}{3}(\overline{S}_i)^{3/2} \tag{13.2}$$

where, $\overline{z}_t$ is the classical turning point and $\overline{S}_i$ is the zeros of the Airy function $(\overline{Ai}(-\overline{S}_i)=0)$.

Using (13.1) and (13.2) leads to the DRof the 2D electrons in accumulation layers of HD non-linear optical materials under the condition of weak electric field limit as

$$\frac{\hbar^2\overline{k}_s^2}{2\overline{m}_{||}^*}=\overline{L}_6(\overline{E},i,\eta_g) \tag{13.3}$$

where

$$\overline{L}_6(\overline{E},i,\eta_g)=\frac{\overline{T}_{21}(\overline{E},\eta_g)-\overline{L}_3(\overline{E},i,\eta_g)}{\overline{L}_4(\overline{E},\overline{i},\eta_g)},\overline{L}_3(\overline{E},i,\eta_g)=\overline{S}_i[\overline{T'}_{21}(\overline{E},\eta_g)]^{2/3}\left[\frac{\hbar|e|\overline{F}_s}{\sqrt{2m_{||}^*}}\right]^{2/3}$$

and

$$\overline{L}_4(\overline{E},i,\eta_g)\left[\frac{\overline{T}_{21}(\overline{E},\eta_g)}{\overline{T}_{22}(\overline{E},\eta_g)}+\overline{L}_3(\overline{E},i,\eta_g)\frac{\overline{T}_{21}(\overline{E},\eta_g)}{\overline{T'}_{21}(\overline{E},\eta_g)T_{22}(\overline{E},\eta_g)}.\frac{2}{3}\left\{\frac{\overline{T'}_{21}(\overline{E},\eta_g)}{\overline{T}_{21}(\overline{E},\eta_g)}-\frac{\overline{T'}_{22}(\overline{E},\eta_g)}{\overline{T}_{22}(\overline{E},\eta_g)}\right\}\right]$$

The EEM in this case can be written as

$$\overline{m}^{*}(\overline{E}'_f, i, \eta_g) = \overline{m}^{*}_{||}\text{Re}\, al\ part\ of\ [\overline{L}'_6(\overline{E}'_f, i, \eta_g)] \tag{13.4}$$

where

$$\overline{E}'_f = eV_g - \frac{e^2\overline{n}_s\overline{d}_{ex}}{\varepsilon_{ox}} + \overline{E}_{FB},$$

V_g is the gate voltage, n_s is the surface electron concentration, $\overline{d}_{ox}$ is the thickness of the oxide layer, ε_{ox} is the permittivity of the oxide layer, $\overline{F}_s = \frac{e\overline{n}_s}{\varepsilon_{sc}}$, ε_{sc} is the materials permittivity and $\overline{E}_{FB}$ should be determined from the equation

$$\overline{n}_B = \frac{2\overline{g}_v}{(2\pi)^3}\frac{2\overline{m}^{*}_{\perp}\sqrt{2\overline{m}^{*}_{||}}}{\hbar^3}\ Real\ Part\ of\ \left[\overline{T}_{22}(\overline{E}_{FB}, \eta_g)\sqrt{\overline{T}_{21}(\overline{E}_{FB}, \eta_g)}\right] \tag{13.5}$$

and $\overline{n}_B$ is the bulk electron concentration.

The sub-band energy $\overline{E}_i$ can be determined from the equation

$$0 = \text{Real part of } \overline{L}_6(\overline{E}_i, i, \eta_g) \tag{13.6}$$

The surface electron concentration in the regime of very low temperatures where the quantum effects become prominent can be written as

$$\overline{n}_s = 2\overline{g}_v\ Real\ part\ of\ the\ \sum_{i=0}^{i_{\max}}\left[\left[\frac{\overline{m}^{*}_{\perp}}{2\pi\hbar^2}\overline{L}_6(\overline{E}'_f, i, \eta_g)\right] + \frac{1}{(2\pi)^3}\frac{2\overline{m}^{*}_{\perp}\sqrt{2\overline{m}^{*}_{||}}}{\hbar^3}\overline{t}_i\overline{n}_B\right.$$
$$\left. = \frac{2\overline{g}_v}{(2\pi)^3}\frac{2\overline{m}^{*}_{\perp}\sqrt{2\overline{m}^{*}_{||}}}{\hbar^3}\left[\overline{T}_{22}(\overline{E}_{FB}, \eta_g)\sqrt{\overline{T}_{21}(\overline{E}_{FB}, \eta_g)}\right]\right] \tag{13.7}$$

where $\overline{t}_i = \frac{\overline{E}_{i\max}}{\overline{e}\overline{F}_s(1+\overline{i}_{\max})}$, $\overline{E}_{i\max}$, is the root of the Real part of the equation

$$\overline{T}_{21}(\overline{E}_{i\max}, \eta_g) - \overline{L}_3(\overline{E}_{i\max}, i_{\max}, \eta_g) = 0 \tag{13.8a}$$

Using (1.31f) and (13.7) we can study the entropy in this case.

In what follows, we shall discuss the entropy in inversion layers of non-linear optical materials for the purpose of relative comparison. In the presence of a surface electric field F_s along z direction and perpendicular to the surface, the (2.2) assumes the form

$$\overline{\psi}_1(\overline{E} - |e|\overline{F}_s\overline{z}) = \psi_2(\overline{E} - |e|\overline{F}_s\overline{z})\overline{k}_s^2 + \psi_3(\overline{E} - |e|\overline{F}_s\overline{z})\overline{k}_z^2 \tag{13.8b}$$

where,

$$\psi_1(\overline{E}) = \gamma(\overline{E}), \psi_2(\overline{E}) = \overline{f}_2(\overline{E}) \text{ and } \psi_3(\overline{E}) = \overline{f}_2(\overline{E})$$

Using (13.2) and (13.8b), under the weak electric field limit, one can write,

$$\int_0^{\overline{z}_t} \sqrt{\overline{A}_7(\overline{E}) - |e|\overline{F}_s \overline{z}\overline{D}_7(\overline{E})}\, d\overline{z} = \frac{2}{3}(\overline{S}_i)^{3/2} \tag{13.9}$$

in which,

$$\overline{A}_7(\overline{E}) \equiv \left[\frac{\psi_1(\overline{E}) - \psi_2(\overline{E})\overline{k}_s^2}{\psi_3(\overline{E})}\right] \overline{D}_7(\overline{E}) \equiv \left[\overline{B}_7(\overline{E}) - \overline{A}_7(\overline{E})\overline{C}_7(\overline{E})\right],$$

$$\overline{B}_7(\overline{E}) \equiv \left[\frac{(\psi_1(\overline{E}))' - (\psi_2(\overline{E}))'\overline{k}_s^2}{\psi_3(\overline{E})}\right] \text{and } \overline{C}_7(\overline{E}) \equiv \left[\frac{(\psi_3(\overline{E}))'}{\psi_3(\overline{E})}\right].$$

Thus, the 2D electron dispersion law in inversion layers of nonlinear optical materials under the weak electric field limit can approximately be written as

$$\psi_1(\overline{E}) = \overline{P}_7(\overline{E}, i)\overline{k}_s^2 + \overline{Q}_7(\overline{E}, i) \tag{13.10}$$

where,

$$\overline{P}_7(\overline{E}, i) \equiv \left[\psi_2(\overline{E}) - \left(\frac{2\overline{t}_2(\overline{E})}{3[\overline{t}_1(\overline{E})]^{1/3}}\right)\psi_3(\overline{E})\overline{S}_i(|e|\overline{F}_2)^{2/3}\right],$$

$$\overline{t}_2(\overline{E}) \equiv \left[\frac{[\psi_2(\overline{E})]'}{\psi_3(\overline{E})} - \left(\frac{\psi_2(\overline{E})[\psi_3(\overline{E})]'}{[\psi_3(\overline{E})]^2}\right)\right], \overline{t}_1(\overline{E}) = \left[\frac{[\psi_1(\overline{E})]'}{\psi_3(\overline{E})} - \left(\frac{\psi_3(E)[\psi_3(\overline{E})]'}{[\psi_3(\overline{E})]^2}\right)\right]$$

and

$$\overline{Q}_7(\overline{E}, i) \equiv \overline{S}_i\psi_3(\overline{E})[|e|\overline{F}_s\overline{t}_1(\overline{E})]^{2/3}.$$

The EEM in the x–y plane can be expressed as

$$\overline{m}^*(\overline{E}_{Fiw}, i) = \left(\frac{\hbar^2}{2}\right)\overline{G}_7(\overline{E}, i)\Big|_{\overline{E}=\overline{E}_{Fw}} \tag{13.11}$$

where,

$$\overline{G}_7(\overline{E}, i) \equiv [\overline{P}_7(\overline{E}, i)]^{-2}\left[\overline{P}_7(\overline{E}, i)\left\{(\psi_1(\overline{E}))' - (\overline{Q}_7(\overline{E}, i))'\right\} - \left\{\psi_1(\overline{E}) - (\overline{Q}_7(\overline{E}, i))\right\}(\overline{P}_7(\overline{E}, i))'\right]$$

and $\overline{E}_{Fiw}$ is the Fermi energy under the weak electric field limit as measured from the edge of the conduction band at the surface in the vertically upward direction. Thus, we observe that EEM is the function of subband index, the Fermi energy and

other band constants due to the combined influence of the crystal filed splitting constant and the anisotropic spin-orbit splitting constants, respectively.

The subband energy ($\overline{E}_{n_{iw1}}$) in this case can be obtained from (13.10) as

$$\psi_1(\overline{E}_{n_{iw1}}) = \overline{Q}_7(\overline{E}_{n_{iw1}}, i) \tag{13.12}$$

The general expression of the 2D total DOS function in this case can be written as

$$\overline{N}_{2D_i}(\overline{E}) = \frac{2\overline{g}_v}{(2\pi)^2}\sum_{i=0}^{i_{\max}} \frac{\partial}{\partial \overline{E}}\left[\overline{A}(\overline{E}, i)\overline{H}(\overline{E} - \overline{E}_{n_i})\right] \tag{13.13}$$

where $\overline{A}(\overline{E}, i)$ is the area of the constant energy 2D wave vector space for inversion layers and $\overline{E}_{n_i}$ is the corresponding subband energy.

Using (13.10) and (13.13), the total 2D DOS function under the weak electric field limit can be expressed as

$$\overline{N}_{2D_i}(\overline{E}) = \frac{\overline{g}_v}{(2\pi)^2}\sum_{i=0}^{i_{\max}} \left[\overline{G}_7(\overline{E}, i)\overline{H}(\overline{E} - \overline{E}_{n_{iw1}})\right] \tag{13.14a}$$

The electron concentration in this case can be written as

$$\overline{n}_0 = \frac{\overline{g}_v}{(2\pi)}\sum_{i=0}^{i_{\max}}\left[\overline{G}_7(\overline{E}_{Fiw}) + \sum_{\overline{r}=1}^{\overline{s}}\overline{L}(\overline{r})\left[\overline{G}_7(\overline{E}_{Fiw})\right]\right] \tag{13.14b}$$

Using (1.31f) and (13.13b) we can study the entropy in this case.

13.2.2 Entropy in accumulation and inversion layers of III–V, ternary, and quaternary materials

(a) Using the substitutions $\delta = 0$, $\Delta_{||} = \Delta_{\perp} = \Delta$ and $\overline{m}^*_{||} = \overline{m}^*_{\perp} = \overline{m}_c$, (13.3) under the condition of weak electric field limit, assumes the form

$$\overline{T}_{90}(\overline{E}, \eta_g) = \frac{\hbar^2\overline{k}_s^2}{2\overline{m}_c} + \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s\left[\overline{T}_{90}(\overline{E}, \eta_g)\right]}{\sqrt{2\overline{m}_c}}\right]^{2/3} \tag{13.15}$$

where,

$$\overline{T}_{90}(\overline{E}, \eta_g) = \overline{T}_{31}(\overline{E}, \eta_g) + i\overline{T}_{32}(\overline{E}, \eta_g)$$

(13.15) represents the entropy of the 2D electrons in accumulation layers of HD III–V, ternary and quaternary materials under the weak electric field limit whose bulk electrons obey the HD three-band model of Kane. Since the electron energy

spectrum in accordance with the HD three-band model of Kane is complex in nature, (13.15) will also be complex. The both complexities occur due to the presence of poles in the finite complex plane of the dispersion relation of the materials in the absence of band tails.

The EEM can be expressed as

$$\overline{m}^{*}(\overline{E'}_f, i, \eta_g) = \overline{m}_c \ \textit{Real part of} \ \overline{P'}_{3HD}(\overline{E'}_f, i, \eta_g) \tag{13.16}$$

where,

$$\overline{P}_{3HD}(\overline{E'}_f, i, \eta_g) = \left[\overline{T}_{90}(\overline{E'}_f, i, \eta_g) - \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s[\overline{T}_{90}(\overline{E'}_f, \eta_g)]'}{\sqrt{2\overline{m}_c}}\right]^{2/3}\right]$$

Thus, one can observe that the EEM is a function of the subband index, surface electric field, the Fermi energy and the other spectrum constants due to the combined influence of E_g and Δ.

The subband energy $\overline{E}_{i1}$ is given by

$$0 = \ \textit{Real part of} \ \left[\overline{T}_{90}(\overline{E}_{i1}, \eta_g) - \overline{S}_i\left[\hbar|e|\overline{F}_s\left[\overline{T}_{90}(\overline{E}_{i1}, \eta_g)\right]'.(2\overline{m}_c)^{-1/2}\right]^{2/3}\right] \tag{13.17}$$

The DOS function can be written as

$$\overline{N}_{2D_i}(E) = \frac{\overline{m}_c\overline{g}_v}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}\left[\overline{P}_{3HD}(\overline{E}, i, \eta_g)\overline{H}(\overline{E} - \overline{E}_{i1})\right] \tag{13.18}$$

Thus the DOS function is complex in nature.

The surface electron concentration is given by

$$\overline{n}_S\ \overline{g}_v\ \textit{Real part of the} \sum_{i=0}^{i_{\max}}\left[\left[\frac{\overline{m}_c}{\pi\hbar^2}\overline{P}_{3HD}(\overline{E'}_f, \overline{i}, \eta_g)\right] + \frac{1}{3\pi^2}\left(\frac{2\overline{m}_c}{\hbar^2}\right)^{3/2}\overline{t}_i\left[\overline{T}_{90}(\overline{E}_{FB}, \eta_g)\right]^{3/2}\right] \tag{13.19}$$

where $\overline{E}_{FB}$ should be determined from the following equation

$$\overline{n}_B = \frac{\overline{g}_v}{3\pi^2}\left(\frac{2\overline{m}_c}{\hbar^2}\right)^{3/2}\textit{Real part of the}\ [\overline{T}_{90}(\overline{E}_{FB}, \eta_g)]^{3/2} \tag{13.20}$$

Using (1.31f) and (13.19) we can study the entropy in this case.

Using the substitutions $\delta = 0$, $\Delta_{||} = \Delta_{\perp} = \Delta$ and $\overline{m}^{*}_{||} = \overline{m}^{*}_{\perp} = \overline{m}_c$, (13.10) under the condition of weak electric field limit, assumes the form

$$\overline{I}_{11}(\overline{E}) = \frac{\hbar^2 \overline{k}_s^2}{2\overline{m}_c} + \overline{S}_i \left[\frac{\hbar |e| \overline{F}_s [\overline{I}_{11}(\overline{E})]}{\sqrt{2\overline{m}_c}} \right]^{2/3} \tag{13.21}$$

(13.21) represents the dispersion relation of the 2D electrons in inversion layers of III–V, ternary and quaternary materials under the weak electric field limit whose bulk electrons obey the three-band model of Kane.

The EEM can be expressed as

$$\overline{m}^*(\overline{E}_{Fiw}, i) = \overline{m}_c [\overline{P}_3(\overline{E}, i)] \Big|_{\overline{E} = \overline{E}_{Fiw}} \tag{13.22}$$

where,

$$\overline{P}_3(\overline{E}, i) = \left\{ [\overline{I}_{11}(\overline{E})]' - \left\{ \frac{2}{3} \overline{S}_i \left[\frac{\hbar |e| \overline{F}_s}{\sqrt{2\overline{m}_c}} \right]^{2/3} \{ [\overline{I}_{11}(\overline{E})]' \}^{-1/3} [\overline{I}_{11}(\overline{E})]' \right\} \right\}.$$

Thus, one can observe that the EEM is a function of the subband index, surface electric field, the Fermi energy and the other spectrum constants due to the combined influence of $\overline{E}_{g_0}$ and Δ.

The subband energy ($\overline{E}_{n_{iw2}}$) in this case can be obtained from the (13.21) as

$$\overline{I}_{11}(\overline{E}_{n_{iw2}}) = \overline{S}_i \left[\frac{\hbar |e| \overline{F}_s [\overline{I}_{11}(\overline{E}_{n_{iw2}})]}{\sqrt{2\overline{m}_c}} \right]^{2/3} \tag{13.23}$$

Thus the 2D total DOS function in weak electric field limit can be expressed as

$$\overline{N}_{2D_i}(\overline{E}) = \frac{\overline{m}_c \overline{g}_v}{\pi \hbar^2} \sum_{i=0}^{i_{\max}} [\overline{P}_3(\overline{E}, i) \overline{H}(\overline{E} - \overline{E}_{n_{iw2}})] \tag{13.24a}$$

The electron concentration can be written as

$$\overline{n}_{2Dw} = \frac{\overline{g}_v \overline{m}_c}{\pi \hbar^2} \sum_{i=0}^{i_{\max}} [\overline{P}_{4w}(\overline{E}_{Fiw}, i) + \overline{Q}_{4w}(\overline{E}_{Fiw}, i)] \tag{13.24b}$$

where,

$$\overline{P}_{4w}(\overline{E}_{Fiw}, i) \equiv \left\{ \overline{I}_{11}(\overline{E}_{Fiw}) - \overline{S}_i \left[\frac{\hbar e \overline{F}_s [\overline{I}_{11}(\overline{E}_{Fiw})]}{\sqrt{2\overline{m}_c}} \right]^{2/3} \right\}$$

and

$$\overline{Q}_4(\overline{E}_{Fiw}, i) \equiv \sum_{\overline{r}=1}^{\overline{s}} \left\{ \overline{L}(\overline{r}) [\overline{P}_4(\overline{E}_{Fiw}, i)] \right\}$$

Using (1.31f) and (13.24b) we can study the entropy in this case.

(a) Using the constraints $\Delta >> \overline{E}_{g_0}$ *or* $\Delta << \overline{E}_{g_0}$, (13.21), under the low electric field limit, assumes the form

$$\gamma_2(\overline{E}, \eta_g) = \frac{\hbar^2 \overline{k}_s^2}{2\overline{m}_c} + \overline{S}_i \left[\frac{\hbar |e| \overline{F}_s [\gamma_2(\overline{E}, \eta_g)]'}{\sqrt{2\overline{m}_c}} \right]^{2/3} \tag{13.25}$$

(13.25) represents the dispersion relation of the 2D electrons in - accumulation layers of HD III-V, ternary and quaternary materials under the weak electric field limit whose bulk electrons obey the HD two band model of Kane.

The EEM can be expressed as

$$\overline{m}^*(\overline{E}'_f, i, \eta_g) = \overline{m}_c \overline{P}'_{3HD1}(\overline{E}'_f, i, \eta_g) \tag{13.26}$$

where,

$$\overline{P}_{3HD1}(\overline{E}'_f, i, \eta_g) = \left[\gamma_2(\overline{E}'_f, \eta_g) - \overline{S}_i \left[\frac{\hbar |e| \overline{F}_s [\gamma_2(\overline{E}'_f, \eta_g)]'}{\sqrt{2\overline{m}_c}} \right]^{2/3} \right]$$

Thus, one can observe that the EEM is a function of the subband index, surface electric field, the Fermi energy and the other spectrum constants due to the combined influence of $\overline{E}_{g_0}$ and Δ.

The subband energy $\overline{E'}_{i1}$ is given by

$$0 = \left[\gamma_2(\overline{E'}_{i1}, \eta_g) - \overline{S}_i \left[\hbar |e| \overline{F}_s \left[\gamma_2(\overline{E'}_{i1}, \eta_g) \right]' (2\overline{m}_c)^{-1/2} \right]^{2/3} \right] \tag{13.27}$$

The DOS function can be written as

$$\overline{N}_{2D_i}(\overline{E}) = \frac{\overline{m}_c \overline{g}_v}{\pi\hbar^2} \sum_{i=0}^{i_{\max}} [\overline{P}_{3HD1}(\overline{E}, i, \eta_g) \overline{H}(\overline{E} - \overline{E}_{i2})] \tag{13.28}$$

Thus, the DOS function is complex in nature.

The surface electron concentration is given by

$$\overline{n}_S = \overline{g}_v \sum_{i=0}^{i_{\max}} \left[\left[\frac{\overline{m}_c}{\pi\hbar^2} \overline{P}_{3HD1}(\overline{E'}_f, i, \eta_g) \right] + \frac{1}{3\pi^2} \left(\frac{2\overline{m}_c}{\hbar^2} \right)^{3/2} \overline{t}_i \left[\gamma_2(\overline{E}_{FB}, \eta_g) \right]^{3/2} \right] \tag{13.29}$$

where $\overline{E}_{FB}$ should be determined from the following equation

$$\overline{n}_B = \frac{\overline{g}_v}{3\pi^2}\left(\frac{2\overline{m}_c}{\hbar^2}\right)^{3/2}\left[\gamma_2(\overline{E}_{FB},\eta_g)\right]^{3/2} \tag{13.30}$$

Using (1.31f), (13.29) and (13.30) we can study the entropy in this case.

Using the constraints $\Delta >> \overline{E}_{g_0}$ *or* $\Delta << \overline{E}_{g_0}$, (13.21) under the low electric field limit assumes the form

$$\overline{E}(1+\alpha\overline{E}) = \frac{\hbar^2\overline{k}_s^2}{2\overline{m}_c} + \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s(1+2\alpha\overline{E})}{\sqrt{2\overline{m}_c}}\right]^{2/3} \tag{13.31}$$

For large values of i, $i, \overline{S}_i \rightarrow \left[\frac{3\pi}{2}\left(i+\frac{3}{4}\right)\right]^{2/3}$ [5], and the (13.31) gets simplified as

$$\overline{E}(1+\alpha\overline{E}) = \frac{\hbar^2\overline{k}_s^2}{2\overline{m}_c} + \left[\frac{3\pi\hbar|e|\overline{F}_s}{2}\left(i+\frac{3}{4}\right)\frac{(1+2\alpha\overline{E})}{\sqrt{2\overline{m}_c}}\right]^{2/3} \tag{13.32}$$

(13.32) was derived for the first time by Antcliffe *et al.* [3].

The EEM in this case is given by

$$\overline{m}^*(\overline{E}_{Fiw}, i) = \overline{m}_c[\overline{P}_6(\overline{E}, i)]|_{\overline{E}=\overline{E}_{Fiw}} \tag{13.33}$$

where,

$$\overline{P}_6(\overline{E}, i) \equiv \left\{1 + 2\alpha\overline{E} - \frac{4\alpha}{3}\overline{S}_i\left[\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}_c}}\right]^{2/3}\left\{1+2\alpha\overline{E}\right\}^{-1/3}\right\}$$

Thus, one can observe that the EEM is a function of the subband index, surface electric field and the Fermi energy due to the presence of band nonparabolicity only.

The subband energies $(\overline{E}_{n_{iw3}})$ are given by

$$(\overline{E}_{n_{iw3}})(1+\alpha\overline{E}_{n_{iw3}}) = \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s(1+2\alpha\overline{E}_{n_{iw3}})}{\sqrt{2\overline{m}_c}}\right]^{2/3} \tag{13.34}$$

The total 2D DOS function can be written as

$$\overline{N}_{2D}(\overline{E}) = \frac{\overline{m}_c\overline{g}_v}{\pi\hbar^2}\sum_{i=0}^{i\max}\left\{\left[1 + 2\alpha\overline{E} - \frac{4\alpha}{3}\overline{S}_i\left[\frac{\hbar|e|\overline{F}}{\sqrt{2\overline{m}_c}}\right]^{2/3}(1+2\alpha\overline{E})^{-1/3}\right]\overline{H}(\overline{E}-\overline{E}_{n_{iw3}})\right\} \tag{13.35a}$$

Under the condition $\alpha E << 1$, the use of (13.29) and the Fermi–Dirac integral leads to the expression of $\overline{n}_{2Dw}$ as

$$\overline{n}_{2Dw} = \left(\frac{\overline{g}_v\overline{m}_c\overline{k}_B\overline{T}}{\pi\hbar^2}\right)\sum_{i=0}^{i\max}\left\{\left[1+\overline{D}_i+2\alpha\overline{E}_{n_{iw3}}\right]\overline{F}_0(\eta_{iw}) + 2\alpha\overline{k}_B\overline{T}\overline{F}_1(\eta_{iw})\right\} \tag{13.35b}$$

where,

$$\overline{D}_i \equiv \frac{4\alpha\overline{S}_i}{3}\left(\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}_c}}\right)^{2/3} \text{ and } \eta_{iw} \equiv \left[\frac{\overline{E}_{Fiw} - \overline{E}_{n_{iw3}}}{\overline{k}_B\overline{T}}\right]$$

For all values of $\alpha\overline{E}_{Fiw}$, the $\overline{n}_{2Dw}$ can be written as

$$\overline{n}_{2Dw} = \left(\frac{\overline{g}_v\overline{m}_c}{\pi\hbar^2}\right)\sum_{i=0}^{i_{\max}}\left[\overline{P}_{5w}(\overline{E}_{Fiw}, i) + \overline{Q}_{5w}(\overline{E}_{Fiw}, i)\right] \tag{13.35c}$$

where,

$$\overline{P}_{5w}(\overline{E}_{Fiw}, i) \equiv \left[\overline{E}_{Fiw}(1+\alpha\overline{E}_{Fiw}) - \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}_c}}(1+2\alpha\overline{E}_{Fiw})\right]^{2/3}\right]$$

and

$$\overline{Q}_{5w}(\overline{E}_{Fiw}, i) \equiv \sum_{\overline{r}=1}^{\overline{s}}\overline{L}(\overline{r})\overline{P}_{5w}(\overline{E}_{Fiw}, i)$$

Using (1.31f) and (13.35c) we can study the entropy in this case.

(b) Using the constraints $\alpha \to 0$, (13.25) under the low electric field limit assumes the form

$$\gamma_3(\overline{E}, \eta_g) = \frac{\hbar^2\overline{k}_s^2}{2\overline{m}_c} + \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s[\gamma_3(\overline{E}, \eta_g)]'}{\sqrt{2\overline{m}_c}}\right]^{2/3} \tag{13.36}$$

(13.36) represents the dispersion relation of the 2D electrons in accumulation layers of HD III–V,

Ternary, and quaternary materials under the weak electric field limit whose bulk electrons obey the HD parabolic band model.

The EEM can be expressed as

$$\overline{m}^*(\overline{E'}_f, i, \eta_g) = \overline{m}_c\overline{P'}_{3HD2}(\overline{E'}_f, i, \eta_g) \tag{13.37}$$

where

$$\overline{P}_{3HD2}(\overline{E'}_f, i, \eta_g) = \left[\gamma_3(\overline{E'}_f, \eta_g) - \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s[\gamma_3(\overline{E'}_f, \eta_g)]'}{\sqrt{2\overline{m}_c}}\right]^{2/3}\right]$$

Thus, one can observe that the EEM is a function of the subband index, surface electric field, the Fermi energy and other spectrum constants due to the combined influence of $\overline{E}_{g_0}$ and Δ.

The subband energy $\overline{E}_{i2}$, is given by

$$0 = \left[\gamma_3(\overline{E}_{i2}, \eta_g) - \overline{S}_i\left[\hbar|e|\overline{F}_s[\gamma_3(\overline{E}_{i2}, \eta_g)]'.(2\overline{m}_c)^{-1/2}\right]^{2/3}\right] \tag{13.38}$$

The DOS function can be written as

$$\overline{N}_{2D_i}(\overline{E}) = \frac{\overline{m}_c\overline{g}_v}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}\left[\overline{P}_{3HD2}(\overline{E}, i, \eta_g)\overline{H}(\overline{E} - \overline{E}_{i3})\right] \tag{13.39}$$

The surface electron concentration is given by

$$\overline{n}_S = \overline{g}_v\sum_{i=0}^{i_{\max}}\left[\left[\frac{\overline{m}_c}{\pi\hbar^2}P_{3HD2}(\overline{E'}_f, i, \eta_g)\right] + \frac{1}{3\pi^2}\left(\frac{2\overline{m}_c}{\hbar^2}\right)^{3/2}\overline{t}_i[\gamma_3(\overline{E}_{FB}, \eta_g)]^{3/2}\right] \tag{13.40}$$

where $\overline{E}_{FB}$ should be determined from the following equation

$$\overline{n}_B = \frac{\overline{g}_v}{3\pi^2}\left(\frac{2\overline{m}_c}{\hbar^2}\right)^{3/2}\left[\gamma_3(\overline{E}_{FB}, \eta_g)\right]^{3/2} \tag{13.41}$$

Using (1.31f) and (13.40), we can study the entropy in this case.

For $\alpha \to 0$, as for inversion layers, whose bulk electrons are defined by the parabolic energy bands, we can write

$$\overline{E} = \frac{\hbar^2\overline{k}_s^2}{2\overline{m}_c} + \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}_c}}\right]^{2/3} \tag{13.42}$$

(13.32) is valid for all values of the surface electric field [1].

The electric subband energy $(\overline{E}_{n_{i4}})$ assumes the form, from (13.32) as

$$\overline{E}_{n_{i4}} = \overline{S}_i\left[\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}_c}}\right]^{2/3} \tag{13.43}$$

The total density-of-states function can be written using (13.33) as

$$\overline{N}_{2D}(\overline{E}) = \frac{\overline{m}_c\overline{g}_v}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}\overline{H}(\overline{E} - \overline{E}_{n_{i4}}) \tag{13.44a}$$

The use of (13.34) leads to the expression of $\overline{n}_{2Di}$ as [1]

$$\overline{n}_{2Di} = \frac{\overline{g}_v\overline{m}_c\overline{k}_B\overline{T}}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}\overline{F}_0(\eta_i) \tag{13.44b}$$

where

$$\eta_i \equiv (\overline{k}_B \overline{T})^{-1} \left[\overline{E}_{Fi} - \overline{S}_i \left[\frac{\hbar |e| \overline{F}_s}{\sqrt{2\overline{m}_c}} \right]^{2/3} \right]$$

$\overline{E}_{Fi}$ is the Fermi energy as measured from the edge of the conduction band at the surface.

Using (1.31f) and (13.44b), we can study the entropy in this case.

13.2.3 Entropy in accumulation and inversion layers of II–VI materials

The use of (2.105) and (13.2) leads to the expression of the quantization integral as

$$\frac{\sqrt{2\overline{m}^*_{||}}}{\hbar} \int_0^{\overline{z}_t} \left[\gamma_3(\overline{E}, \eta_g) - |e| \overline{F}_s \overline{z} \gamma'_3(\overline{E}, \eta_g) - \overline{a'}_0 \overline{k}_s^2 \mp (\overline{\lambda}_0) \overline{k}_s \right] \tag{13.45}$$

where,

$$\overline{z}_t \equiv \left(|e| \overline{F}_s \gamma'_3(\overline{E}, \eta_g) \right)^{-1} \left[\gamma_3(\overline{E}, \eta_g) - \overline{a'}_0 \overline{k}_s^2 \mp (\overline{\lambda}_0) \overline{k}_s \right]$$

Therefore, the 2D electron dispersion law for accumulation layers of HD II–VI materials can be expressed as

$$\gamma_3(\overline{E}, \eta_g) = \overline{a'}_0 \overline{k}_s^2 \pm (\overline{\lambda}_0) \overline{k}_s + \overline{S}_i \left[\frac{\hbar |e| \overline{F}_s \gamma'_3(\overline{E}, \eta_g)}{\sqrt{2\overline{m}^*_{||}}} \right]^{2/3} \tag{13.46}$$

The area of the 2D surface as enclosed by the (13.46) can be expressed as

$$\overline{A}(\overline{E}, \eta_g, i) = \frac{\pi}{\overline{a'}_0^2} \Delta_{10}(\overline{E}, \eta_g, i) \tag{13.47}$$

where

$$\Delta_{10}(\overline{E}, \eta_g, i) = \left[(\overline{\lambda}_0)^2 - 2\overline{a'}_0 \left[-\gamma_3(\overline{E}, \eta_g) + \overline{S}_i \left(\frac{\hbar |e| \overline{F}_s \gamma'_3(\overline{E}, \eta_g)}{\sqrt{2\overline{m}^*_{||}}} \right)^{2/3} \right] \right]$$

The EEM in this case assumed the form

$$\overline{m}^*(\overline{E}_f', \eta_g, i) = \overline{m}^*_{\perp} \Delta_{10}(\overline{E}_f', \eta_g, i) \tag{13.48}$$

The subband energy $\overline{E}_{i2}$ can be written as

$$\gamma_3(\overline{E}_{i2}, \eta_g) = \overline{S}_i \left(\frac{\hbar |e| \overline{F}_s \gamma'_3(\overline{E}_{i2}, \eta_g)}{\sqrt{2\overline{m}^*_{||}}} \right)^{2/3} \tag{13.49}$$

The surface electron concentration can be written as

$$\overline{n}_S = \overline{g}_v \sum_{i=0}^{i_{\max}} \left[\left[\left(\frac{\overline{m}^*_{\perp}}{\pi\hbar^2} \right) \left[\Delta_{10}(\overline{E}'_f, \eta_g, i) + \Delta_{11}(\overline{E}'_f, \eta_g, i) \right] \right] + \frac{\overline{t}_i}{2} \left(\frac{\overline{k}_0 \overline{T}}{\pi \overline{b}'_0} \right)^{3/2} \left(\frac{\overline{b}'_0}{\overline{a}'_0} \right) \left[\overline{F}_{1/2} \left(\frac{\overline{E}_{FB}}{\overline{k}_B \overline{T}} \right) + \frac{(\overline{\lambda}_0)^2}{2\overline{a}'_0 \overline{k}_B \overline{T}} \overline{F}_{-1/2} \left(\frac{\overline{E}_{FB}}{\overline{k}_B \overline{T}} \right) \right] \right] \tag{13.50}$$

$\overline{E}_{FB}$ can be determined from the following equation

$$\overline{n}_B = \frac{\overline{g}_v}{2} \left(\frac{\overline{k}_0 \overline{T}}{\pi \overline{b}'_0} \right)^{3/2} \left(\frac{\overline{b}'_0}{\overline{a}'_0} \right) \left[\overline{F}_{1/2} \left(\frac{\overline{E}_{FB}}{\overline{k}_B \overline{T}} \right) + \frac{(\overline{\lambda}_0)^2}{2\overline{a}'_0 \overline{k}_B \overline{T}} \overline{F}_{-1/2} \left(\frac{\overline{E}_{FB}}{\overline{k}_B \overline{T}} \right) \right] \tag{13.51}$$

Using (1.31f) and (13.50), we can study the entropy in this case.

The expression of the quantization integral for inversion layers in this case as

$$\frac{\sqrt{2\overline{m}^*_{||}}}{\hbar} \int_0^{\overline{z}_t} \left[\overline{T} - |e| \overline{F}_s \overline{z} - \overline{a}'_0 \overline{k}_s^2 \mp (\overline{\lambda}_0) \overline{k}_s \right]^{1/2} d\overline{z} = \frac{2}{3} (\overline{S}_i)^{3/2} \tag{13.52}$$

where

$$\overline{z}_t \equiv (|e| \overline{F}_s)^{-1} \left[\overline{E} - \overline{a}'_0 \overline{k}_s^2 \mp (\overline{\lambda}_0) \overline{k}_s \right]$$

Therefore, the 2D electron dispersion law for *n*-channel inversion layers of II–VI materials can be expressed for all values of $\overline{F}_s$ as

$$\overline{E} = \overline{a}'_0 \overline{k}_s^2 \mp (\overline{\lambda}_0) \overline{k}_s + \overline{S}_i \left(\frac{\hbar |e| \overline{F}_s}{\sqrt{2\overline{m}^*_{||}}} \right)^{2/3} \tag{13.53}$$

The area of the 2D surface as enclosed by (13.43) can be expressed as

$$\overline{A}(\overline{E}, i) = \frac{\pi (\overline{m}^*_{\perp})^2}{\hbar^4} \left[\left\{ 2(\overline{\lambda}_0)^2 - \frac{2\hbar^2}{\overline{m}^*_{\perp}} \overline{S}_i \left(\frac{\hbar |e| \overline{F}_s}{\sqrt{2\overline{m}^*_{||}}} \right)^{2/3} + \frac{2\hbar^2 \overline{E}}{\overline{m}^*_{\perp}} \right\}$$

$$-2(\bar{\lambda}_0)\left[(\bar{\lambda}_0)^2-\frac{2\hbar^2}{\overline{m}^*_{\perp}}\overline{S}_i\left(\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}^*_{||}}}\right)^{2/3}+\frac{2\hbar^2\overline{E}}{\overline{m}^*_{\perp}}\right]^{1/2}\Bigg] \tag{13.54}$$

The EEM is given by

$$\overline{m}^*(\overline{E}_{Fi},i)=\overline{m}^*_{\perp}\left[1-\frac{\rho_{71}}{\sqrt{\overline{E}_{Fi}+\rho_{72}}}\right] \tag{13.55}$$

where $\overline{E}_{Fi}$ is the Fermi energy in this case,

$$\rho_{71}\equiv\frac{\bar{\lambda}_0}{2\sqrt{\bar{a}'_0}}\ \textit{and}\ \rho_{72}\equiv\left[(\rho_{71})^2-\left(\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}^*_{||}}}\right)^{2/3}\right].$$

Thus, EEM depends on both the Fermi energy and the subband index due to the presence of the term $\bar{\lambda}_0$.

The subband energy $(\overline{E}_{n_{i6}})$ can be written as

$$\overline{E}_{n_{i6}}=\overline{S}_i\left(\frac{\hbar|e|\overline{F}_s}{\sqrt{2\overline{m}^*_{||}}}\right)^{2/3} \tag{13.56a}$$

The total 2D density-of-states function can be written as

$$\overline{N}_{2D_i}(\overline{E})=\frac{\overline{m}^*_{\perp}\overline{g}_v}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}\left\{\left[1-\frac{\rho_{71}}{\sqrt{\overline{E}+\rho_{72}}}\right]H(\overline{E}-\overline{E}_{n_{i6}})\right\} \tag{13.56b}$$

The surface electron concentration assumes the form

$$\overline{n}_{2Di}=\frac{\overline{g}_v\overline{m}^*_{\perp}\bar{k}_B\overline{T}}{\pi\hbar^2}\left\{\sum_{i=0}^{i_{\max}}\left[\overline{F}_0(\eta_i)-\left\{\frac{\bar{\lambda}_0\bar{f}_7(\overline{E}_{Fi},i)}{2\sqrt{\bar{a}'_0\bar{k}_B\overline{T}}}\right\}\right]\right\} \tag{13.56c}$$

where

$$\eta_i\equiv\left[\frac{\overline{E}_{Fi}-\overline{E}_{n_{i6}}}{\bar{k}_B\overline{T}}\right]\bar{f}_7(\overline{E}_{Fi},i)\equiv\left[2\left[\sqrt{\eta_i+\delta_{72}}-\sqrt{\delta_{72}}\right]+\sum_{\bar{r}=1}^{\bar{s}}\left\{2(1-2^{1-2r})\zeta(2\bar{r})\frac{(-1)^{2r-1}(2r-1)!}{(\eta_i+\delta_{72})^{2r}}\right\}\right]$$

and

$$\delta_{72} \equiv \frac{\left(\overline{\lambda}_0\right)^2}{4\overline{a'}_0 \overline{k}_B \overline{T}}$$

Using (1.31f) and (13.56c) we can study the entropy in this case.

13.2.4 Entropy in accumulation and inversion layers of IV–VI materials

The 2D electron dispersion relation in accumulation layers of IV–VI materials can be written as

$$\theta_1(\overline{E}, i, \eta_g)k_x^2 + \theta_2(\overline{E}, i, \eta_g)k_y^2 = \theta_3(\overline{E}, i, \eta_g) \tag{13.57}$$

where

$$\theta_1(\overline{E}, i, \eta_g) = \left[\overline{F}_1(\overline{E}, \eta_g) + \overline{S}_i(e\overline{F}_s\overline{a}_1(\overline{E}, \eta_g))^{2/3}\overline{F}_2(\overline{E}, \eta_g)\right]$$

$$\overline{a}_1(\overline{E}, \eta_g) = \frac{1}{\overline{F}_2(\overline{E}, \eta_g)}\left[\frac{\overline{F'}_2(\overline{E}, \eta_g)}{\overline{F}_2(\overline{E}, \eta_g)}\overline{F}_1(\overline{E}, \eta_g) - \overline{F'}_1(\overline{E}, \eta_g)\right]$$

$$\theta_2(\overline{E}, i, \eta_g) = \left[\left[\overline{F}_1(\overline{E}, \eta_g) + \frac{2\overline{a}_2(\overline{E}, \eta_g)}{3\overline{a}_1(\overline{E}, \eta_g)}\left(e\overline{F}_s\overline{a}_1(\overline{E}, \eta_g)\right)^{2/3}\overline{S}_i\overline{F}_1(\overline{E}, \eta_g)\right]\right]$$

$$a_2(\overline{E}, \eta_g) = \frac{1}{\overline{F}_2(\overline{E}, \eta_g)}\left[\frac{\overline{F'}_2(\overline{E}, \eta_g)}{\overline{F}_2(\overline{E}, \eta_g)}\overline{F}_1(\overline{E}, \eta_g) - \overline{F'}_1(\overline{E}, \eta_g)\right]$$

$$\theta_3(\overline{E}, i, \eta_g) = \left[1 + \frac{2\overline{C}(\overline{E}, \eta_g)}{3\overline{a}_1(\overline{E}, \eta_g)}\overline{S}_i\left(e\overline{F}_s\overline{a}_1(\overline{E}, \eta_g)\right)^{2/3}\overline{F}_2(\overline{E}, \eta_g)\right] \text{ and } \overline{C}(\overline{E}, \eta_g) = \left[\frac{\overline{F'}_2(\overline{E}, \eta_g)}{\overline{F}_2^2(\overline{E}, \eta_g)}\right]$$

EEM can be expressed as

$$\overline{m}^*(\overline{E}, i, \eta_g) = \frac{\hbar^2}{2}\theta'_4(\overline{E}'_f, i, \eta_g) \tag{13.58}$$

where

$$\theta_4(\overline{E}'_f, i, \eta_g) = \frac{\theta_3(\overline{E}'_f, i, \eta_g)}{\sqrt{\theta_1(\overline{E}'_f, i, \eta_g)\theta_2(\overline{E}'_f, i, \eta_g)}}$$

The subband energy $\overline{E}_{i3}$ is given by

$$\theta_3(\overline{E}_{t3}, i, \eta_g) = 0 \tag{13.59}$$

The 2D electron concentration in accumulation layer of IV–VI materials under the condition of extreme degeneracy and low electric field limit can be written as

$$\overline{n}_S = \overline{g}_v \; Real\ part\ of \sum_{i=0}^{i\max}\left[\theta_4(\overline{E}'_f, i, \eta_g) + \frac{\overline{t}_i}{3\pi^2}\left[\overline{F}_1(\overline{E}_{FB}, \eta_g)\sqrt{\overline{F}_2(\overline{E}_{FB}, \eta_g)}\right]^{-1}\right] \tag{13.60}$$

where $\overline{E}_{FB}$ can be determined from the equation

$$\overline{n}_B = \overline{g}_v \; Real\ part\ of \left[\frac{1}{3\pi^2}\left[\overline{F}_1(\overline{E}_{FB}, \eta_g)\sqrt{\overline{F}_2(\overline{E}_{FB}, \eta_g)}\right]^{-1}\right] \tag{13.61}$$

Using (1.31f) and (13.60) we can study the entropy in this case.

The 2D electron dispersion relation of the inversion layers of IV–VI materials in the low electric field limit can be written as

$$\overline{k}_s^2 = \beta_3(\overline{E}, i) \tag{13.62}$$

where

$$\beta_3(\overline{E}, i) = \frac{\beta_1(\overline{E}, i)}{\beta_2(\overline{E}, i)},$$

$$\beta_1(\overline{E}, \overline{i}) = 1 - \left[\frac{\overline{e}\overline{F}_s\overline{V}'_2(\overline{E})}{\overline{V}_2^2(\overline{E})}\right]^{2/3}\overline{S}_i\overline{V}_2(\overline{E}),\ \overline{V}_2(\overline{E}) = \left[\frac{2(\overline{A})^2}{\overline{E}_{g_0}(1+\alpha_1\overline{E})} + \frac{(\overline{S}+\overline{Q})^2}{\Delta''_c(1+\alpha_3\overline{E})}\right](2\overline{E})^{-1},$$

$$\beta_2(\overline{E}, i) = \left[\overline{V}_1(\overline{E}) + \left[\frac{\overline{e}\overline{F}_s\overline{V}'_2(\overline{E})}{\overline{V}_2^2(\overline{E})}\right]\right]^{2/3}\overline{S}_i\overline{V}_2(\overline{E})\frac{2}{3}\frac{\overline{V}_2^2(\overline{E})}{\overline{V}'_2(\overline{E})}\left[\frac{\overline{V}_1(\overline{E})\overline{V}'_2(\overline{E})}{\overline{V}_2^2(\overline{E})} - \frac{\overline{V}'_1(E)}{\overline{V}_2(E)}\right]$$

and

$$\overline{V}_1(E) = \left[\frac{(\overline{R})^2}{\overline{E}_{g_0}(1+\alpha_1\overline{E})} + \frac{(\overline{S})^2}{\Delta'_c(1+\alpha_2\overline{E})} + \frac{(\overline{Q})^2}{\Delta''_c(1+\alpha_3\overline{E})}\right](2\overline{E})^{-1}$$

EEM can be expressed as

$$\overline{m}^*(\overline{E}_{Fi}, i) = \frac{\hbar^2}{2}\beta'_3(\overline{E}_{Fi}, i) \tag{13.63}$$

The subband energy $(\overline{E}_{i4})$ can be written as

$$0 = \beta_3(\overline{E}_{i4}, i) \tag{13.64a}$$

The electron concentration can be given as

$$\overline{n}_0 = \frac{\overline{g}_v}{2\pi}\left[\sum_{i=0}^{i\max}\sqrt{\beta_3(\overline{E}_{Fi}, i)} + \sum_{\overline{r}=1}^{\overline{s}}\overline{L}(\overline{r})\left[\sqrt{\beta_3(\overline{E}_{Fi}, i)}\right]\right] \tag{13.64b}$$

Using (1.31f) and (16.64), we can study the entropy in this case.

13.2.5 Entropy in accumulation and inversion layers of stressed III–V materials

The 2D electron entropy in accumulation layers of stressed III–V materials can be written as

$$\theta_{13}(\overline{E},i,\eta_g)\overline{k}_x^2+\theta_{23}(\overline{E},\overline{i},\eta_g)\overline{k}_y^2=\theta_{33}(\overline{E},\overline{i},\eta_g) \tag{13.65}$$

where

$$\theta_{13}(\overline{E},i,\eta_g)=\left[\overline{f}_1(\overline{E},i,\eta_g)+\overline{S}_i\left(\overline{e}\overline{F}_s\overline{a}_{13}(\overline{E},\eta_g)\right)^{2/3}\overline{f}_3(\overline{E},\eta_g)\right]$$

$$a_{13}(\overline{E},\eta_g)=\frac{1}{\overline{f}_3(\overline{E},\eta_g)}\left[\frac{\overline{f'}_3(\overline{E},\eta_g)}{\overline{f}_3(\overline{E},\eta_g)}\overline{f}_1(\overline{E},\eta_g)-\overline{f'}_1(\overline{E},\eta_g)\right]$$

$$\theta_{23}(\overline{E},i,\eta_g)=\left[\left[\overline{f}_2(\overline{E},\eta_g)+\frac{2a_{23}(\overline{E},\eta_g)}{3a_{13}(\overline{E},\eta_g)}\left(\overline{e}\overline{F}_s\overline{a}_{13}(\overline{E},\eta_g)\right)^{2/3}\overline{S}_i\overline{f}_2(\overline{E},\eta_g)\right]\right]$$

$$a_{23}(\overline{E},\eta_g)=\frac{1}{\overline{f}_3(\overline{E},\eta_g)}\left[\frac{\overline{f'}_3(\overline{E},\eta_g)}{\overline{f}_3(\overline{E},\eta_g)}\overline{f}_2(\overline{E},\eta_g)-\overline{f'}_2(\overline{E},\eta_g)\right]$$

$$\theta_{33}(\overline{E},i,\eta_g)=\left[1+\frac{2\overline{C}_3(\overline{E},\eta_g)}{3\overline{a}_{13}(\overline{E},\eta_g)}\overline{S}_i\left(e\overline{F}_s\overline{a}_{13}(\overline{E},\eta_g)\right)^{2/3}\overline{f}_3(\overline{E},\eta_g)\right]\text{ and }\overline{C}_3(\overline{E},\eta_g)=\left[\frac{\overline{f}'_3(\overline{E},\eta_g)}{\overline{f}_3^2(\overline{E},\eta_g)}\right],$$

and

$$\overline{f}_1(\overline{E},\eta_g),\overline{f}_2(\overline{E},\eta_g),\overline{f}_3(\overline{E},\eta_g),\overline{P}_{11}(\overline{E},\eta_g),\overline{Q}_{11}(\overline{E},\eta_g)\text{ and }\overline{S}_{11}(\overline{E},\eta_g)$$

are defined in Chapter 2, respectively.

EEM can be expressed as

$$\overline{m}^*(\overline{E'}_f,i,\eta_g)=\frac{\hbar^2}{2}\theta'_{43}(\overline{E'}_f,i,\eta_g) \tag{13.66}$$

where

$$\theta_{43}(\overline{E'}_f,i,\eta_g)=\frac{\theta_{33}(\overline{E'}_f,i,\eta_g)}{\sqrt{\theta_{13}(\overline{E'}_f,i,\eta_g)\theta_{23}(\overline{E'}_f,i,\eta_g)}}$$

The subband energy $\overline{E}_{i33}$ is given by

$$\theta_{33}(\overline{E}_{i33}, i, \eta_g) = 0 \tag{13.67}$$

The 2D electron concentration in accumulation layers of stressed III–V materials under the condition of extreme degeneracy and low electric field limit can be written as

$$\overline{n}_S = \overline{g}_v \; Real\ part\ of \sum_{i=0}^{i_{\max}} \left[\theta_{43}(\overline{E'}_f, i, \eta_g) + \frac{\overline{t}_i}{3\pi^2}\left[\overline{f}_1(\overline{E}_{FB}, \eta_g)\overline{f}_2(\overline{E}_{FB}, \eta_g)\overline{f}_3(\overline{E}_{FB}, \eta_g)\right]^{-1/2}\right] \tag{13.68}$$

The E_{FB} can be determined from the following equation

$$\overline{n}_B = \overline{g}_v \left[\overline{f}_1(\overline{E}_{FB}, \eta_g)\overline{f}_2(\overline{E}_{FB}, \eta_g)\overline{f}_3(\overline{E}_{FB}, \eta_g)\right]^{-1/2} \tag{13.69}$$

Using (1.31f) and (13.68) we can study the entropy in this case.

The expression of the entropy of the 2D electrons in inversion layers of stressed III–V materials under the low electric field limit as

$$\left[\overline{T}_{57}(\overline{E}, i)\right]\overline{k}_x^2 + \left[\overline{T}_{67}(\overline{E}, i)\right]\overline{k}_y^2 = \overline{T}_{77}(\overline{E}, i) \tag{13.70}$$

where

$$\overline{T}_{57}(\overline{E}, i) = \left[\overline{E} - \alpha_1 + \frac{2}{3}\overline{S}_i\left(\frac{|e|^2}{\varepsilon_{sc}}\right)^{2/3}(\overline{n}_{2Dw})^{2/3}\overline{L}_{17}(\overline{E})\right]$$

$$\overline{L}_{17}(\overline{E}) = \left[\frac{(\overline{E} - \alpha_1)}{(\overline{E} - \alpha_3)^{2/3}[\overline{T}_{47}(\overline{E})]^{1/3}} - (\overline{E} - \alpha_3)^{1/3}[\overline{T}_{47}(\overline{E})]^{-1/3}\right],$$

$$[\overline{T}_{47}(\overline{E})] = \left[\{\rho_5(\overline{E})\}' - \left(\frac{\rho(\overline{E})}{\overline{E} - \alpha_3}\right)\right], \overline{T}_{67}(\overline{E}, i) = \left[\overline{E} - \overline{T}_2 + \frac{2}{3}\overline{S}_i\left(\frac{|e|^2}{\varepsilon_{sc}}\right)^{2/3}(\overline{n}_{2Dw})^{2/3}\overline{L}_{27}(\overline{E})\right],$$

$$\overline{L}_{27}(\overline{E}) = \left[\frac{(\overline{E} - \alpha_2)}{(\overline{E} - \alpha_3)^{2/3}[\overline{T}_{47}(E)]^{1/3}} - \left(\frac{(\overline{E} - \alpha_3)^{1/3}}{[\overline{T}_{47}(\overline{E})]^{1/3}}\right)\right],$$

$$\overline{T}_{77}(\overline{E}, i) = \left[\rho_5(\overline{E}) - S_i\left(\frac{|e|^2}{\varepsilon_{sc}}\right)^{2/3}(\overline{n}_{2Dw})^{2/3}L_{37}(\overline{E}), L_{37}(\overline{E}) \equiv (\overline{E} - \alpha_3)^{1/3}[\overline{T}_{47}(\overline{E})]\right]^{2/3}$$

and

$$\rho_5(\overline{E}) \equiv \left[\overline{t}_1\overline{E}^3 - \overline{t}_2\overline{E}^2 + \overline{t}_3\overline{E} + \overline{t}_4\right],$$

The area of the 2D surface under the weak electric field limit can be written as

$$\overline{A}(\overline{E},i)=\frac{\pi\overline{T}_{77}(\overline{E},i)}{\sqrt{\overline{T}_{57}(\overline{E},i)\overline{T}_{67}(\overline{E},i)}} \tag{13.71}$$

The sub-band energies $(\overline{E}_{n_{iw8}})$ in this case are defined by

$$\overline{T}_{47}(\overline{E}_{n_{iw8}})=\overline{S}_i\left(\frac{|e|^2}{\varepsilon_{sc}}\right)^{2/3}(\overline{n}_{2Dw})^{2/3}\overline{L}_{37}(\overline{E}_{n_{iw8}}) \tag{13.72}$$

The expression of EEM in this case can be written as

$$\overline{m}^*(\overline{E}_{Fiw},i)=\frac{\hbar^2}{2}\overline{L}_{47}(\overline{E},i)|_{\overline{E}=\overline{E}_{Fiw}} \tag{13.73}$$

where

$$\overline{L}_{47}(\overline{E},i)\equiv\left[\frac{1}{\overline{T}_{57}(\overline{E},i)\overline{T}_{67}(\overline{E},i)}\right]\left[\{\overline{T}_{77}(\overline{E},i)\}'[\overline{T}_{57}(\overline{E},i)\overline{T}_{67}(\overline{E},i)]^{1/2}-\left(\frac{\overline{T}_{77}(\overline{E},i)}{2}\right)\right.$$
$$\left.\left\{\{\overline{T}_{57}(\overline{E},i)\}'\left[\frac{\overline{T}_{67}(\overline{E},i)}{\overline{T}_{57}(\overline{E},i)}\right]^{1/2}+\{\overline{T}_{67}(\overline{E},i)\}'\left[\frac{\overline{T}_{57}(\overline{E},i)}{\overline{T}_{67}(\overline{E},i)}\right]^{1/2}\right\}\right.$$

The total 2D DOS function can be expressed as

$$\overline{N}_{2D}(\overline{E})=\frac{\overline{g}_v}{2\pi}\sum_{i=0}^{i_{\max}}\{\overline{L}_{47}(\overline{E},i)\overline{H}(\overline{E}-\overline{E}_{n_{iw8}})\} \tag{13.74a}$$

The surface electron concentration under the weak electric field limit assumes the form

$$\overline{n}_{2Dw}=\frac{\overline{g}_v}{(2\pi)}\left\{\sum_{i=0}^{i_{\max}}[\overline{P}_{8w}(\overline{E}_{Fwi},i)+\overline{Q}_{8w}(\overline{E}_{Fwi},i)]\right\} \tag{13.74b}$$

where

$$\overline{P}_{8w}(\overline{E}_{Fwi},i)\equiv\frac{\overline{T}_{77}(\overline{E}_{Fwi},i)}{\sqrt{\overline{T}_{57}(\overline{E}_{Fwi},i)\overline{T}_{67}(\overline{E}_{Fwi},i)}}\ \textit{and}\ \overline{Q}_{8w}(\overline{E}_{Fwi},i)\equiv\sum_{\overline{r}=1}^{\overline{s}}\overline{L}(\overline{r})\overline{P}_{8w}(\overline{E}_{Fwi},i)$$

Using (1.31f) and (13.74b), we can study the entropy in this case.

13.2.6 Entropy in accumulation and inversion layers of germanium

The 2D entropy in accumulation layers of Ge can be written as

$$\frac{\hbar^2\overline{k}_x^2}{2\overline{m}_1^*}+\frac{\hbar^2\overline{k}_y^2}{2\overline{m}_2^*}=\gamma_{10}(\overline{E},i,\eta_g) \tag{13.75}$$

where

$$\gamma_{10}(\overline{E},i,\eta_g)=\left[\gamma_3(\overline{E},\eta_g)\left[1+\alpha\gamma_3(\overline{E},\eta_g)\right]-\overline{S}_i\left[\frac{\hbar^2e\overline{F}_s\gamma'_3(\overline{E},\eta_g)}{\sqrt{2\overline{m}_3^*}}\right]^{2/3}\right.$$
$$\left.\left[1+2\alpha\gamma_3.5(\overline{E},\eta_g)\right]+\alpha\left[\overline{S}_i\left[\frac{\hbar e\overline{F}_s\gamma'_3(\overline{E},\eta_g)}{\sqrt{2\overline{m}_3^*}}\right]^{2/3}\right]^2\right]$$

The EEM can be expressed as

$$\overline{m}^*(\overline{E'}_f,i,\eta_g)=\sqrt{\overline{m}_1^*\overline{m}_2^*}\left[\gamma'_{10}(\overline{E},i,\eta_g)\right] \tag{13.76}$$

The band nonparabolicity and heavy doping makes the mass quantum number dependent.

The subband energy $\overline{E}_{i14}$ can be written as

$$\gamma_{10}(\overline{E}_{i14},i,\eta_g)=0 \tag{13.77}$$

The surface electron concentration in accumulation layers can be written as

$$\overline{n}_s=2\overline{g}_v\sum_{i=0}^{i_{\max}}\left[\left[\frac{\sqrt{\overline{m}_1^*\overline{m}_2^*}}{\pi\hbar^2}[\gamma_{10}(\overline{E'}_f,i,\eta_g)]+\overline{t}_i\frac{8\pi\overline{m}_\perp^*\sqrt{2\overline{m}_{||}^*}}{\hbar^3}[2\gamma_3(\overline{E}_{FB},\eta_g)]\right]^{3/2}\right.$$
$$\left.\left[1+\frac{4\alpha}{5}\gamma_3(\overline{E}_{FB},\eta_g)\right]\right] \tag{13.78}$$

where E_{FB} can be determined from the following equation

$$\overline{n}_B=\overline{g}_v\left[\frac{8\pi\overline{m}_\perp^*\sqrt{2\overline{m}_{||}^*}}{\hbar^3}\left[2\gamma_3(\overline{E}_{FB},\eta_g)\right]^{3/2}\left[1+\frac{4\alpha}{5}\gamma_3(\overline{E}_{FB},\eta_g)\right]\right] \tag{13.79}$$

Using (1.31f) and (13.78) we can study the entropy in this case.

The 2D electron dispersion law in inversion layers of Ge at low electric field limit can be expressed as

$$\frac{\hbar^2\overline{k}_x^2}{2\overline{m}_1^*}+\frac{\hbar^2\overline{k}_y^2}{2\overline{m}_2^*}=\left[\overline{E}(1+\alpha\overline{E})+\alpha\overline{E}_{i20}^2-\overline{E}_{i20}(1+2\alpha\overline{E})\right] \tag{13.80}$$

where,

$$\overline{E}_{i20}=\overline{S}_i\left(\frac{\hbar e\overline{F}_s}{\sqrt{2\overline{m}_3}}\right)^{2/3}$$

The area of 2D space is

$$\overline{A}=\frac{2\pi\sqrt{\overline{m}_1\overline{m}_2}}{\hbar^2}\left[\overline{E}(1+\alpha\overline{E})+\alpha\overline{E}_{i20}^2-\overline{E}_{i20}(1+2\alpha\overline{E})\right] \tag{13.81}$$

EEM assumes the form

$$\overline{m}^*(\overline{E}_{Fiw},i)=\sqrt{\overline{m}_1\overline{m}_2}\left[1+2\alpha\overline{E}_{Fiw}-\overline{E}_{i20}2\alpha\right] \tag{13.82}$$

Thus, EEM is the function of both Fermi energy and quantum number due to band nonparabolicity.

The DOS function is given by

$$\overline{N}_{2D}(\overline{E})=\frac{2\overline{g}_v}{(2\pi)^2}.\frac{2\pi\sqrt{\overline{m}_1\overline{m}_2}}{\hbar^2}\sum_{i=0}^{i_{\max}}\left[1+2\alpha\overline{E}-2\alpha\overline{E}_{i20}\right]\overline{H}(\overline{E}-\overline{E}_{i20}) \tag{13.83a}$$

The electron concentration can be given as

$$\overline{n}_s=\frac{\overline{g}_v\overline{k}_B\overline{T}\sqrt{\overline{m}_1\overline{m}_2}}{\pi\hbar^2}\sum_{i=0}^{i_{\max}}\left[\overline{F}_0(\eta_{i20})+2\alpha\overline{k}_B\overline{T}\overline{F}_1(\eta_{i20})\right] \tag{13.83b}$$

where

$$\eta_{i20}=\frac{\overline{E}_{Fi\omega}-\overline{E}_{i20}}{\overline{k}_B\overline{T}}$$

Using (1.31f) and (13.83b), we can study the entropy in this case.

13.3 Open research problems

R.13.1 Investigate the entropy in the presence of an arbitrarily oriented electric quantization for accumulation layers of tetragonal materials. Study all the special cases for III–V, ternary and quaternary materials in this context.

R.13.2 Investigate the entropy in accumulation layers of IV–VI, II–VI, and stressed Kane-type compounds in the presence of an arbitrarily oriented quantizing electric field.

R.13.3 Investigate the entropy in accumulation layers of all the materials as stated in R.1.1 of Chapter 1 in the presence of an arbitrarily oriented quantizing electric field.

R.13.4 Investigate the entropy in the presence of an arbitrarily oriented nonquantizing magnetic field in accumulation layers of tetragonal materials by including the electron spin. Study all the special cases for III–V, ternary and quaternary materials in this context.

R.13.5 Investigate the entropy in accumulation layers of IV–VI, II–VI, and stressed Kane-type compounds in the presence of an arbitrarily oriented nonquantizing magnetic field by including the electron spin.

R.13.6 Investigate the entropy in accumulation layers of all the materials as stated in R.1.1 of Chapter 1 in the presence of an arbitrarily oriented non-quantizing magnetic field by including electron spin.

R.13.7 Investigate the entropy in accumulation layers for all the problems from R.13.1 to R.13.6 in the presence of an additional arbitrarily oriented electric field.

R.13.8 Investigate the entropy in accumulation layers for all the problems from R.13.1 to R.13.3 in the presence of arbitrarily oriented crossed electric and magnetic fields.

R.13.9 Investigate the entropy in accumulation layers for all the problems from R.13.1 to R.13.8 in the presence of surface states.

R.13.10 Investigate the entropy in accumulation layers for all the problems from R.13.1 to R.13.8 in the presence of hot electron effects.

R.13.11 Investigate the entropy in accumulation layers for all the problems from R.13.1 to R.13.6 by including the occupancy of the electrons in various electric subbands.

R. 13.12 investigate the problems from R.13.1 to R.13.11 for the appropriate p-channel accumulation layers.

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14 Appendix E: Entropy in HDs under cross-fields configuration

The reading of old good books is like conversation with the finest men of the past centuries.

14.1 Introduction

The influence of crossed electric and quantizing magnetic fields on the transport properties of materials having various band structures are relatively less investigated as compared with the corresponding magnetic quantization, although the cross-fields are fundamental with respect to the addition of new physics and the related experimental findings. In 1966, Zawadzki and Lax [1] formulated the electron dispersion law for III–V materials in accordance with the two-band model of Kane under cross-fields configuration that generates the interest to study this particular topic of semiconductor science in general [2–14].

In Section 14.2.1 of theoretical background, the entropy in HD nonlinear optical materials in the presence of crossed electric and quantizing magnetic fields has been investigated by formulating the electron dispersion relation. Section 14.2.2 reflects the study of the entropy in HD III–V, ternary, and quaternary compounds as a special case of Section 14.2.1. Section 14.2.3 contains the study of the entropy for the HD II–VI materials in the present case. In Section 14.2.4, the entropy under cross-fields configuration in HD IV–VI materials has been investigated in accordance with the models of the Cohen, the Lax nonparabolic ellipsoidal and the parabolic ellipsoidal respectively. In Section 14.2.5, the entropy for the HD-stressed Kane-type materials has been investigated. Sections 14.2.6, 14.2.7, 14.2.8, 14.2.9, and 14.2.10 discuss the entropys in QWs of the above HD materials in the presence of cross-fields configuration, respectively. This appendix presents three open research problems.

14.2 Theoretical background

14.2.1 Entropy in HD nonlinear optical materials under cross-fields configuration

The (2.26) of Chapter 2 can be expressed as

$$\overline{T}_{22}(\overline{E},\eta_g) = \frac{\overline{p}_s^2}{2\overline{m}_{\perp}^*} + \frac{\overline{p}_z^2}{2\overline{M}_{||}}\overline{T}_{22}(\overline{E},\eta_g)\left[\overline{T}_{21}(\overline{E},\eta_g)\right]^{-1} \tag{14.1}$$

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where

$$\overline{p}_s = \hbar\overline{k}_s \text{ and } \overline{p}_z = \hbar\overline{k}_z$$

We know that from electromagnetic theory that,

$$\vec{B} = \nabla \times \vec{A} \tag{14.2}$$

where $\vec{A}$ is the vector potential. In the presence of quantizing magnetic field $\overline{B}$ along $\overline{z}$ direction, (14.2) assumes the form

$$\begin{aligned}
\frac{\partial \overline{A}_z}{\partial \overline{y}} - \frac{\partial \overline{A}_y}{\partial \overline{z}} &= 0 \\
\frac{\partial \overline{A}_x}{\partial \overline{z}} - \frac{\partial \overline{A}_z}{\partial \overline{x}} &= 0 \\
\frac{\partial \overline{A}_y}{\partial \overline{x}} - \frac{\partial \overline{A}_x}{\partial \overline{y}} &= B
\end{aligned} \tag{14.3}$$

where, $\hat{i}$, $\hat{j}$ and $\hat{k}$ are orthogonal triads. Thus, we can write

$$\begin{aligned}
\frac{\partial \overline{A}_z}{\partial \overline{y}} - \frac{\partial \overline{A}_y}{\partial \overline{z}} &= 0 \\
\frac{\partial \overline{A}_x}{\partial \overline{z}} - \frac{\partial \overline{A}_z}{\partial \overline{x}} &= 0 \\
\frac{\partial \overline{A}_y}{\partial \overline{x}} - \frac{\partial \overline{A}_x}{\partial \overline{y}} &= B
\end{aligned} \tag{14.4}$$

This particular set of equations is being satisfied for $\overline{A}_x = 0$, $\overline{A}_y = \overline{B}_x$ *and* $\overline{A}_z = 0$.

Therefore in the presence of the electric field $\overline{E}_o$ along x-axis and the quantizing magnetic field B along z-axis for the present case following (14.1), we can approximately write,

$$\overline{T}_{22}(\overline{E}, \eta_g) + |e|\overline{E}_o \hat{x}p(e, \eta_g) = \frac{\hat{p}_x^2}{2\overline{m}_\perp^*} + \frac{\left(\hat{p}_x - |e|\overline{B}\hat{x}\right)^2}{2\overline{m}_\perp^*} + \frac{\hat{p}_z^2}{2\overline{a}(\overline{E}, \eta_g)} \tag{14.5}$$

where

$$\rho(\overline{E}) \equiv \frac{\partial}{\partial \overline{E}}\left[\overline{T}_{22}(\overline{E}, \eta_g)\right]$$

and

$$\alpha\left(\overline{E}, \eta_g\right) \equiv \overline{m}_{||}^* \left[\overline{T}_{22}(\overline{E}, \eta_g)\right]^{-1} \left[\overline{T}_{21}(\overline{E}, \eta_g)\right]$$

Let us define the operator $\hat{\theta}$ as

$$\hat{\theta} = -\hat{p}_y + |e|\overline{B}\hat{x} - \frac{\overline{m}_{\perp}^{*}\overline{E}_o\rho(\overline{E},\eta_g)}{\overline{B}} \tag{14.6}$$

Eliminating the operator $\hat{x}$, between (14.5) and (14.6) the dispersion relation of the conduction electron in tetragonal semiconductors in the presence of cross fields configuration is given by

$$\overline{T}_{22}(\overline{E},\eta_g) = \left[\left(\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_{01}\right)\right] + \left(\frac{\left[\hbar\overline{k}_z(\overline{E})\right]^2}{2\overline{a}(\overline{E},\eta_g)}\right) - \left(\frac{\overline{E}_0\hbar\overline{k}_y\rho(\overline{E},\eta_g)}{\overline{B}}\right) - \left(\frac{\overline{M}_{\perp}\rho^2(\overline{E},\eta_g)\overline{E}_o^2}{2\overline{B}^2}\right) \tag{14.7}$$

where,

$$\omega_{01} = \frac{|e|\overline{B}}{\overline{m}_{\perp}^{*}}$$

The EEMs along $\overline{Z}$ *and* $\overline{Y}$ directions can, respectively be expressed from (14.7) as

$$\overline{m}_z^{*}(\overline{E}_{FBDH},\eta_g,\overline{n},\overline{E}_0) = Real\ part\ of\ \left[\overline{a}'(\overline{E}_{FBDH},\eta_g)\left[\overline{T}_{22}\left(\overline{E}_{FBDH},\eta_g\right) - \left(n+\frac{1}{2}\right)\hbar\omega_{01} + \frac{\overline{M}_{\perp}\rho^2(\overline{E}_{FBDH},\eta_g)\overline{E}_0^2}{2\overline{B}^2}\right] + \left[\overline{a}(\overline{E}_{FBDH},\eta_g)\left[\overline{T}'_{22}(\overline{E}_{FBDH},\eta_g) + \frac{\overline{M}_{\perp}\rho(\overline{E}_{FBDH},\eta_g)\rho'(\overline{E}_{FBDH},\eta_g)\overline{E}_0^2}{\overline{B}^2}\right]\right] \tag{14.8}$$

and

$$\overline{m}_y^{*}\left(\overline{E}_{FBDH},\eta_g,\overline{n},\overline{E}_0\right) = \left(\frac{\overline{B}}{\overline{E}_0}\right)^2 Real\ part\ of\ \left[\rho\left(\overline{E}_{FBDH},\eta_g\right)^{-3}\left[\overline{T}_{22}\left(\overline{E}_{FBDH},\eta_g\right) - \left(\overline{n}+\frac{1}{2}\right)\hbar\omega_{01} + \frac{\overline{M}_{\perp}\rho^2(\overline{E}_{FBDH},\eta_g)\overline{E}_0^2}{2\overline{B}^2}\right]\right.$$
$$\left[\rho\left(\overline{E}_{FBDH},\eta_g\right)\left[\overline{T}_{22}\left(\overline{E}_{FBDH},\eta_g\right) + \frac{\overline{M}_{\perp}\rho(\overline{E}_{FBDH},\eta_g)\rho'(\overline{E}_{FBDH},\eta_g)\overline{E}_0^2}{\overline{B}^2}\right]\right.$$
$$\left.\left. - \left[\overline{T}_{22}(\overline{E}_{FBDH},\eta_g) - \left(\overline{n}+\frac{1}{2}\right)\hbar\omega_{01}\frac{\overline{M}_{\perp}\rho^2(\overline{E}_{FBDH},\eta_g)\overline{E}_0^2}{2\overline{B}^2}\right]\rho'\left(\overline{E}_{FBDH},\eta_g\right)\right]\right] \tag{14.9}$$

where $\overline{E}_{FBHD}$ is the Fermi energy in the presence of cross-fields configuration and heavy doping as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization.

When $\overline{m}_z^*(\overline{E}_{FBHD}, \eta_g, \overline{n}, \overline{E}_0) \to \infty$, which is a physically justified result. The dependence of EEM along y direction on the Fermi energy, electric field, magnetic field and the magnetic quantum number is an intrinsic property of cross fields together with the fact in the present case of heavy doping, EEM exists in the band gap. Another characteristic feature of cross-field is that various transport coefficients will be sampled dimension dependent. These conclusions are valid for even isotropic parabolic energy bands and cross fields introduce the index dependent anisotropy in the effective mass.

The formulation of DR requires the expression of the electron concentration which can, in general, be written excluding the electron spin as

$$\overline{n}_o = \frac{-\overline{g}_v}{\overline{L}_x \pi^2} \sum_{\overline{n}=0}^{\overline{n}_{\max}} \int_{\overline{E}_0}^{\infty} \overline{I}(\overline{E}, \eta_g) \frac{\partial \overline{f}_o}{\partial \overline{E}} d\overline{E} \tag{14.10}$$

where $\overline{L}_x$ is the sample length along $\overline{x}$ direction, $\overline{E}_0$ is determined by the equation

$$\overline{I}(\overline{E}, \eta_g) = 0 \tag{14.11}$$

where,

$$\overline{I}(\overline{E}, \eta_g) = \int_{\overline{x}_l(\overline{E}, \eta_g)}^{\overline{x}_h(\overline{E}, \eta_g)} \overline{k}_z(\overline{E}) d\overline{k}_y$$

in which,

$$\overline{x}_l(\overline{E}, \eta_g) \equiv \frac{-\overline{E}_0 \overline{M}_\perp \rho(\overline{E}, \eta_g)}{\hbar \overline{B}} \text{ and } \overline{x}_h(\overline{E}, \eta_g) \equiv \frac{|e|\overline{B}\overline{L}_x}{\hbar} + \overline{x}_1(\overline{E}, \eta_g)$$

Thus, we get

$$\overline{I}(\overline{E},\eta_g)=\frac{2}{3}\left[\frac{\overline{B}\sqrt{2\overline{a}(\overline{E},\eta_g)}}{\bar{h}^2\overline{E}_0\rho(\overline{E},\eta_g)}\left[\left[\overline{T}_{22}(\overline{E},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\frac{\bar{h}|e|\overline{B}}{\overline{m}_\perp^*}+|e|\overline{E}_0\overline{L}_x\rho(\overline{E},\eta_g)\right.\right.\right.$$
$$\left.\left.\left.-\frac{\overline{m}_\perp^*\overline{E}_0^2\left[\rho(\overline{E},\eta_g)\right]^2}{2\overline{B}^2}\right]^{\frac{3}{2}}-\left[\left[\overline{T}_{22}(\overline{E},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\frac{\bar{h}|e|\overline{B}}{\overline{m}_\perp^*}-\frac{\overline{m}_\perp^*\overline{E}_0^2[\rho(\overline{E},\eta_g)]^2}{2\overline{B}^2}\right]^{\frac{3}{2}}\right]\right]\right] \tag{14.12}$$

Therefore, the electron concentration is given by

$$\overline{n}_0 = \left(\frac{2\overline{g}_v\overline{B}\sqrt{2}}{3\overline{L}_x\pi^2\hbar^2\overline{E}_0}\right) \textit{Real part of} \sum_{\overline{n}=0}^{\overline{n}_{\max}}\left[\overline{T}_{41HD}(\overline{n}, \overline{E}_{FBHD}, \eta_g) + \overline{T}_{42HD}(\overline{n}, \overline{E}_{FBHD}, \eta_g)\right] \tag{14.13}$$

where

$$\overline{T}_{41HD}(\overline{n},\overline{E}_{FBHD},\eta_g) \equiv \frac{\sqrt{\overline{a}(\overline{E}_{FBHD},\eta_g)}}{\rho(\overline{E}_{FBHD},\eta_g)}$$

$$\left[\left[\overline{T}_{22}\left(\overline{E}_{FBHD},\eta_g\right) - \left(\overline{n}+\frac{1}{2}\right)\frac{\hbar|e|\overline{B}}{\overline{M}_{\perp}} + |e|\overline{E}_0\overline{L}_x\rho(\overline{E}_{FBHD},\eta_g) - \frac{\overline{m}^{*}_{\perp}\left[\rho(\overline{E}_{FBHD},\eta_g)\right]^2}{2\overline{B}^2}\right]^{\frac{3}{2}}\right.$$

$$\left. - \left[\overline{T}_{22}(\overline{E}_{FBHD},\eta_g) - \left(\overline{n}+\frac{1}{2}\right)\frac{\hbar|e|\overline{B}}{\overline{m}^{*}_{\perp}} - \frac{\overline{m}^{*}_{\perp}\overline{E}_0^2\left[\rho(\overline{E}_{FBHD},\eta_g)\right]^2}{2\overline{B}^2}\right]^{\frac{3}{2}}\right]$$

where $\overline{E}_{FBHD}$ is the fermic energy in this case.

and

$$\overline{T}_{42HD}(\overline{n},\overline{E}_{FBHD},\eta_g) \equiv \sum_{\overline{r}=1}^{\overline{s}}\left[\overline{L}(\overline{r})\overline{T}_{41HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\right]$$

Using (1.31f) and (14.13) we can study the entropy in this case.

14.2.2 Entropy in HD Kane-type III–V materials under cross-fields configuration

(a) Under the conditions $\delta = 0$, $\Delta_{||} = \Delta_{\perp} = \Delta$ *and* $m^{*}_{||} = m_{\perp} = m_c$, (14.7) assumes the form

$$\overline{T}_{33}(\overline{E},\eta_g) = \left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0 + \frac{\left[\hbar\overline{k}_z(\overline{E})\right]^2}{2\overline{m}_c} - \frac{E_0}{B}\hbar k_y\left\{\overline{T}_{33}(\overline{E},\eta_g)\right\}' - \frac{m_c E_0^2\left[\left\{\overline{T}_{33}(\overline{E},\eta_g)\right\}\right]^2}{} \tag{14.14}$$

where

$$\overline{T}_{33}(\overline{E},\eta_g) = \overline{T}_{31}(\overline{E},\eta_g) + i\overline{T}_{32}(\overline{E},\eta_g)$$

The use of (14.14) leads to the expressions of the EEM s' along $\overline{z}$ *and* $\overline{y}$ directions as

$$\overline{m}^{*}_{z}(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0) = \overline{m}_c \, Real\, part\, of\, \left[\left\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\right\}'' + \frac{\overline{m}_c\overline{E}_0^2\left\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\right\}\left\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\right\}''}{\overline{B}^2}\right] \tag{14.15}$$

$$\overline{m}_y^*\left(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0\right)=\left(\frac{\overline{B}}{\overline{E}_0}\right)^2 Real\ part\ of\ \left[\left[\{T_{33}(\overline{E}_{FBHD},\eta_g)\}'\right]^{-1}\right.$$
$$\left.+\left[\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0+\frac{\overline{m}_c\overline{E}_0^2[\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\}'']^2}{2\overline{B}^2}\right]\right]$$
$$\left[\frac{-\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\}''}{[\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\}']^2}\left[\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0\right.\right.$$
$$\left.\left.+\frac{m_cE_0^2[\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\}']}{2\overline{B}^2}\right]+1\frac{m_cE_0^2\{\overline{T}_{33}(\overline{E}_{FBHD},\eta_g)\}''}{\overline{B}^2}\right] \tag{14.16}$$

The Landau energy $(\overline{E}_{n_1})$ can be written as

$$\overline{T}_{33}(\overline{E}_{n_1},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{m}_c\overline{E}_0{}^2\left[\left\{\overline{T}_{33}(\overline{E}_{n_1},\eta_g)\right\}'\right]^2}{2\overline{B}^2} \tag{14.17}$$

The electron concentration in this case assumes the form

$$\overline{n}_0=\frac{2\overline{g}_v\overline{B}\sqrt{2\overline{m}_c}}{3\overline{L}_x\pi^2\hbar^2\overline{E}_0}Real\ Part\ of\ \sum_{\overline{n}=0}^{\overline{n}_{\max}}\left[\overline{T}_{43HD}(\overline{n},\overline{E}_{FB},\eta_g)+\overline{T}_{44HD}(\overline{n},\overline{E}_{FB},\eta_g)\right] \tag{14.18}$$

where,

$$\overline{T}_{43HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\left[\left[\overline{T}_{33}(\overline{E}_{FB},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left[\{\overline{T}_{33}(\overline{E}_{FB},\eta_g)\}'\right]^2\right.\right.$$
$$\left.+|e|E_0L_x\left[\{\overline{T}_{33}(\overline{E}_{FB},\eta_g)\}'\right]\right]^{\frac{3}{2}}-\left[\overline{T}_{33}(\overline{E}_{FB},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0\right.$$
$$\left.\left.-\frac{m_cE_0^2}{2B^2}\left[\{\overline{T}_{33}(\overline{E}_{FB},\eta_g)\}'\right]^2\right]^{\frac{3}{2}}\frac{1}{\left[\{\overline{T}_{33}(\overline{E}_{FB},\eta_g)\}'\right]}$$

and

$$\overline{T}_{44HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\sum_{\overline{r}=1}^{\overline{s}}\left[\overline{L}(\overline{r})\overline{T}_{44HD}\left(\overline{n},\overline{E}_{FBHD},\eta_g\right)\right]$$

Using (1.31f) and (14.18), we can study the entropy in this case

(b) Under the condition $\Delta\gg\overline{E}_{g_0}$, (14.15) assumes the form

$$\gamma_2(\overline{E},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{E}_0}{\overline{B}}\hbar k_y\gamma_2^{'}(\overline{E},\eta_g)-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma_2^{'}(\overline{E},\eta_g)\right)+\frac{\left[\hbar\overline{k}_z(\overline{E})\right]^2}{2\overline{m}_c} \tag{14.19}$$

The use of (14.20) leads to the expressions of the EEM s' along *z and y* directions as

$$\overline{m}_z^*(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0)=\overline{m}_c\left[\left\{\gamma_2(\overline{E}_{FBHD},\eta_g)\right\}^{''}+\frac{\overline{m}_c\overline{E}_o^2\left\{\gamma_2(\overline{E}_{FBHD},\eta_g)\right\}^{'}\left\{\gamma_2(\overline{E}_{FBHD},\eta_g)\right\}^{''}}{\overline{B}^2}\right] \tag{14.20}$$

$$\overline{m}_y^*(\overline{E}_{FBHD},\eta_g,n,E_0)=\left(\frac{\overline{B}}{\overline{E}_0}\right)^2\frac{1}{\left[\left\{\gamma_2(\overline{E}_{FBHD},\eta_g)\right\}^{'}\right]}\left[\gamma_2(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0+\frac{m_cE_o^2\left[\left\{\gamma_2(\overline{E}_{FBHD},\eta_g)\right\}^{'}\right]^2}{2\overline{B}^2}\right]$$

$$\left[\frac{-\{\gamma_2(\overline{E}_{FBHD},\eta_g)^{''}}{\left[\{\gamma_2(\overline{E}_{FBHD},\eta_g)\}^{'}\right]^2}\left[\gamma_2(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0+\frac{\overline{m}_c\overline{E}_o^2\left[\left\{\gamma_2(\overline{E}_{FBHD},\eta_g)\right\}^{'}\right]^2}{2\overline{B}^2}\right]+1+\frac{\overline{m}_c\overline{E}_o^2\{\gamma_2(\overline{E}_{FBHD},\eta_g)\}^{''}}{\overline{B}^2}\right] \tag{14.21}$$

The Landau energy $(\overline{E}_{n_2})$ can be written as

$$\gamma_2(\overline{E},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma_2^{'}(\overline{E}_{n_2},\eta_g)\right)^2 \tag{14.22}$$

The expressions for $\overline{n}_0$ in this case assume the forms

$$\overline{n}_0=\frac{2\overline{g}_v\overline{B}\sqrt{2\overline{m}_c}}{3\overline{L}_x\pi^2\hbar^2\overline{E}_0}\sum_{\overline{n}=0}^{\overline{n}_{\max}}\left[\overline{T}_{47HD}(\overline{n},\overline{E}_{FBHD},\eta_g)+\overline{T}_{48HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\right] \tag{14.23}$$

where

$$\overline{T}_{47HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\left[\left[\gamma_2(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0+|e|\overline{E}_0\overline{L}_x\left(\gamma^{'}{}_2(\overline{E}_{FBHD},\eta_g)\right)-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma_2(\overline{E}_{FBHD},\eta_g)\right)^2\right]^{\frac{3}{2}}-\left[\left[(\gamma_2(\overline{E}_{FBHD},\eta_g))-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma_2(\overline{E}_{FBHD},\eta_g)\right)^2\right]^{\frac{3}{2}}\right]\left[\gamma^{'}{}_2(\overline{E}_{FBHD},\eta_g)\right]\Bigg]^{-1}$$

and

$$\overline{T}_{48HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\sum_{\overline{r}=0}^{\overline{s}}\left[\overline{L}(\overline{r})\overline{T}_{47HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\right]$$

Using (1.31f) and (14.23) we can study the entropy in this case.

(c) For $\alpha\to 0$ and we can write,

$$\gamma_3(\overline{\mathrm{E}},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{E}_0}{B}\hbar k_y\gamma_3^{'}(\overline{\mathrm{E}},\eta_g)-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma'_3(\overline{\mathrm{E}},\eta_g)\right)^2+\frac{\left[\hbar\overline{k}_z(\overline{E})\right]^2}{2\overline{m}_c} \tag{14.24}$$

The use of (14.25) leads to the expressions of the EEMs along z and y directions as

$$\overline{m}_z^*(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0)=\overline{m}_c\left[\left\{\gamma_3(\overline{E}_{FBHD},\eta_g)''+\frac{\overline{m}_c\overline{E}_0^2\left\{\gamma_3(\overline{E}_{FBHD},\eta_g)\right\}^{'}\left\{\gamma_3(\overline{E}_{FBHD},\eta_g)\right\}''}{\overline{B}^2}\right\}\right] \tag{14.25}$$

$$\begin{aligned}\overline{m}_y^*(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0)=&\left(\frac{\overline{B}}{\overline{E}_0}\right)^2\frac{1}{\left[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}^{'}\right]}\left[\gamma_3(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0\right.\\&\left.+\frac{\overline{m}_c\overline{E}_0^2[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}']^2}{2\overline{B}^2}\right]\\&\left[\frac{-\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}''}{[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}']^2}\left[\gamma_3(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0+\frac{\overline{m}_c\overline{E}_0^2\left[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}'\right]^2}{2\overline{B}^2}\right]\right.\\&\left.+1+\frac{\overline{m}_c\overline{E}_0^2\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}''}{\overline{B}^2}\right]\end{aligned} \tag{14.26}$$

The Landau energy $(\overline{E}_{n_3})$ can be written as

$$\gamma_3(\overline{E}_{n_3},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma'_3(\overline{E}_{n_3},\eta_g)\right)^2 \tag{14.27}$$

The expressions for n_0 in this case assume the forms

$$\overline{n}_0=\frac{2\overline{g}_v\overline{B}\sqrt{2\overline{m}_c}}{3\overline{L}_x\pi^2\hbar^2\overline{E}_0}\sum_{\overline{n}=0}^{\overline{n}_{\max}}\left[\overline{T}_{49HD}(\overline{\mathrm{n}},\overline{E}_{FBHD},\eta_g)+\overline{T}_{50HD}(\overline{\mathrm{n}},\overline{E}_{FBHD},\eta_g)\right] \tag{14.28}$$

where

$$\overline{T}_{49HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\left[\left[\gamma'_3(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0+|e|\overline{E}_0\overline{L}_x\left(\gamma'_3(\overline{E}_{FBHD},\eta_g)\right)-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma'_3(\overline{E}_{FBHD},\eta_g)\right)^2\right]^{3/2}-\left[\left(\gamma'_3(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\frac{\overline{m}_c\overline{E}_0^2}{2\overline{B}^2}\left(\gamma'_3(\overline{E}_{FBHD},\eta_g)\right)^2\right]^{3/2}\right]\left[\gamma'_3(\overline{E}_{FBHD},\eta_g)\right]^{-1}$$

and

$$\overline{T}_{50HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\sum_{\overline{r}=0}^{\overline{s}}\left[\overline{L}(\overline{r})\overline{T}_{49HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\right]$$

Using (1.31f) and (14.28), we can study the entropy in this case.

14.2.3 Entropy in HD II–VI materials under cross-fields configuration

The electron energy spectrum in HD II-VI Materials in the presence of electric field E_0 along x direction and quantizing magnetic field B along z direction can approximately be written as

$$\gamma_3(\overline{E},\eta_g)=\beta_1(\overline{n},\overline{E}_0)-\frac{\overline{E}_0}{\overline{B}}\hbar k_y\gamma'_3(\overline{E},\eta_g)-\frac{\overline{m}^*_{||}\overline{E}_0^2}{2\overline{B}^2}\left(\gamma'_3(\overline{E},\eta_g)\right)^2+\frac{\left[\hbar\overline{k}_z(\overline{E})\right]^2}{2\overline{m}^*_{||}} \tag{14.29}$$

where

$$\beta_1(\overline{n},\overline{E}_0)\equiv\left[\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_0-\left(\frac{\overline{E}_0^2\overline{m}^*_{\perp}}{2\overline{B}^2}\right)+\overline{D}\left\{\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_{02}-\left(\frac{\overline{E}_0^2\overline{m}^*_{\perp}}{2\overline{B}^2}\right)\right\}^{\frac{1}{2}}\right]\omega_{02}\equiv\frac{|e|\overline{B}}{\overline{m}^*_{\perp}}$$

and

$$\overline{D}\equiv\pm\frac{\overline{\lambda}_0\sqrt{2\overline{m}^*_{\perp}}}{\hbar}$$

The use of (14.30) leads to the expressions of EEMsalong z and y directions as

$$\overline{m}^*_z(\overline{E}_{FBHD},\eta_g,n,E_0)=\overline{m}^*_{||}\left[\left\{\gamma_3(\overline{E}_{FBHD},\eta_g)\right\}''+\frac{\overline{m}^*_{||}\overline{E}_0^2\left\{\gamma_3(\overline{E}_{FBHD},\eta_g)\right\}'\left\{\gamma_3(\overline{E}_{FBHD},\eta_g)\right\}''}{\overline{B}^2}\right] \tag{14.30}$$

$$\overline{m}_y^*(\overline{E}_{FBHD},\eta_g,\mathrm{n},\mathrm{E}_0)=\left(\frac{\overline{B}}{\overline{E}_0}\right)^2\frac{1}{\left[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}'\right]}\left[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}\right.$$
$$\left.-\beta_1(\overline{n},\overline{E}_0)+\frac{\overline{m}_{||}^*\overline{E}_0^2[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}']^2}{2\overline{B}^2}\right]$$
$$\left[\frac{-\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}''}{[-\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}']^2}\left[\gamma_3(\overline{E}_{FBHD},\eta_g)-\beta_1(n,E_0)+\frac{\overline{m}_{||}^*\overline{E}_0^2[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}']^2}{2\overline{B}^2}\right]\right.$$
$$\left.+1+\frac{\overline{m}_{||}^*\overline{E}_0^2[\{\gamma_3(\overline{E}_{FBHD},\eta_g)\}']}{\overline{B}^2}\right] \tag{14.31}$$

The Landau energy $(\overline{E}_{n_4})$ can be written as

$$\gamma_3(\overline{E}_{n_4},\eta_g)=\beta_1(n,E_0)-\frac{\overline{m}_{||}^*\overline{E}_0^2}{2\overline{B}^2}(\gamma'_3(\overline{E}_{n_4},\eta_g))^2 \tag{14.32}$$

The expression for $\overline{n}_0$ in this case assumes the form

$$\overline{n}_0=\frac{2\overline{g}_v\overline{B}\sqrt{2\overline{m}_c}}{3\overline{L}_x\pi^2\hbar^2\overline{E}_0}\sum_{\overline{n}=0}^{\overline{n}_{\max}}\left[\overline{T}_{53HD}(\overline{\mathrm{n}},\overline{E}_{FBHD},\eta_g)+\overline{T}_{54HD}(\overline{\mathrm{n}},\overline{E}_{FBHD},\eta_g)\right] \tag{14.33}$$

where

$$\overline{T}_{53HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\left[[\gamma_3(\overline{E}_{FBHD},\eta_g)-\beta_1(\overline{n},\overline{E}_0)+|e|\overline{E}_0\overline{L}_x(\gamma'_3(\overline{E}_{FBHD},\eta_g))\right.$$
$$\left.-\frac{\overline{m}_{||}^*\overline{E}_0^2}{2\overline{B}^2}(\gamma'_3(\overline{E}_{FBHD},\eta_g))^2\right]^{3/2}-\left[\gamma_3(\overline{E}_{FBHD},\eta_g)-\beta_1(\overline{n},\overline{E}_0)\right.$$
$$\left.-\frac{\overline{m}_{||}^*\overline{E}_0^2}{2\overline{B}^2}(\gamma'_3(\overline{E}_{FBHD},\eta_g))^2\right]^{3/2}\left[\gamma'_3(\overline{E}_{FBHD},\eta_g)\right]^{-1}$$

and

$$\overline{T}_{54HD}(\overline{\mathrm{n}},\overline{E}_{FBHD},\eta_g)\equiv\sum_{\overline{r}=0}^{\overline{s}}\left[\overline{L}(\overline{r})\overline{T}_{53HD}(\overline{\mathrm{n}},\overline{E}_{FBHD},\eta_g)\right]$$

Using (1.31f) and (14.33), we can study the entropy in this case.

14.2.4 Entropy in HD IV–VI materials under cross-fields configuration

The (2.143) can be written as

$$\frac{\overline{p}_s^2}{2\overline{M}_1^*(\overline{E},\eta_g)}+\frac{\overline{p}_z^2}{2\overline{M}_3^*(\overline{E},\eta_g)}=\overline{g}(\overline{E},\eta_g) \tag{14.34}$$

where

$$\overline{M}_1^*(\overline{E},\eta_g)=\left[\frac{(\overline{R})}{\overline{E}_{g_0}}\left\{\overline{c}_1(\alpha_1,\overline{E},\overline{E}_{g_0})-i\overline{D}_1(\alpha_1,\overline{E},\overline{E}_{g_0})\right\}+\frac{(\overline{S})}{\Delta_c}\left\{\overline{c}_2(\alpha_2,\overline{E},\overline{E}_{g_0})\right.\right.$$
$$\left.\left.-i\overline{D}_2(\alpha_2,\overline{E},\overline{E}_{g_0})\right\}\frac{(\overline{Q})}{\Delta_c}\left\{\overline{c}_3(\alpha_3,\overline{E},\overline{E}_{g_0})-i\overline{D}_3(\alpha_3,\overline{E},\overline{E}_{g_0})\right\}\right]^{-1}$$

$$\overline{M}_3^*(\overline{E},\eta_g)=\left[\frac{2(\overline{A})^2}{E_g}\left\{\overline{c}_1(\alpha_1,\overline{E},\overline{E}_{g_0})-i\overline{D}_1(\alpha_1,\overline{E},\overline{E}_{g_0})\right\}\right.$$
$$\left.+\frac{(\overline{S}+\overline{Q})^2}{\Delta_c}\left\{\overline{c}_3(\alpha_3,\overline{E},\overline{E}_{g_0})-i\overline{D}_3(\alpha_3,\overline{E},\overline{E}_{g_0})\right\}\right]^{-1}$$

and

$$\overline{g}^*(\overline{E},\eta_g)=2\hbar^2\gamma_0(\overline{E},\eta_g)$$

In the presence of quantizing magnetic field $\overline{B}$ along $\overline{z}$ direction and the electric field along x-axis, from above equation we obtain

$$\frac{\hat{p}_x{}^2}{2\overline{M}_1^*(\overline{E},\eta_g)}+\frac{(\hat{p}_y-|e|\overline{B}\hat{x})^2}{2\overline{M}_1^*(\overline{E},\eta_g)}+\frac{\hat{p}_z{}^2}{2\overline{M}_3^*(\overline{E},\eta_g)}=\overline{g}^*(\overline{E},\eta_g)+|e|\overline{E}_0\hat{x}\rho_1^*(\overline{E},\eta_g) \tag{14.35}$$

where

$$\rho_1^*(\overline{E},\eta_g)=\frac{\partial}{\partial\overline{E}}\left[\overline{g}^*(\overline{E},\eta_g)\right]$$

Let us define the operator $\hat{\theta}$ as

$$\hat{\theta}=-\hat{p}_y+|e|\overline{B}\hat{x}-\frac{\rho_1^*(\overline{E},\eta_g)\overline{E}_0\left[\overline{M}_1^*(\overline{E},\eta_g)\right]}{\overline{B}} \tag{14.36}$$

Eliminating $\hat{x}$, between the above two equations, the dispersion relation of the conduction electrons in HD-stressed Kane-type semiconductors in the presence of cross fields configuraration can be expressed as

$$\overline{g}^{*}(\overline{E},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\bar{\hbar}\overline{\omega}_{i1}(E,\eta_g)+\frac{\bar{\hbar}^2\overline{k}_z^2}{2\overline{M}_3^{*}(\overline{E},\eta_g)}-\frac{\overline{E}_0}{\overline{B}}\rho_1^{*}(\overline{E},\eta_g)\bar{\hbar}\overline{k}_y-\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho_1^{*}(\overline{E},\eta_g)\right]^2\overline{M}_1^{*}(\overline{E},\eta_g) \tag{14.37}$$

where

$$\omega_{i1}(\overline{E},\eta_g)=e\overline{B}[\overline{M}_1^{*}(\overline{E},\eta_g)]^{-1}$$

The use of (14.41) leads to the expressions of the EEMs along z and y directions as

$$\begin{aligned}\overline{m}_z^{*}(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0)=\text{Real part of }&\left[\left[\overline{M}_3^{*}(\overline{E}_{FBHD},\eta_g)\right]^{'}\left[\overline{g}^{*}(\overline{E}_{FBHD},\eta_g)\right.\right.\\&-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_i(\overline{E}_{FBHD},\eta_g)+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho_1^{*}(\overline{E}_{FBHD},\eta_g)^2\overline{M}_1^{*}(\overline{E}_{FBHD},\eta_g)\right]\\&+\left[\overline{M}_3^{*}(\overline{E}_{FBHD},\eta_g)\right]\left[\left[\overline{g}^{*}(\overline{E}_{FBHD},\eta_g)\right]'-\left(\overline{n}+\frac{1}{2}\right)\hbar\left[\omega_i(\overline{E}_{FBHD},\eta_g)\right]'\end{aligned} \tag{14.38}$$

and

$$\begin{aligned}\overline{m}_y^{*}(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0)=(\overline{B}/\overline{E}_0)^2\text{Real part of }&\left[\rho_1^{*}(\overline{E}_{FBHD},\eta_g)\right]^{-3}\left[\overline{g}^{*}(\overline{E}_{FBHD},\eta_g)\right.\\&-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_{i1}(\overline{E}_{FBHD},\eta_g)+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho^{*}(\overline{E}_{FBHD},\eta_g)^2\overline{M}_1^{*}(\overline{E}_{FBHD},\eta_g)\right]\\&\left[\left[\left[\rho_1^{*}(\overline{E}_{FBHD},\eta_g)\right]\left[\overline{g}^{*}(\overline{E}_{FBHD},\eta_g)\right]'-(\overline{n}+\frac{1}{2})\hbar\left[\omega_i(\overline{E}_{FBHD},\eta_g)\right]'\right.\right.\\&+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\left[\rho_1^{*}(\overline{E}_{FBHD},\eta_g)^2\left[\overline{M}_1^{*}(\overline{E}_{FBHD},\eta_g)\right]'\right]-\left[\rho_1^{*}(\overline{E}_{FBHD},\eta_g)\right]^{'}\right.\\&\left.\left.\left[\overline{g}^{*}(\overline{E}_{FBHD},\eta_g)-(\overline{n}+\frac{1}{2})\hbar\omega_{i1}(\overline{E}_{FBHD},\eta_g)\right]\right.\end{aligned} \tag{14.39}$$

The Landau level energy $\overline{E}_{n_9}$ in this case can be expressed through the equation

$$\overline{g}^{*}(\overline{E}_{n_9},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_{i1}(\overline{E}_{n_9},\eta_g)-\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho_1^{*}(E_{n_9},\eta_g)\right]^2\overline{M}_1^{*}(\overline{E}_{n_9},\eta_g) \tag{14.40}$$

The electron concentration can be written as

$$\overline{n}_0=\frac{2\overline{B}}{3\overline{L}_x\pi^2\bar{\hbar}^2\overline{E}_0}\text{Real part of }\sum_{\overline{n}=0}^{\overline{n}_{\max}}\left[\overline{T}_{4131HD}(\overline{n},\overline{E}_{FBHD},\eta_g)+\overline{T}_{4141HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\right] \tag{14.41}$$

where

$$\overline{T}_{4131HD}(\overline{n},\overline{E}_{FBHD},\eta_g)=\left[\frac{\sqrt{2\overline{M}_3^*(\overline{E}_{FBHD},\eta_g)}}{\rho_1^*(\overline{E}_{FBHD},\eta_g)}\right]\Big[[\overline{T}_{51}(\overline{n},\overline{E}_{FBHD},\eta_g)+\frac{\overline{E}_0}{\overline{B}}\rho_1^*(\overline{E}_{FBHD},\eta_g)\hbar x_{hHD1}(\overline{E}_{FBHD},\eta_g)\rho_1^*(\overline{E}_{FBHD},\eta_g)\Big]^{3/2}-\Big[\overline{T}_{51}(\overline{n},\overline{E}_{FBHD},\eta_g)+\frac{\overline{E}_0}{\overline{B}}\rho_1^*(\overline{E}_{FBHD},\eta_g)\hbar\overline{x}_{hHD1}(\overline{E}_{FBHD},\eta_g)\rho_1^*(\overline{E}_{FBHD},\eta_g)\Big]^{3/2}\Big]$$

$$\overline{T}_{51}(\overline{n},\overline{E}_{FBHD},\eta_g)=\left[\overline{g}^*(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_{i1}(\overline{E}_{FBHD},\eta_g)+\frac{\overline{M}_1^*(\overline{E}_{FBHD},\eta_g)E_0^2}{2B^2}\left[\rho_1^*(\overline{E}_{FBHD},\eta_g)\right]^2\right]$$

$$\overline{x}_{1HD1}(\overline{E}_{FBHD},\eta_g)=\frac{-\overline{M}_1^*(\overline{E}_{FBHD},\eta_g)\overline{E}_0\left[\rho_1^*(\overline{E}_{FBHD},\eta_g)\right]}{\overline{B}},\overline{x}_{hHD1}(\overline{E}_{FBHD},\eta_g)=\frac{|e|\overline{BL}_x}{\hbar}+\overline{x}_{1HD1}(\overline{E}_{FBHD},\eta_g)$$

and

$$\overline{T}_{4141HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\sum_{\overline{r}=1}^{\overline{s}}\left[\overline{L}(\overline{r})\overline{T}_{4131HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\right]$$

Using (1.31f) and (14.41), we can study the entropy in this case.

14.2.5 Entropy in HD stressed materials under cross-fields configuration

In this case we get

$$\frac{\overline{p}_x^2}{2\overline{M}_1^*(\overline{E},\eta_g)}+\frac{\overline{p}_y^2}{2\overline{M}_2^*(\overline{E},\eta_g)}+\frac{\overline{p}_z^2}{2\overline{M}_3^*(\overline{E},\eta_g)}=\overline{G}^*(\overline{E},\eta_g) \tag{14.42}$$

where

$$m_1^*(\overline{E},\eta_g)=\left[2\hbar^2\left[\gamma_0(\overline{E},\eta_g)-\overline{I}(1)\overline{T}_{17}\right]\right]^{-1},$$

$$\overline{T}_{17}\equiv\left[\overline{E}_{g_0}-\overline{C}_1\varepsilon-(\overline{a}_0+\overline{C}_1)\varepsilon+\frac{3}{2}\overline{b}_0\varepsilon_{xx}-\frac{\overline{b}_0}{2}\varepsilon+\left(\frac{\sqrt{3}}{2}\right)\varepsilon_{xy}\overline{d}_0\right]$$

$$\overline{m}_2^*(\overline{E},\eta_g)=\left[2\hbar^2\left[\gamma_0(\overline{E},\eta_g)-\overline{I}(1)\overline{T}_{27}\right]\right]^{-1},$$

$$\overline{T}_{27}\equiv\left[\overline{E}_{g_0}-\overline{C}_1\varepsilon-(\overline{a}_0+\overline{C}_1)\varepsilon+\frac{3}{2}\overline{b}_0\varepsilon_{xx}-\frac{\overline{b}_0}{2}\varepsilon+\left(\frac{\sqrt{3}}{2}\right)\varepsilon_{xy}\overline{d}_0\right]$$

$$\overline{m}_3^*(\overline{E},\eta_g)=\left[2\hbar^2\left[\gamma_0(\overline{E},\eta_g)-\overline{I}(1)\overline{T}_{37}\right]\right]^{-1},$$

$$\overline{T}_{37}\equiv\left[\overline{E}_{g_0}-\overline{C}_1\varepsilon-(\overline{a}_0+\overline{C}_1)\varepsilon+\frac{3}{2}\overline{b}_0\varepsilon_{xx}-\frac{\overline{b}_0}{2}\varepsilon+\left(\frac{\sqrt{3}}{2}\right)\varepsilon_{xy}\overline{d}_0\right]$$

and the other symbols are mentioned in Chapter 2.

In the presence of quantizing magnetic field $\overline{B}$ *along* $\overline{z}$ direction and the electric field along *x*-axis, from (14.46) one obtains

$$\frac{\hat{p}_x{}^2}{2\overline{M}_1^*(\overline{E},\eta_g)}+\frac{\left(\hat{p}_y-|e|\overline{B}\hat{x}\right)^2}{2\overline{M}_2^*(\overline{E},\eta_g)}+\frac{\hat{p}_z{}^2}{2\overline{M}_3^*(\overline{E},\eta_g)}=\overline{G}^*(\overline{E},\eta_g)+|e|\overline{E}_0\hat{x}\left[\frac{\overline{m}_1^*(\overline{E},\eta_g)}{\overline{m}_2^*(\overline{E},\eta_g)}\right]^{\frac{1}{2}}\rho^*(\overline{E},\eta_g) \tag{14.43}$$

where

$$\rho^*(\overline{E},\eta_g)=\frac{\partial}{\partial\overline{E}}\left[\overline{G}^*(\overline{E},\eta_g)\right]$$

Let us define the operator $\hat{\theta}$ as

$$\hat{\theta}=-\hat{p}_y+|e|\overline{B}\hat{x}-\frac{\rho^*(\overline{E},\eta_g)\overline{E}_0\left[\overline{m}_1^*(\overline{E},\eta_g)\overline{m}_2^*(\overline{E},\eta_g)\right]^{1/2}}{\overline{B}} \tag{14.44a}$$

Eliminating $\hat{x}$, between the above two equations, the dispersion relation of the conduction electrons in HD-stressed Kane-type semiconductors in the presence of cross fields configuration can be expressed as

$$\overline{G}^*(\overline{E},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\overline{\omega}_i(\overline{E},\eta_g)+\frac{\hbar^2\overline{k}_z^2}{2\overline{m}_3^*(\overline{E},\eta_g)}-\frac{\overline{E}_0}{\overline{B}}\rho^*(\overline{E},\eta_g)\left[\frac{\overline{m}_1^*(\overline{E},\eta_g)}{\overline{m}_2^*(\overline{E},\eta_g)}\right]^{1/2}\hbar\overline{k}_y$$
$$-\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho^*(\overline{E},\eta_g)\right]^2\overline{m}_1^*(\overline{E},\eta_g) \tag{14.44b}$$

where

$$\omega_i(\overline{E},\eta_g)=e\overline{B}[\overline{m}_1^*(\overline{E},\eta_g)\overline{m}_2^*(\overline{E},\eta_g)]^{-\frac{1}{2}}$$

The use of (14.44b) leads to the expressions of the EEMs along *z* and *y* directions as

$$\overline{m}_z^*(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0)=\left[\left[\overline{m}_3^*(\overline{E}_{FBHD},\eta_g)\right]'\left[\overline{G}^*(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_i(\overline{E}_{FBHD},\eta_g)\right.\right.$$
$$+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho^*(\overline{E}_{FBHD},\eta_g)^2\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\right]+\left[\overline{m}_3^*(\overline{E}_{FBHD},\eta_g)\right]$$
$$\left[\left[\overline{G}^*(\overline{E}_{FBHD},\eta_g)\right]'-\left(\overline{n}+\frac{1}{2}\right)\hbar\left[\omega_i(\overline{E}_{FBHD},\eta_g)\right]'\right.$$
$$+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[2[\rho^*(\overline{E}_{FBHD},\eta_g)[\rho^*(\overline{E}_{FBHD},\eta_g)'\right]$$
$$\left.\left.\left[\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\right]+\left[\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\right]'\left[\rho^*(\overline{E}_{FBHD},\eta_g)\right]^2\right]\right]\right] \tag{14.45}$$

$$\overline{m}_y^*(\overline{E}_{FBHD},\eta_g,\overline{n},\overline{E}_0)=(\overline{B}/\overline{E}_0)^2\left[\overline{m}_4^*(\overline{E}_{FBHD},\eta_g)\right]^{-3}\left[\overline{G}^*(\overline{E}_{FBHD},\eta_g)\right.$$
$$-\left(\overline{n}+\frac{1}{2}\right)\hbar\overline{\omega}_i(\overline{E}_{FBHD},\eta_g)+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho^*(\overline{E}_{FBHD},\eta_g)^2\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\right]$$
$$\left[\left[\overline{m}_4^*(\overline{E}_{FBHD},\eta_g)\right]\left[\left[\overline{G}^*(\overline{E}_{FBHD},\eta_g)\right]'-(\overline{n}+\frac{1}{2})\hbar\left[\omega_i(\overline{E}_{FBHD},\eta_g)\right]'\right.\right.$$
$$\left.+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\left[\rho^*(\overline{E}_{FBHD},\eta_g)^2\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\right]\right]\right]\left[\overline{m}_4^*(\overline{E}_{FBHD},\eta_g)\right]'$$
$$\left[\overline{G}^*(\overline{E}_{FBHD},\eta_g)\right]-\left(\overline{n}+\frac{1}{2}\right)\hbar\overline{\omega}_i(\overline{E}_{FBHD},\eta_g)$$
$$\left.+\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho^*(\overline{E}_{FBHD},\eta_g)^2\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\right]\right] \tag{14.46}$$

where

$$\overline{m}_4^*(\overline{E}_{FBHD},\eta_g)=\left[\left[\rho^*(\overline{E}_{FBHD},\eta_g)\right]\left[\frac{m_1^*(\overline{E}_{FBHD},\eta_g)}{m_2^*(\overline{E}_{FBHD},\eta_g)}\right]^{\frac{1}{2}}\right]$$

The Landau level energy (E_{n_g}) in this case can be expressed through the equation

$$\overline{G}^*(\overline{E}_{n_9},\eta_g)=\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_i(\overline{E}_{n_8},\eta_g)-\frac{\overline{E}_0^2}{2\overline{B}^2}\left[\rho^*(\overline{E}_{n_8},\eta_g)\right]^2\overline{m}_1^*(\overline{E}_{n_8},\eta_g) \tag{14.47}$$

The electron concentration can be written as

$$\overline{n}_0=\frac{2\overline{B}}{3\overline{L}_x\pi^2\hbar^2\overline{E}_0}\sum_{\overline{n}=0}^{\overline{n}_{\max}}\left[\overline{T}_{413HD}(\overline{n},\overline{E}_{FBHD},\eta_g)+\overline{T}_{414HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\right] \tag{14.48}$$

where

$$\overline{T}_{413HD}(\overline{n},\overline{E}_{FBHD},\eta_g)=\left[\frac{\sqrt{2\overline{m}_3^*(\overline{E}_{FBHD},\eta_g)}}{\rho^*(\overline{E}_{FBHD},\eta_g)}\right]\left[\left[\overline{T}_5(\overline{n},\overline{E}_{FBHD},\eta_g)+\frac{\overline{E}_0}{\overline{B}}\rho^*(\overline{E}_{FBHD},\eta_g)\hbar\overline{x}_{hHD}(\overline{E}_{FBHD},\eta_g)\rho^*(\overline{E}_{FBHD},\eta_g)\right]^{\frac{3}{2}}-\left[\overline{T}_5(\overline{n},\overline{E}_{FBHD},\eta_g)+\frac{\overline{E}_0}{\overline{B}}\rho^*(\overline{E}_{FBHD},\eta_g)\hbar\overline{x}_{lHD}(\overline{E}_{FBHD},\eta_g)\rho^*(\overline{E}_{FBHD},\eta_g)\right]^{\frac{3}{2}}\right],$$

$$\overline{T}_5(\overline{n},\overline{E}_{FBHD},\eta_g)=\left[\overline{G}^*(\overline{E}_{FBHD},\eta_g)-\left(\overline{n}+\frac{1}{2}\right)\hbar\omega_i(\overline{E}_{FBHD},\eta_g)+\frac{\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\overline{E}_0^2}{2\overline{B}^2}\left[\rho^*(\overline{E}_{FBHD},\eta_g)\right]^2\right]$$

$$\overline{x}_{lHD}(\overline{E}_{FBHD},\eta_g)=\frac{-\overline{m}_1^*(\overline{E}_{FBHD},\eta_g)\overline{E}_0\left[\rho^*(\overline{E}_{FBHD},\eta_g)\right]}{\overline{B}},\overline{x}_{hHD}(\overline{E}_{FBHD},\eta_g)=\frac{|e|\overline{BL}_x}{\hbar}+\overline{x}_{lHD}(\overline{E}_{FBHD},\eta_g)$$

and

$$\overline{T}_{414HD}(\overline{n},\overline{E}_{FBHD},\eta_g)\equiv\sum_{\overline{r}=1}^{\overline{s}}\overline{L}(\overline{r})\overline{T}_{413HD}(\overline{n},\overline{E}_{FBHD},\eta_g)$$

Using (1.31f) and (14.48), we can study the entropy in this case.

14.3 Open research problems

R.14.1 Investigate the entropy in the presence of an arbitrarily oriented quantizing magnetic and crossed electric fields in HD tetragonal materials by including broadening and the electron spin. Study all the special cases for HD III–V, ternary, and quaternary materials in this context.

R.14.2 Investigate the entropy for all models of HD IV–VI, II–VI, and stressed Kane-type compounds in the presence of an arbitrarily oriented quantizing magnetic and crossed electric fields by including broadening and electron spin.

R.14.3 Investigate the entropy for all the materials as stated in R.1.1 of Chapter 1 in the presence of an arbitrarily oriented quantizing magnetic and crossed electric fields by including broadening and electron spin.

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15 Appendix F: The numerical values of the energy band constants of few materials

Whenever we meet a man of high intellect, let us ask him what he reads

	Materials	Numerical Values of the Energy Band Constants
1	The conduction electrons of *n*-Cadmium Germanium Arsenide can be described by three types of band models	1. The values of the energy band constants in accordance with the generalized electron dispersion relation of nonlinear optical materials are as follows $\bar{E}_{g_0} = 0.57eV, \Delta_{\|\|} = 0.30eV, \Delta_{\perp} = 0.36eV$, $\bar{m}^*_{\|\|} = 0.034m_0, \bar{m}^*_{\perp} = 0.039\bar{m}_0, \bar{T} = 4\bar{K}, \bar{\delta} = -0.21eV, \bar{g}_v = 1$, $\varepsilon_{sc} = 18.4\varepsilon_0$ (ε_{sc} and ε_0 are the permittivity of the semiconductor material and free space, respectively) and $\bar{W}(electron\ affinity) = 4eV$ [1] 2. In accordance with the three-band model of Kane, the spectrum constants are given by $\Delta = (\Delta_{\|\|} + \Delta_{\perp})/2 = 0.33eV, \bar{E}_{g_0} = 0.57eV, \bar{m}_c = (\bar{m}^*_{\|\|} + \bar{m}^*_{\perp})/2 = 0.0365\bar{m}_0$ and $\bar{\delta} = 0eV$ 3. In accordance with two-band model of Kane, the spectrum constants are given by $\bar{E}_{g_0} = 0.57eV$ and $\bar{m}_c = 0.0365\bar{m}_0$
2	*n*-Indium arsenide	The values $\bar{E}_{g_0} = 0.36eV, \Delta = 0.43eV, \bar{m}_c = 0.026\bar{m}_0, \bar{g}_v = 1$, $\varepsilon_{sc} = 12.25\varepsilon_0$ are valid for three-band model of Kane.
4	*n*-Gallium aluminium arsenide	$\bar{E}_{g_0} = (1.424 + 1.266\bar{x} + 0.26\bar{x}^2)eV$, $\Delta = (0.34 - 0.5\bar{x})eV, \bar{g}_v = 1, \bar{m}_c = [0.066 + 0.088\bar{x}]\bar{m}_0$, $\varepsilon_{sc} = [13.18 - 3.12\bar{x}]\varepsilon_0$
5	*n*-Mercury cadmium telluride	$\bar{E}_{g_0} = (-0.302 + 1.93\bar{x} + 5.35 \times 10^{-4}(1-2x)T - 0.810\bar{x}^2 + 0.832\bar{x}^3)eV$, $\Delta = (0.63 + 0.24\bar{x} - 0.27\bar{x}^2)eV, \bar{m}_c = 0.1\bar{m}_0\bar{E}_{g_0}(eV)^{-1}, \bar{g}_v = 1$, $\varepsilon_{sc} = [20.262 - 14.812x + 5.22795\bar{x}^2]\varepsilon_0$ [1, 2] and $\bar{W} = (4.23 - 0.813(\bar{E}_{g_0} - 0.083))eV$
6	*n*-Indium gallium arsenide phosphide lattice matched to indium phosphide	$\bar{E}_{g_0} = (1.337 - 0.73\bar{y} + 0.13\bar{y}^2)eV, \Delta = (0.114 + 0.26y - 0.22\bar{y}^2)eV$, $\bar{y} = (0.1896 - 0.4052\bar{x})/(0.1896 - 0.0123\bar{x}), \bar{m}_c = (0.08 - 0.039\bar{y})\bar{m}_0$, $\bar{g}_v = 1, \varepsilon_{sc} = [10.65 + 0.1320\bar{y}]\varepsilon_0$ *and* $\bar{W}(\bar{x}, \bar{y}) = [5.06(1-\bar{x})\bar{y} + 4.38(1-\bar{x})(1-\bar{y}) + 3.64\bar{x}\,\bar{y} + 3.75\{\bar{x}(1-\bar{y})\}]eV$
7	*n*-Indium antimonide	$\bar{E}_{g_0} = 0.2352eV, \Delta = 0.81eV, \bar{m}_c = 0.01359\bar{m}_0, \bar{g}_v = 1, \varepsilon_{sc} = 15.56\varepsilon_0$ [1]
8	*n*-Gallium antimonide	The values of $\bar{E}_{g_0} = 0.81eV, \Delta = 0.80eV, \bar{P} = 9.48 \times 10^{-10}eV\bar{m}$, $\bar{\varsigma}_0 = -2.1, \bar{v}_0 = -1.49, \bar{\omega}_0 = 0.42, \bar{g}_v = 1$ [1–19] and $\varepsilon_{sc} = 15.85\varepsilon_0$ [1–19] are valid for the model of Seiler et. al.
9	*n*-Cadmium sulphide	$\bar{m}^*_{\|\|} = 0.7\bar{m}_0, \bar{m}^*_{\perp} = 1.5\bar{m}_0, \bar{C}_0 = 1.4 \times 10^{-8}eV\bar{m}, \bar{g}_v = 1$ [1], $\varepsilon_{sc} = 15.5\varepsilon_0$ [53] and $\bar{W} = 4.5eV$ [8]

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(continue)

	Materials	Numerical Values of the Energy Band Constants
10	*n*-Lead telluride	The values $\bar{m}_t^- = 0.070\bar{m}_0$, $\bar{m}_l^- = 0.54\bar{m}_0$, $\bar{m}_t^+ = 0.010\bar{m}_0$, $\bar{m}_l^+ = 1.4\bar{m}_0$, $\bar{P}_{\|} = 141\bar{m}eV\bar{n}\bar{m}$, $\bar{P}_{\perp} = 486\bar{m}eV\bar{n}\bar{m}$, $\bar{E}_{g_0} = 190\bar{m}eV$, $\bar{g}_v = 4$ [1], $\varepsilon_{sc} = 33\varepsilon_0$ [1, 18] and $\bar{W} = 4.6eV$ are valid for the Dimmock model [20]. The values $\bar{m}_1 = 0.0239\bar{m}_0$, $\bar{m}_2 = 0.024\bar{m}_0$, $\bar{m}_2{}' = 0.31\bar{m}_0$, $\bar{m}_3 = 0.24\bar{m}_0$ [21] are valid for the Cohen model [21–23] .
11	Stressed *n*-Indium antimonide	The values $m_c = 0.048m_o$, $E_{g_0} = 0.081eV$, $B_2 = 9\times10^{-10}eVm$, $C_1 = 3eV$, $C_2 = 2eV$, $\bar{a}_0 = -10eV$, $\bar{b}_0 = -1.7eV$, $\bar{d}_0 = -4.4eV$, $S_{xx} = 0.6\times10^{-3}(kbar)^{-1}$, $S_{yy} = 0.42\times10^{-3}(kbar)^{-1}$, $S_{zz} = 0.39\times10^{-3}(kbar)^{-1}$, $S_{xy} = 0.5\times10^{-3}(kbar)^{-1}$, $\varepsilon_{xx} = \sigma S_{xx}$, $\varepsilon_{yy} = \sigma S_{yy}$, $\varepsilon_{zz} = \sigma S_{zz}$, $\varepsilon_{xy} = \sigma S_{xy}$, σ is the stress in kilobar, $g_v = 1$ [24] are valid for the model of Seiler et. al. [24].
12	Bismuth	$E_{g_0} = 0.0153eV$, $m_1 = 0.00194m_0$, $m_2 = 0.313m_0$, $m_3 = 0.00246m_0$, $m'_2 = 0.36m_0$, $g_v = 3$ [25],$M_2 = 1.25m_0$, $M_2{}' = 0.36m_0$ [25, 26]
13	Mercury telluride	$m_v^* = 0.028m_0$, $g_v = 1$, $\varepsilon_\infty = 15.2\varepsilon_0$ [27]
14	Platinum antimonide	For valence bands, along <100> direction, $\bar{\lambda}_0 = (0.02/4)eV$, $\bar{l} = (-0.32/4)eV$, $\bar{v} = (0.39/4)eV$, $\bar{n} = (-0.65/4)eV$, $\bar{a} = 0.643nm$, $I = 0.30(eV)^2$, $\bar{\delta}_0 = 0.02eV$, $g_v = 6$[32], $\varepsilon_{sc} = 30\varepsilon_0$ [28–30] and $\phi_w \approx 3.0eV$ [31, 32]. For conduction bands, along <111> direction, $g_v = 8$[28–32], $\bar{\lambda}_0 = (0.33/4)eV$, $\bar{l} = (1.09/4)eV$, $\bar{v} = (0.17/4)eV$ and $\bar{n} = (0.22/4)eV$
15	Germanium	$E_{g_0} = 0.785eV$, $m_{\|}^* = 1.57m_0$, $m_{\perp}^* = 0.0807m_0$ [1] and $g_v = 4$
16	Tellurium	The values $\psi_1 = 6.7\times10^{-16}meVm^2$, $\psi_2 = 4.2\times10^{-16}meVm^2$, $\psi_3 = 6\times10^{-8}meVm$ and $\psi_4 = \left(3.6\times10^{-8}meVm\right)$ [33] are valid for the model of Bouat et. al. [33].
17	Lead germanium telluride	The values $g_v = 4$ [34–40] and $\phi_w \approx 6eV$ [34–40] are valid for the model of Vassilev [38]
18	Cadmium antimonide	The values $a_1 = -32.3\times10^{-20}eVm^2$, $b_1 = -60.7\times10^{-20}eVm^2$, $a_2 = -16.3\times10^{-20}eVm^2$, $b_2 = -24.4\times10^{-20}eVm^2$, $a_3 = -91.9\times10^{-20}eVm^2$, $b_3 = -105\times10^{-20}eVm^2$, $A = 2.92\times10^{-10}eVm$, $B = -3.47\times10^{-10}eVm$, $G_3 = 1.3\times10^{-10}eVm$, $\Delta_3 = 0.070eV$ [40]
19	Cadmium diphosphide	The values $\beta_1 = 8.6\times10^{-21}eVm^2$, $\beta_2 = 1.8\times10^{-21}(eVm)^2$, $\beta_4 = 0.0825eV$, $\beta_5 = -1.9\times10^{-19}eVm^2$are valid for the model of Chuiko [41–43].
20	Zinc diphosphide	The values$\beta_1 = 8.7\times10^{-21}eVm^2$, $\beta_2 = 1.9\times10^{-21}(eVm)^2$, $\beta_4 = 0.0875eV$, $\beta_5 = -1.9\times10^{-19}eVm^2$are valid for the model of Chuiko [31–43]

(continue)

	Materials	Numerical Values of the Energy Band Constants
21	Bismuth telluride	The values $E_{g_0} = 0.145eV$, $\bar{\alpha}_{11} = 4.9$, $\bar{\alpha}_{22} = 5.92$, $\bar{\alpha}_{33} = 9.5$, $\bar{\alpha}_{23} = 4.22$, $g_v = 6$[44–51] and $\phi_w = 5.3eV$ [51]
22		
23	Antimony	The values $\alpha_{11} = 16.7$, $\alpha_{22} = 5.98$, $\alpha_{33} = 11.61$, $\alpha_{23} = 7.54$ [50] and $W = 4.63eV$ are valid for the model of Ketterson [50]
24	Zinc selenide	$m_{c2} = 0.16m_0$, $\Delta_2 = 0.42eV$, $E_{g_{02}} = 2.82eV$
25	Lead selenide	$m_t^- = 0.23m_0$, $m_l^- = 0.32m_0$, $m_t^+ = 0.115m_0$, $m_l^+ = 0.303m_0$, $P_{\|\|} \approx 138meVnm$, $P_\perp = 471meVnm$, $E_{g_0} = 0.28eV$ [53], $\varepsilon_{sc} = 21.0\varepsilon_0$.

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