Sitangshu Bhattacharya Kamakhya Prasad Ghatak

# Effective Electron Mass in Low-Dimensional Semiconductors



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Sitangshu Bhattacharya Kamakhya Prasad Ghatak

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Sitangshu Bhattacharya
Department of Electronics Systems
Engineering, Nano Scale Device
Research Laboratory
Indian Institute of Science
Bangalore
India

Kamakhya Prasad Ghatak Department of Electronics and Communication Engineering National Institute of Technology Agartala, Tripura West India

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The first author dedicates this book to his beautiful and wonderful wife Rekha Verma, the source of inspiration to complete this monograph

The second author dedicates this monograph to the Jadavpur University, Kolkata for accepting him as the first recipient of the Degree of Doctor of Engineering in 1991 since the University inception in 1955

### **Preface**

The merging of the concept of introduction of asymmetry of the wave vector space of the charge carriers in semiconductors with the modern techniques of fabricating nanostructured materials such as MBE, MOCVD, and FLL in one, two, and three dimensions (such as UFs, nipi structures, inversion, and accumulation layers, quantum wire superlattices, carbon nanotubes, nanowires, quantum dots, magneto inversion and accumulation layers, quantum dot superlattices, etc.) spawns not only useful quantum effect devices but also unearths new concepts in the realm of low-dimensional materials science and related disciplines. It is worth remarking that these semiconductor nanostructures occupy a paramount position in the entire arena of nanoscience and technology by their own right and find extensive applications in quantum registers, resonant tunneling diodes and transistors, quantum switches, quantum sensors, quantum logic gates, hetero-junction fieldeffect transistors, quantum well and nanowire transistors, high-speed digital networks, high-frequency microwave circuits, quantum cascade lasers, high-resolution terahertz spectroscopy, superlattice photo-oscillator, advanced integrated circuits, superlattice photocathodes, thermoelectric devices, superlattice coolers, intermediate-band solar cells, micro-optical systems, high performance infrared imaging systems, band-pass filters, thermal sensors, optical modulators, optical switching systems, single electron/molecule electronics, nanotube-based diodes, and other nano-electronic devices. Knowledge regarding these quantized structures may be gained from original research contributions in scientific journals, proceedings of various international conferences, and different review articles respectively. Mathematician Simmons rightfully tells us [1] that the mathematical knowledge is said to be doubling in every 10 years and in this context we can also envision the extrapolation of the Moore's law by projecting it in the perspective of the advancement of new research and analyses, in turn, generating novel concepts particularly in the area of nanoscience and technology [2]. In this context, it may be noted that the available books on solid-state and allied sciences cannot afford to cover even an entire chapter excluding few pages on the Effective Electron Mass (EEM) in Low-Dimensional Semiconductors.

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The effective mass of the carriers in semiconductors, 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 [3]. The carrier degeneracy in semiconductors influences the effective mass when it is energy dependent. Under degenerate conditions, only the electrons at the Fermi surface of n-type semiconductors participate in the conduction process and hence, the effective mass of the electrons corresponding to the Fermi level 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 EEM in degenerate n-type semiconductors under the degree of carrier degeneracy. In recent years, various energy wave vector dispersion relations have been proposed [4–10] 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 quantising magnetic field under magnetic quantization, with the quantizing electric field as in inversion layers, with the nano-thickness as in UFs and nanowires and with superlattice period as in the quantum confined superlattices of small gap semiconductors with graded interfaces having various carrier energy spectra [11–57].

This book, divided into three parts which contain nine chapters and three Appendices, is partially based on our ongoing researches on the effective mass from 1980 and an attempt has been made to present a cross section of the effective mass for a wide range of low-dimensional semiconductors with varying carrier energy spectra under various physical conditions. The first part deals with the influence of quantum confinement on the EEM in non-parabolic semiconductors. Chapter 1 investigates the EEM in UFs of nonlinear optical materials on the basis of a generalized electron dispersion law introducing the anisotropies of the effective electron masses and the spin orbit splitting constants respectively together with the inclusion of the crystal field splitting within the framework of the k.p formalism. The results of III-V (e.g. InAs, InSb, GaAs, etc.), ternary (e.g. Hg<sub>1-x</sub>Cd<sub>x</sub>Te), quaternary (e.g. In<sub>1-x</sub>Ga<sub>x</sub>As<sub>1-v</sub>P<sub>v</sub> lattice matched to InP) compounds form a special case of our generalized analysis under certain limiting conditions. The EEM in UFs of II-VI, Bi, IV-VI, stressed Kane-type semiconductors, Te, GaP, PtSb<sub>2</sub>, Bi<sub>2</sub>Te<sub>3</sub>, Ge and GaSb compounds have also been investigated by using the appropriate energy band structures for these materials. The importance of the aforementioned semiconductors has also been described in the same chapter. It is well known that the semiconductor superlattices find extensive applications in avalanche photodiodes, photo-detectors, electro-optic modulators, etc. In Chap. 2 the EEM in nipi structures of nonlinear optical, III-V, II–VI, IV–VI, and stressed Kane-type semiconductors has been studied.

In recent years, there has been considerable interest in the study of the inversion layers which are formed at the surfaces of semiconductors in metal—oxide—semiconductor field-effect transistors (MOSFET) under the influence of a sufficiently strong electric field applied perpendicular to the surface by means of a large gate bias. In such layers, the carriers form a two-dimensional gas and are free to move

parallel to the surface while their motion is quantized perpendicular to it leading to the formation of electric subbands [58]. In Chap. 3, the EEM in *n*-channel inversion layers of nonlinear optical, III–V, II–VI, IV–VI stressed Kane-type semiconductors, Ge and GaSb has been investigated.

The effects of quantizing magnetic field on the band structures of compound semiconductors are more 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 [59-63] of various materials having different carrier dispersion relations [64]. In Chap. 4, the EEM in nonlinear optical, III-V. II-VI, Bi. IV-VI, stressed Kane-type semiconductors, Te, GaP, PtSb<sub>2</sub>, Bi<sub>2</sub>Te<sub>3</sub>, Ge, GaSb and II-V compounds have also been studied under magnetic quantization. Since Iijima's discovery [65], carbon nanotubes (CNTs) have been recognized as fascinating materials with nanometer dimensions uncovering new phenomena in different areas of nanoscience and technology. The remarkable physical properties of these quantum materials make them ideal candidates to reveal new phenomena in nano-electronics. Chapter 5 contains the study of the EEM in nanowires of the nonlinear optical, III-V, II-VI, Bi, IV-VI, stressed Kane-type semiconductors, Te, GaP, PtSb<sub>2</sub> Bi<sub>2</sub>Te<sub>3</sub>, Ge, GaSb and II-V semiconductors together with CNTs respectively.

With the advent of nanophotonics, there has been considerable interest in studying the optical processes in semiconductors and their nanostructures [66–67]. It appears from the literature that investigations have been carried out on the assumption that the carrier energy spectra are invariant quantities in the presence of intense light waves, which is not fundamentally true. The physical properties of semiconductors in the presence of light waves which change the basic dispersion relation have been relatively less investigated in the literature [68, 69]. The second part of this book studies the influence of light waves of the EEM in opto-electronic semiconductors and Chap. 6 investigates the influence of light waves on the EEM in quantum confined III-V, ternary, and quaternary semiconductors. Under external photo excitation the electron dispersion relation changes profoundly and the EEM has been studied by formulating a new electron dispersion law on the basis of k,p formalism. In the same chapter the influence of magnetic quantization on the EEM has been investigated. The same chapter also explores the effect of light waves on the EEM for 2D systems (e.g. UFs, nipi structures, and inversion layers), 1D systems (such as quantum wire effective mass superlattices, and quantum wire superlattices with graded interfaces) and the influence of quantizing magnetic field on the EEM for effective mass superlattices, and superlattices with graded interfaces respectively.

With the advent of nanodevices, the inbuilt electric field becomes so large that the electron energy spectrum changes fundamentally and the single Chap. 7 of the third part investigates the influence of intense electric field on the EEM in II–V, ternary

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and quaternary semiconductors. The same chapter also explores the influence of electric field on the 2D systems (e.g. UFs, nipi structures and inversion layers) and 1D systems (such as, nano wire effective mass superlattices, and nano wire superlattices with graded interfaces) in this context. Chapter 8 contains the applications and brief review of experimental results. Chapter 9 contains the conclusion and the scope for future research.

It may be noted that the influence of crossed electric and quantizing magnetic fields on the transport properties of semiconductors 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. 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 dispersion relations of the conduction electrons in semiconductors become modified and for which the electron moves in both the z and y directions. The motion along y-direction is purely due to the presence of  $E_0$  along x-axis and in the absence of electric field, the EEM along y-axis tends to infinity which indicates the fact that the electron motion along y-axis is forbidden. The EEM of the isotropic, bulk semiconductors 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 EEM along z-axis is a constant quantity. In 1966, Zawadzki and Lax [70] formulated the electron dispersion law for III-V semiconductors 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 [71–77].

Appendix A investigates the EEM under cross field configuration in nonlinear optical, III-V, II-VI, Bi, IV-VI, and stressed Kane-type semiconductors and ultra thin films of the aforementioned materials. It is an amazing fact that though heavily doped semiconductors have been deeply studied in the literature but the study of the carrier transport in heavily doped materials through proper formulation of the Boltzmann transport equation which needs in turn, the corresponding heavily doped carrier energy spectra is still one of the open research problems [78–81]. Appendix B attempts to touch the enormous field of active research with respect to EEM of heavily doped compound semiconductors in a nutshell. Appendix C deals with the EEM in III-V, II-VI, IV-VI, HgTe/CdTe, and strained layer heavily doped superlattices with graded interfaces and effective mass superlattices of the said constituent materials. In these appendices no graphs together with results and discussions are being presented since we feel that the readers will enjoy the complex computer algorithm to investigate the EEM in the respective case generating new physics and thereby transforming each appendix into a short monograph by considering various materials having different dispersion relations. Since there is no existing book devoted totally to the EEM in low-dimensional semiconductors to the best of our knowledge, we hope that this book will be a useful reference source for the present and the next generation of readers and researchers of materials and allied sciences in general. In spite of our Preface xi

joint efforts, the production of error-free first edition of any book from every point of view enjoys permanently the domain of impossibility theorems and the same stands very true for this monograph also. Various expressions of this book have been appearing for the first time in printed form. The suggestions of the readers for the development of this book will be highly appreciated for the purpose of future edition, if any.

In this book, from Chap. 1 till the end, we have presented 250 open research problems in this particular topic. The problems presented here are the integral part of this book and will be useful for the readers to initiate their own contributions on the effective mass. This aspect is also important for Ph.D. aspirants and researchers. Each chapter ends with a table containing the main results excluding the last two and the Appendices.

In this monograph, we have investigated various dispersion relations of different quantized structures and the corresponding electron statistics to study effective mass. Our theoretical formulation of the density-of-states effective mass of tetragonal materials based on our generalized electron dispersion relation agrees well with the available experimental data as given elsewhere [82]. Thus, in this book, the readers will get a lot of information regarding quantum confined low-dimensional materials having different band structures. Although the name of the book is extremely specific, from the content, one can infer that it should be useful in graduate courses on materials science, nanoscience and technology, solid-state science, semiconductor physics, and nanostructured devices in many universities and institutes. Last but not the least, we do hope that our humble effort will kindle the desire to delve deeper into this fascinating topic by anyone engaged in materials research and device development either in academics or in industries.

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Acknowledgment by Kamakhya Prasad Ghatak

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Like the first author, I am ever grateful to Professor A. N. Chakravarti, my Ph.D. thesis advisor and mentor who convinced a 21-year-old Circuit theorist that theoretical semiconductor science is the hidden dual dance of quantum mechanics and statistical mechanics, and even to appreciate the incredible beauty, he placed a stiff note for me to understand deeply the Course of Theoretical Physics, the Classics of Landau–Lifshitz together with the two-volume classics of Morse-Feshbach 35 years ago. I am grateful to Professor P. K. Bose, Director, National Institute of Technology, Agartala, Tripura my present mentor at the last phase of my academic life and a very pivotal person in my academic career, for instigating me to carry out extensive research by ignoring all the difficulties. I express my gratitude to Professors R. K. Poddar and R. N. Basu, Ex-Vice Chancellors of the University of Calcutta, Professors S. K. Sen and A. N. Basu, Ex-Vice Chancellors of Jadavpur University, and Professor D. K. Basu, Ex-Vice Chancellor of Burdwan and Tripura Universities, the five pivotal persons in the research growth of my career. I am grateful to Professors S. C. Dasgupta, P. K. Choudhury, M. Mitra and S. Sarkar of the Department of Mathematics of the then Bengal Engineering College (presently Bengal Engineering and Science University), Shibpur, Howrah for creating the interest in various topics of Engineering Mathematics when I was pursuing the bachelor degree in the branch of Electronics and Telecommunication Engineering 40 years ago. I am indebted to Late Professor C. K. Majumdar of the Department of Physics of the University of Calcutta for lighting the fire for Theoretical Physics. I express my gratitude to Professors H. L. Hartnagel, D. Bimberg, W. L. Freeman, and W. Schommers for various academic interactions spanning the last two decades. The well-known scientist Late Professor P. N. Butcher has been a steady hidden force since 1987, before his demise, with respect to our scripting the series in band structure-dependent properties of nanostructured materials. He insisted to me repeatedly regarding it and to tune with his high rigorous academic standard, my colleagues and I wrote the Einstein Relation in Compound Semiconductors and their Nanostructures, Springer Series in Materials Science, Vol. 116, 2009 as the first one, Photoemission from Optoelectronic Materials and their Nanostructures, Springer Series in Nanostructure Science and Technology, 2009 as the second one, "Thermoelectric Power in Nano-Structured Materials Under Strong Magnetic Fields", Springer Series in Materials Science, Vol. 137, 2010 as the third one, "Fowler-Nordheim Field Emission :Effects in Semiconductor Nanostructures", Springer Series in Solid State Sciences, Vol 170, 2012 as the fourth one, and the present monograph as the fifth one.

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Bangalore, India Tripura, India S. Bhattyacharya K. P. Ghatak

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### Part I Influence of Quantum Confinement on the Effective Electron Mass (EEM) in Non-Parabolic Semiconductors

### Chapter 1 The EEM in Ultrathin Films (UFs) of Nonparabolic Semiconductors

### 1.1 Introduction

The concept of the effective mass of the carriers in semiconductors is one of the basic pillars in the realm of solid state and related sciences [1]. It must be noted that among the various definitions of the effective electron mass (e.g effective acceleration mass, density-of-state effective mass, concentration effective mass, conductivity effective mass, Faraday rotation effective mass, etc) [2], it is the effective momentum mass that should be regarded as the basic quantity [3]. This is due to the fact that it is this mass which appears in the description of transport phenomena and all other properties of the conduction electrons in a semiconductor with arbitrary band nonparabolicity [3]. It can be shown that it is the effective momentum mass which enters in various transport coefficients and plays the most dominant role in explaining the experimental results of different scattering mechanisms through Boltzmann's transport equation [4, 5]. The carrier degeneracy in semiconductors influences the effective mass when it is energy dependent. Under degenerate conditions, only the electrons at the Fermi surface of n-type semiconductors participate in the conduction process and hence, the effective momentum mass of the electrons (EEM) corresponding to the Fermi level would be of interest in electron transport under such conditions. The Fermi energy is again determined by the carrier energy spectrum and the electron statistics and therefore, these two features would determine the dependence of the EEM in degenerate n-type semiconductors under the degree of carrier degeneracy. In recent years, various energy wave vector dispersion relations have been proposed [6–38] which have created the interest in studying the EEM in such materials under external conditions. The nature of these variations has been investigated in the literature [39–85]. Some of the significant features, which have emerged from these studies, are:

- (a) The EEM increases monotonically with electron concentration.
- (b) The EEM increases with doping in heavily doped materials in the presence of band tails

- (c) The nature of variations is significantly influenced by the energy band constants of various materials having different band structures.
- (d) The EEM oscillates with inverse quantizing magnetic field due to SdH effect. The EEM in Bismuth under magnetic quantization depends both on the Fermi energy and on the magnetic quantum number due to the presence of band nonparabolicity only.
- (e) The EEM increases with the magnitude of the quantizing electric field in n-channel inversion layers of III-V semiconductors and depend on the subband index for both low and high electric field limits.
- (f) The EEM in ultrathin films of nonlinear optical materials depends on the Fermi energy and size quantum numbers due to the specific dispersion relations.
- (g) The EEM has significantly different values in superlattices and also in the presence of quantum confined superlattices of small gap semiconductors with graded interfaces.

In recent years, with the advent of fine lithographical methods [86, 87] molecular beam epitaxy [88], organometallic vapor-phase epitaxy [89], and other experimental techniques, the restriction of the motion of the carriers of bulk materials in one (ultrathin films, NIPI structures, inversion, and accumulation layers), two (nanowires) and three (quantum dots, magnetosize quantized systems, magneto accumulation layers, magneto inversion layers, quantum dot superlattices, magneto ultrathin film superlattices, and magneto NIPI structures) dimensions have in the last few years, attracted much attention not only for their potential in uncovering new phenomena in nanoscience but also for their interesting quantum device applications [90–93]. In ultrathin films (UFs), 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 carrier 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 semiconductors [94–98]. The low-dimensional heterostructures based on various materials are widely investigated because of the enhancement of carrier mobility [99]. These properties make such structures suitable for applications in ultrathin film lasers [100], heterojunction FETs [101, 102], high-speed digital networks [103–106], high-frequency microwave circuits [107], optical modulators [108], optical switching systems [109], and other devices. The constant energy 3D wave-vector space of bulk semiconductors becomes 2D wave-vector surface in UFs 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 EEM in UFs of nonparabolic semiconductors having different band structures. At first we shall investigate the EEM in UFs of nonlinear optical compounds which are being used in nonlinear optics and light emitting diodes [110]. 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

1.1 Introduction 5

of the nonlinear optical compounds, Kildal [111] 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 the two aforementioned band constants are the significant physical features of the said materials [112–114]. In Sect. 1.2.1, the EEM in UFs of nonlinear optical semiconductors has been investigated 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 k.p formalism. The III-V compounds find applications in infrared detectors [115], quantum dot light emitting diodes [116], quantum cascade lasers [117], ultrathin film wires [118], optoelectronic sensors [119], high electron mobility transistors [120], etc. The electron energy spectrum of III-V semiconductors can be described by the three- and two-band models of Kane [121, 122], together with the models of Stillman et al. [123], Newson and Kurobe [124] and, Palik et al. [125] 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  $Hg_{1-x}Cd_x$ Te 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  $30 \,\mu\text{m}$  [126] by adjusting the alloy composition.  $\text{Hg}_{1-x}\text{Cd}_x$  Te finds extensive applications in infrared detector materials and photovoltaic detector arrays in the 8–12 µm wave bands [127]. The above uses have generated the  $Hg_{1-x}Cd_x$ Te 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 subband physics because the relevant material constants can easily be experimentally measured [128]. 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 photodetectors [129], hetero-junction lasers [130], light emitting diodes [131] and avalanche photodiodes[132], field effect transistors, detectors, switches, modulators, solar cells, filters, and new types of integrated optical devices are made from the quaternary systems [133]. It may be noted that all types of band models as discussed for III-V semiconductors are also applicable for ternary and quaternary compounds. In Sect. 1.2.2, the EEM in UFs of III-V, ternary and quaternary semiconductors has been studied in accordance with the said band models and the simplified results for wide gap materials having parabolic energy bands under certain limiting conditions have further been demonstrated as a special case and thus confirming the compatibility test.

The II-VI semiconductors are being used in nanoribbons, 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 [134–141]. The carrier energy spectra in II-VI compounds are defined by the Hopfield model [142] where the splitting of the two-spin states by the spin-orbit coupling and the crystalline field has been taken into account. The Sect. 1.2.3 contains the investigation of the EEM in UFs of II-VI compounds.

In recent years, Bismuth (Bi) nanolines have been fabricated and Bi also finds use in array of antennas which leads to the interaction of electromagnetic waves

with such Bi-nanowires [143, 144]. Several dispersion relations of the carriers have been proposed for Bi. Shoenberg [145, 146] experimentally verified that the de Haas-Van Alphen and cyclotron resonance experiments supported the ellipsoidal parabolic model of Bi, although, the magnetic field dependence of many physical properties of Bi supports the two-band model [147]. The experimental investigations on the magneto-optical and the ultrasonic quantum oscillations support the Lax ellipsoidal nonparabolic model [147]. Kao [148], Dinger and Lawson [149] and Koch and Jensen [150] demonstrated that the Cohen model [151] is in conformity with the experimental results in a better way. Besides, the hybrid model of bismuth, as developed by Takoka et al., also finds use in the literature [152]. McClure and Choi [153] derived a new model of Bi and they showed that it can explain the data for a large number of magneto-oscillatory and resonance experiments.

In Sect. 1.2.4, the EEM in UFs of Bi has been formulated in accordance with the aforementioned energy band models for the purpose of relative assessment. Besides, under certain limiting conditions all the results for all the models of 2D systems are reduced to the well-known result of the EEM in UFs of wide gap materials. This above statement exhibits the compatibility test of our theoretical analysis.

Lead chalcogenides (PbTe, PbSe, and PbS) are IV-VI nonparabolic semiconductors whose studies over several decades have been motivated by their importance in infrared IR detectors, lasers, light-emitting devices, photovoltaics, and high temperature thermoelectrics [154–158]. PbTe, in particular, is the end compound of several ternary and quaternary high performance high temperature thermoelectric materials [159–163]. It has been used not only as bulk but also as films [164–167], ultrathin films [168] superlattices [169, 170] nanowires [171] and colloidal and embedded nanocrystals [172–175], and PbTe films doped with various impurities have also been investigated [176–183] 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 [184]. In Sect. 1.2.5, the EEM in UFs of IV-VI semiconductors has been studied taking PbTe, PbSe, and PbS as examples.

The stressed semiconductors are being investigated for strained silicon transistors, quantum cascade lasers, semiconductor strain gages, thermal detectors, and strained-layer structures [185–188]. The EEM in UFs of stressed compounds (taking stressed n-InSb as an example) has been investigated in Sect. 1.2.6 The vacuum deposited Tellurium (Te) has been used as the semiconductor layer in thin-body transistors (TFT) [189] which is being used in  $CO_2$  laser detectors [190], electronic imaging, strain sensitive devices [191, 192], and multichannel Bragg cell [193]. Section 1.2.7 contains the investigation of EEM in UFs of Tellurium.

The n-Gallium Phosphide (n-GaP) is being used in quantum dot light emitting diode [194], 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 [195–197]. In Sect. 1.2.8, the EEM in UFs of n-GaP has been studied. The Platinum Antimonide (PtSb<sub>2</sub>) finds application in device miniaturization, colloidal nanoparticle synthesis, sensors and detector materials and thermo-photovoltaic devices [198–200]. Section 1.2.9 explores the EEM in UFs of PtSb<sub>2</sub>.Bismuth telluride

1.1 Introduction 7

(Bi<sub>2</sub>Te<sub>3</sub>) was first identified as a material for thermoelectric refrigeration in 1954 [201] and its physical properties were later improved by the addition of bismuth selenide and antimony telluride to form solid solutions [202–206]. The alloys of Bi<sub>2</sub>Te<sub>3</sub> are useful compounds for the thermoelectric industry and have been investigated in the literature [202–206]. In Sect. 1.2.10, the EEM in UFs of Bi<sub>2</sub>Te<sub>3</sub> 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 [207–210]. In Sect. 1.2.11, the EEM has been studied in UFs of Ge. Gallium Antimonide (GaSb) finds applications in the fiber optic transmission window, heterojunctions, and ultrathin films. A complementary heterojunction 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 [211–216]. In Sect. 1.2.12, the EEM in UFs of GaSb has been studied. Section 1.3 contains the result and discussions pertaining to this chapter. The last Sect. 1.4 contains open research problems.

### 1.2 Theoretical Background

### 1.2.1 The EEM in UFs of Nonlinear Optical Semiconductors

The form of k.p matrix for nonlinear optical compounds can be expressed extending Bodnar [112] as

$$H = \begin{bmatrix} H_1 & H_2 \\ H_2^+ & H_1 \end{bmatrix} \tag{1.1}$$

where,

$$H_{1} \equiv \begin{bmatrix} E_{g0} & 0 & P_{\parallel}k_{z} & 0 \\ 0 & (-2\Delta_{\parallel}/3) & (\sqrt{2}\Delta_{\perp}/3) & 0 \\ P_{\parallel}k_{z} & (\sqrt{2}\Delta_{\perp}/3) & -(\delta + \frac{1}{3}\Delta_{\parallel}) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$H_2 \equiv \begin{bmatrix} 0 & -f_{,+} & 0 & f_{,-} \\ f_{,+} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ f_{,+} & 0 & 0 & 0 \end{bmatrix}$$

in which  $E_{g_0}$  is the band gap in the absence of any field,  $P_{\parallel}$  and  $P_{\perp}$  are the momentum matrix elements parallel and perpendicular to the direction of crystal axis respectively,

 $\delta$  is the crystal-field splitting constant,  $\Delta_{\parallel}$  and  $\Delta_{\perp}$  are the spin-orbit splitting constants parallel and perpendicular to the C-axis respectively,  $f_{,\pm} \equiv \left(P_{\perp}/\sqrt{2}\right)\left(k_x \pm ik_y\right)$  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 semiconductors as

$$\gamma(E) = f_1(E)k_s^2 + f_2(E)k_z^2 \tag{1.2}$$

where,

$$\begin{split} \gamma(E) &\equiv E(E+E_{g_0}) \left[ (E+E_{g_0})(E+E_{g_0}+\Delta_{\parallel}) + \delta \left(E+E_{g_o}+\frac{2}{3}\Delta_{\parallel}\right) \right. \\ &\left. + \frac{2}{9}(\Delta_{\parallel}^2-\Delta_{\perp}^2) \right], \end{split}$$

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,  $k_s^2 = k_x^2 + k_y^2$ ,

$$\begin{split} f_1(E) &\equiv \frac{\hbar^2 E_{g_0} \left( E_{g_0} + \Delta_{\perp} \right)}{\left[ 2m_{\perp}^* \left( E_{g_0} + \frac{2}{3} \Delta_{\parallel} \right) \right]} \\ &\times \left[ \delta \left( E + E_{g_0} + \frac{1}{3} \Delta_{\parallel} \right) + (E + E_{g_0}) \left( E + E_{g_0} + \frac{2}{3} \Delta_{\parallel} \right) + \frac{1}{9} (\Delta_{\parallel}^2 - \Delta_{\parallel}^2) \right] \end{split}$$

$$f_2(E) \equiv \frac{\hbar^2 E_{g_0} \left( E_{g_0} + \Delta_{\parallel} \right)}{\left[ 2m_{\parallel}^* \left( E_{g_0} + \frac{2}{3} \Delta_{\parallel} \right) \right]} \left[ (E + E_{g_0}) \left( E + E_{g_0} + \frac{2}{3} \Delta_{\parallel} \right) \right], \quad \hbar = h/2\pi,$$

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

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (1.2) as

$$\psi_1(E) = \psi_2(E)k_s^2 + \psi_3(E)(n_z\pi/d_z)^2$$
(1.3)

where  $\psi_1(E) = \gamma(E)$ ,  $\psi_2(E) = f_1(E)$ ,  $\psi_3(E) = f_2(E)$ ,  $n_z = 1, 2, 3, ...$ ) and  $d_z$  are the size quantum number and the nano-thickness along the z-direction respectively.

The EEM is defined as the ratio of the electron momentum to the group velocity. The EEM at the Fermi level in the *xy*-plane can be written as

$$m^*(E_F, n_z) = \hbar^2 k_s \left. \frac{\partial k_s}{\partial E} \right|_{E=E_F} \tag{1.4}$$

where  $E_{Fs}$  is the Fermi energy in the presence of size quantization as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization. From (1.3) and (1.4), the EEM in this case can be written as

$$m^{*}(E_{Fs}, n_{z}) = \left(\frac{\hbar^{2}}{2}\right) [\psi_{2}(E_{Fs})]^{-2} \left[ \psi_{2}(E_{Fs}) \left\{ \{\psi_{1}(E_{Fs})\}' - \{\psi_{3}(E_{Fs})\}' \left(\frac{n_{z}\pi}{d_{z}}\right)^{2} \right\} - \left\{ \psi_{1}(E_{Fs}) - \psi_{3}(E_{Fs}) \left(\frac{n_{z}\pi}{d_{z}}\right)^{2} \right\} \{\psi_{2}(E_{Fs})\}' \right]$$

$$(1.5)$$

where, the primes denote the differentiation of the differentiable functions with respect to Fermi energy. Thus, we observe that the EEM is the function of size quantum number and the Fermi energy due to the combined influence of the crystal-field splitting constant and the anisotropic spin-orbit splitting constants respectively. To study the dependence of the EEM as a function of electron concentration per unit area we have to formulate the corresponding density-of-states function (DOS).

The general expression of the total 2D DOS  $(N_{2DT}(E))$  in this case is given by

$$N_{2DT}(E) = \frac{2g_v}{(2\pi)^2} \sum_{n_z=1}^{n_{zmax}} \frac{\partial A(E, n_z)}{\partial E} H(E - E_{n_z})$$
 (1.6)

where,  $g_v$  is the valley degeneracy,  $A(E, n_z)$  is the area of the constant energy 2D wave vector space for UFs,  $H(E - E_{n_z})$  is the Heaviside step function and  $(E_{n_z})$  is the corresponding subband energy. Using (1.3) and (1.6), the expression of the  $N_{2DT}(E)$  for UFs of nonlinear optical semiconductors can be written as

$$N_{2DT}(E) = \left(\frac{g_{\nu}}{2\pi}\right) \sum_{n_z=1}^{n_{z_{max}}} \left[\psi_2(E)\right]^{-2} \left[\psi_2(E) \left\{ \{\psi_1(E)\}' - \{\psi_3(E)\}' \left(\frac{n_z \pi}{d_z}\right)^2 \right\} - \left\{\psi_1(E) - \psi_3(E) \left(\frac{n_z \pi}{d_z}\right)^2 \right\} \left\{\psi_2(E)\}' \right] H(E - E_{n_{z_1}})$$
(1.7)

where, the subband energies  $(E_{n_{z_1}})$  in this case is given by

$$\psi_1(E_{n_{z_1}}) = \psi_2(E_{n_{z_1}})(n_z \pi/d_z)^2$$
(1.8)

Combining (1.7) with the Fermi-Dirac occupation probability factor, integrating between  $E_{n_{z_1}}$  to infinity and applying the generalized Somerfeld's lemma, the 2D carrier statistics in this case assumes the form

$$n_{2D} = \frac{g_v}{2\pi} \sum_{n_x=1}^{n_{x_{max}}} \left[ T_{51} \left( E_{Fs}, n_z \right) + T_{52} \left( E_{Fs}, n_z \right) \right]$$
 (1.9)

where,

$$T_{51}(E_{Fs}, n_z) \equiv \left[ \frac{\psi_1(E_{Fs}) - \psi_3(E_{Fs})(n_z \pi/d_z)^2}{\psi_2(E_{Fs})} \right],$$

$$T_{52}(E_{Fs}, n_z) \equiv \sum_{r=1}^{s} L(r)[T_{51}(E_{Fs}, n_z)],$$

 $L(r) = 2(k_BT)^{2r}(1-2^{1-2r})\xi(2r)\frac{\partial^{2r}}{\partial E_f^{2r}}, k_B$  is the Boltzmann constant, T is the temperature, r is the set of real positive integers whose upper limit is s,  $\xi(2r)$  is the Zeta function of order 2r [217].

### 1.2.2 The EEM in UFs of III-V Semiconductors

The dispersion relation of the conduction electrons of III-V compounds are described by the models of Kane (both three and two bands) [121, 122], Stillman et al. [123], Newson and Kurobe [124] and Palik et al. [125] respectively. For the purpose of complete and coherent presentation, the EEM in UFs of III-V semiconductors have also been investigated in accordance with the aforementioned different dispersion relations for the purpose of relative comparison as follows:

(a) The three-band model of Kane

Under the conditions,  $\delta=0$ ,  $\Delta_{\parallel}=\Delta_{\perp}=\Delta$  (isotropic spin orbit splitting constant) and  $m_{\perp}^*=m_{\perp}^*=m_c$  (isotropic effective electron mass at the edge of the conduction band), (1.2) gets simplified into the form

$$\frac{\hbar^2 k^2}{2m_c} = I_{11}(E), I_{11}(E) \equiv \frac{E(E + E_{g_0})(E + E_{g_0} + \Delta)(E_{g_0} + \frac{2}{3}\Delta)}{E_{g_0}(E_{g_0} + \Delta)(E + E_{g_0} + \frac{2}{3}\Delta)}$$
(1.10)

which is known as the three-band model of Kane [121, 122] and is often used to study the electronic properties of III-V materials.

Thus, under the conditions  $\delta=0$ ,  $\Delta_{\parallel}=\Delta_{\perp}=\Delta$  and  $m_{\parallel}^*=m_{\perp}^*=m_c$ , (1.3) assumes the form

$$\frac{\hbar^2 k_s^2}{2m_c} + \frac{\hbar^2}{2m_c} (n_z \pi / d_z)^2 = I_{11}(E)$$
 (1.11)

Using (1.11) and (1.4), the EEM in x-y plane for this case can be written as

$$m^*(E_{Fs}) = m_c \{I_{11}(E_{Fs})\}'$$
 (1.12)

It is worth noting 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 can be written as

$$N_{2DT}(E) = \left(\frac{m_c g_v}{\pi \hbar^2}\right) \sum_{n_z=1}^{n_{z_{max}}} \left\{ [I_{11}(E)]' H\left(E - E_{n_{z_2}}\right) \right\}$$
(1.13)

where, the subband energies  $E_{n_{z_2}}$  can be expressed as

$$I_{11}(E_{n_{z_2}}) = \frac{\hbar^2}{2m_c} (n_z \pi / d_z)^2$$
 (1.14)

The 2D carrier concentration assumes the form

$$n_{2D} = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z,max}} [T_{53}(E_{Fs}, n_z) + T_{54}(E_{Fs}, n_z)]$$
 (1.15)

where

$$T_{53}(E_{Fs}, n_z) \equiv \left[ I_{11}(E_{Fs}) - \frac{\hbar^2}{2m_c} \left( \frac{n_z \pi}{d_z} \right)^2 \right]$$
 and  $T_{54}(E_{Fs}, n_z) \equiv \sum_{r=1}^s L(r) T_{53}(E_{Fs}, n_z).$ 

Under the inequalities  $\Delta \gg E_{g_0}$  or  $\Delta \ll E_{g_0}$  (1.10) can be expressed as

$$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2m_c}$$
 (1.16)

where,  $\alpha \equiv 1/E_{g_0}$  and is known as band nonparabolicity.

It may be noted that (1.16) 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 optoelectronic materials whose energy band structures obey the aforementioned inequalities. Under the said inequalities (1.11) assumes the form

$$E(1 + \alpha E) = \frac{\hbar^2 k_s^2}{2m_c} + \frac{\hbar^2}{2m_c} \left(\frac{n_z \pi}{d_z}\right)^2$$
 (1.17)

The EEM in this case can be written as

$$m^*(E_{Fs}) = m_c(1 + 2\alpha E_{Fs}) \tag{1.18}$$

Thus, we observe that the EEM in the present case is a function of Fermi energy only due to the presence of band nonparabolicity.

The total 2D DOS function assumes the form

$$N_{2DT}(E) = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z,max}} (1 + 2\alpha E) H\left(E - E_{n_{z_3}}\right)$$
(1.19)

where, the subband energy  $(E_{n_{z_3}})$  can be expressed as

$$\frac{\hbar^2}{2m_c} (n_z \pi / d_z)^2 = E_{n_{z_3}} \left( 1 + \alpha E_{n_{z_3}} \right)$$
 (1.20)

The 2D electron statistics can be written as

$$n_{2D} = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{\infty} \int_{E_{n_{z3}}}^{\infty} \frac{(1 + 2\alpha E)dE}{1 + exp\left(\frac{E - E_{Fs}}{k_B T}\right)}$$

$$= \frac{m_c k_B T g_v}{\pi \hbar^2} \sum_{n_*=1}^{n_{z_{max}}} \left[ (1 + 2\alpha E_{n_{z_3}}) F_0(\eta_{n_1}) + 2\alpha k_B T F_1(\eta_{n_1}) \right]$$
(1.21)

where,  $\eta_{n_1} \equiv (E_{Fs} - E_{n_{z_3}})/k_BT$  and  $F_j(\eta)$  is the one-parameter Fermi-Dirac integral of order j which can be written [218, 219] as

$$F_{j}(\eta) = \left(\frac{1}{\Gamma(j+1)}\right) \int_{0}^{\infty} \frac{x^{j} dx}{1 + \exp(x - \eta)}, \quad j > -1$$
 (1.22)

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

$$F_{j}(\eta) = \left(\frac{\Gamma(-j)}{2\pi\sqrt{-1}}\right) \int_{-\infty}^{+0} \frac{x^{j} dx}{1 + \exp(-x - \eta)}$$
(1.23)

where  $\eta$  is the dimensionless x independent variable.

Under the condition  $\alpha \to 0$ , the expressions of total 2D DOS, for UFs whose bulk electrons are defined by the isotropic parabolic energy bands can, be written as

$$N_{2DT}(E) = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z,max}} H\left(E - E_{n_{z_p}}\right)$$
 (1.24)

The subband energy  $(E_{n_{z_p}})$ , the EEM, and the  $n_{2D}$  can respectively be expressed as

$$E_{n_{zp}} = \frac{\hbar^2}{2m_c} \left(\frac{n_z \pi}{d_z}\right)^2 \tag{1.25}$$

$$m^*(E_{F_S}) = m_C (1.26)$$

and

$$n_{2D} = \frac{m_c k_b T g_v}{\pi \hbar^2} \sum_{n_r=1}^{n_{zmax}} F_0(\eta_{n_2})$$
 (1.27)

where, 
$$\eta_{n_2} \equiv \frac{1}{k_B T} \left[ E_{Fs} - \frac{\hbar^2}{2m_c} \left( \frac{n_z \pi}{d_z} \right)^2 \right]$$

It may be noted that the results of this section are already well known in the literature [220].

(b) The model of Stillman et al.

In accordance with the model of Stillman et al. [123], the electron dispersion law of III-V materials assumes the form

$$E = \bar{t}_{11}k^2 - \bar{t}_{12}k^4 \tag{1.28}$$

where,

$$\bar{t}_{11} \equiv \frac{\hbar^2}{2m_c}; \bar{t}_{12} \equiv \left(1 - \frac{m_c}{m_0}\right)^2 \left(\frac{\hbar^2}{2m_c}\right)^2 \times \left[\left(3E_{g_0} + 4\Delta + \frac{2\Delta^2}{E_{g_0}}\right) \cdot \left\{(E_{g_0} + \Delta)(2\Delta + 3E_{g_0})\right\}^{-1}\right]$$

and  $m_0$  is the free electron mass.

Equation (1.28) can be expressed as

$$\frac{\hbar^2 k^2}{2m_c} = I_{12}(E) \tag{1.29}$$

where, 
$$I_{12}(E) \equiv a_{11} \left[ 1 - (1 - a_{12}E)^{1/2} \right]$$
,  $a_{11} \equiv \left( \frac{\hbar^2 \bar{t}_{11}}{4m_c \bar{t}_{12}} \right)$  and  $a_{12} \equiv \frac{4\bar{t}_{12}}{\bar{t}_{11}^2}$ .

The 2D electron dispersion relation in this case assumes the form

$$\frac{\hbar^2 k_s^2}{2m_c} + \frac{\hbar^2}{2m_c} (n_z \pi / d_z)^2 = I_{12}(E)$$
 (1.30)

Using (1.30) and (1.4), the EEM in x-y plane for this case can be written as

$$m^*(E_{Fs}) = m_c \{I_{12}(E_{Fs})\}'$$
 (1.31)

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 can be written as

$$N_{2DT}(E) = \left(\frac{m_c g_v}{\pi \hbar^2}\right) \sum_{n_*=1}^{n_{z_{max}}} \left\{ [I_{12}(E)]' H(E - E_{n_{z_3}}) \right\}$$
(1.32)

where, the subband energies  $E_{n_{z_3}}$  can be expressed as

$$I_{12}(E_{n_{z_3}}) = \frac{\hbar}{2m_c} (n_z \pi / d_z)^2$$
 (1.33)

The 2D carrier concentration assumes the form

$$n_{2D} = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z_{max}}} \left[ T_{55}(E_{Fs}, n_z) + T_{56}(E_{Fs}, n_z) \right]$$
 (1.34)

where

$$T_{55}(E_{Fs}, n_z) \equiv \left[ I_{12}(E_{Fs}) - \frac{\hbar^2}{2m_c} \left( \frac{n_z \pi}{d_z} \right)^2 \right]$$
 and  $T_{56}(E_{Fs}, n_z) \equiv \sum_{r=1}^s L(r) T_{55}(E_{Fs}, n_z)$ 

### (c) Model of Palik et al.

The energy spectrum of the conduction electrons in III-V semiconductors 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. [125] as

$$E = \frac{\hbar^2 k^2}{2m_c} - \bar{B}_{11}k^4 \tag{1.35}$$

where

$$\begin{split} \bar{B}_{11} &= \left[\frac{\hbar^4}{4E_{g_0}(m_c)^2}\right] \left[\frac{1 + \frac{x_{11}^2}{2}}{1 + \frac{x_{11}}{2}}\right] (1 - y_{11})^2, \\ x_{11} &= \left[1 + \left(\frac{\Delta}{E_{g_0}}\right)\right]^{-1} \text{ and } y_{11} = \frac{m_c}{m_o} \end{split}$$

The (1.35) gets simplified as

$$\frac{\hbar^2 k^2}{2m_a} = I_{13}(E) \tag{1.36}$$

where

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

The 2D electron dispersion relation in this case assumes the form

$$\frac{\hbar^2 k_s^2}{2m_c} + \frac{\hbar^2}{2m_c} (n_z \pi/d_z)^2 = I_{13}(E)$$
 (1.37)

Using (1.37) and (1.4), the EEM in x-y plane for this case can be written as

$$m^*(E_{Fs}) = m_c \{I_{13}(E_{Fs})\}'$$
 (1.38)

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 can be written as

$$N_{2DT}(E) = \left(\frac{m_c g_v}{\pi \hbar^2}\right) \sum_{n_*=1}^{n_{z_{max}}} \left\{ [I_{13}(E)]' H(E - E_{n_{z_4}}) \right\}$$
(1.39)

where, the subband energies  $E_{n_{z_4}}$  can be expressed as

$$I_{13}(E_{n_{z_4}}) = \frac{\hbar}{2m_c} (n_z \pi / d_z)^2$$
 (1.40)

The 2D carrier concentration assumes the form

$$n_{2D} = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z_{max}}} \left[ T_{57}(E_{Fs}, n_z) + T_{58}(E_{Fs}, n_z) \right]$$
(1.41)

where

$$T_{57}(E_{Fs}, n_z) \equiv \left[ I_{13}(E_{Fs}) - \frac{\hbar^2}{2m_c} \left( \frac{n_z \pi}{d_z} \right)^2 \right]$$
 and  $T_{58}(E_{Fs}, n_z) \equiv \sum_{r=1}^s L(r) T_{57}(E_{Fs}, n_z)$ 

### 1.2.3 The EEM in UFs of II-VI Semiconductors

The carrier energy spectra in bulk specimens of II-VI compounds in accordance with Hopfield model [142] can be written as

$$E = a'_{o}k_{s}^{2} + b'_{o}k_{z}^{2} \pm \bar{\lambda}_{o}k_{s} \tag{1.42}$$

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

The dispersion relation of the conduction electrons of UFs of II-VI materials for dimensional quantization along z-direction can be written following (1.42) as

$$E = a'_o k_s^2 + b'_o \left(\frac{n_z \pi}{d_z}\right)^2 \pm \bar{\lambda}_o k_s \tag{1.43}$$

Using (1.43), the EEM in this case can be written as

$$m^*(E_{Fs}, n_z) = m_{\perp}^* \left[ 1 \mp \frac{(\bar{\lambda}_o)}{\left[ (\bar{\lambda}_o)^2 - 4a_o'b_o' \left( \frac{n_z \pi}{d_z} \right)^2 + 4a_o' E_{Fs} \right]^{1/2}} \right]$$
(1.44)

Thus, we can infer that the EEM in the UFs of II-VI compounds is a function of both the size quantum number and the Fermi energy due to the presence of the term  $\bar{\lambda}_o$ .

The subband energy  $E_{n_{z_5}}$  assumes the form

$$E_{n_{zs}} = b_o' (n_z \pi / d_z)^2 \tag{1.45}$$

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

$$A_{\pm}(E, n_z) = \left[ \frac{\pi}{2 \left( a_0' \right)^2} \left[ \left( \overline{\lambda_0} \right)^2 + 2 a_0' \left( E - E_{n_{z_5}} \right) \pm \overline{\lambda_0} \left[ \left( \overline{\lambda_0} \right)^2 + 4 a_0' \left( E - E_{n_{z_5}} \right) \right]^{1/2} \right] \right]$$
(1.46)

The surface electron concentration under the condition of extreme carrier degeneracy can be expressed in this case as

$$n_{2D} = \frac{2g_v}{2(2\pi)^2} \sum_{n_z=1}^{n_{z \max}} \left[ A_+ \left( E_{Fs}, n_z \right) + A_- \left( E_{Fs}, n_z \right) \right]$$
(1.47)

Using (1.46) and (1.47) we get

$$n_{2D} = \frac{g_{\nu} m_{\perp}^*}{\pi \hbar^2} \sum_{n_*=1}^{n_{z \max}} \left( E_{Fs} - E_{n_{z_5}} + (\overline{\lambda})^2 m_{\perp}^* \hbar^{-2} \right)$$
(1.48)

### 1.2.4 The EEM in UFs of Bismuth

#### (a) The McClure and Choi model

The dispersion relation of the carriers in Bi can be written, following the McClure and Choi [153], as

$$E(1 + \alpha E) = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{p_z^2}{2m_3} + \frac{p_y^2}{2m_2} \alpha E \left\{ 1 - \left( \frac{m_2}{m_2'} \right) \right\} + \frac{p_y^4 \alpha}{4m_2 m_2'} - \frac{\alpha p_x^2 p_y^2}{4m_1 m_2} - \frac{\alpha p_y^2 p_z^2}{4m_2 m_3}$$

$$(1.49)$$

where  $p_i \equiv \hbar k_i$ ,  $i = x, y, z, m_1, m_2$  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).

The dispersion relation of the conduction electrons in UFs of Bi for dimensional quantization along  $k_z$  direction can be written following (1.49) for this model as

$$E(1 + \alpha E) = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{\hbar^2}{2m_3} \left(\frac{n_z \pi}{d_z}\right)^2 + \frac{p_y^2}{2m_2} \alpha E \left\{1 - \left(\frac{m_2}{m_2'}\right)\right\} + \frac{p_y^4 \alpha}{4m_2 m_2'} - \frac{\alpha p_x^2 p_y^2}{4m_1 m_2} - \frac{\alpha p_y^2 \hbar^2}{4m_2 m_3} \left(\frac{n_z \pi}{d_z}\right)^2$$

$$(1.50)$$

Equation (1.50) can, approximately, be expressed as

$$\gamma_1(E, n_z) = p_1 k_x^2 + q_1(E) k_y^2 + R_1(E, n_z) k_y^4$$
(1.51)

where,

$$\begin{split} \gamma_1(E,n_z) &\equiv \left[ E(1+\alpha E) - \frac{\hbar^2}{2m_3} \left( \frac{n_z \pi}{d_z} \right)^2 \right], \quad p_1 \equiv \frac{\hbar^2}{2m_1}, \\ q_1(E) &\equiv \frac{\hbar^2}{2m_2} \left[ 1 + \alpha E \left( 1 - \frac{m_2}{m_2'} \right) - \alpha E(1+\alpha E) \right] \end{split}$$

and

$$R_1(E,n_z) \equiv \left[\frac{\alpha\hbar^4}{4m_2m_2'} + \alpha\left(\frac{\hbar^2}{2m_2}\right)^2 \left\{1 + \alpha E\left(1 - \frac{m_2}{m_2'}\right) - \frac{\alpha\hbar^2}{2m_3}\left(\frac{n_z\pi}{d_z}\right)^2\right\}\right]$$

The area enclosed by (1.51) is defined by the following integral:

$$A(E, n_z) = 4 \left[ \frac{R_1(E, n_z)}{p_1} \right]^{1/2} \cdot J_1(E, n_z)$$
 (1.52)

where,

$$J_1(E, n_z) \equiv \int_{0}^{u_o(E, n_z)} \left[ \frac{\gamma_1(E, n_z)}{R_1(E, n_z)} - \frac{q_1(E)k_y^2}{R_1(E, n_z)} - k_y^4 \right]^{1/2} dk_y$$

and

$$u_0(E, n_z) \equiv \left[ \sqrt{\frac{q_1^2(E)}{4R_1^2(E, n_z)} + \frac{\gamma_1(E, n_z)}{R_1(E, n_z)}} - q_1(E) \right]^{1/2}$$

Thus, the area enclosed can be written as

$$A(E, n_z) = \frac{4}{3} \left[ \frac{R_1(E, n_z)}{p_1} \right]^{1/2} \left[ a^2(E, n_z) + b^2(E, n_z) \right]^{1/2}$$

$$\[a^{2}(E, n_{z})F\left[\frac{\pi}{2}, l(E, n_{z})\right] - \left[a^{2}(E, n_{z}) - b^{2}(E, n_{z})\right]E\left[\frac{\pi}{2}, l(E, n_{z})\right]\] (1.53)$$

where,

$$a^2(E,n_z) \equiv \frac{q_1(E)}{2R_1(E,n_z)} + \frac{1}{2} \left[ \frac{q_1^2(E)}{R_1^2(E,n_z)} + \frac{4\gamma_1(E,n_z)}{R_1(E,n_z)} \right]^{1/2},$$

$$b^{2}(E, n_{z}) \equiv \frac{1}{2} \left[ \frac{q_{1}^{2}(E)}{R_{1}^{2}(E, n_{z})} + \frac{4\gamma_{1}(E, n_{z})}{R_{1}(E, n_{z})} \right]^{1/2} - \left( \frac{q_{1}(E)}{2R_{1}(E, n_{z})} \right),$$

$$l(E, n_z) \equiv \frac{b(E, n_z)}{\sqrt{a^2(E, n_z) + b^2(E, n_z)}}, F\left[\frac{\pi}{2}, l(E, n_z)\right] \text{ and } E\left[\frac{\pi}{2}, l(E, n_z)\right]$$

are the complete elliptic integral of the first and second kinds respectively [217] Using (1.53), the EEM can be written as

$$m^*(E_{Fs}, n_z) = \left(\frac{2\hbar^2}{3\pi\sqrt{p_1}}\right) [R_3(E, n_z)]|_{E=E_{Fs}}$$
(1.54)

where.

$$R_{3}(E_{Fs}, n_{z})$$

$$\equiv \frac{1}{2} \left[ R_{1}(E_{Fs}, n_{z}) \right]^{-1/2} \left[ R_{1}(E_{Fs}, n_{z}) \right]' \left[ a^{2}(E_{Fs}, n_{z}) + p^{2}(E_{Fs}, n_{z}) \right]^{1/2}$$

$$\times \left[ a^{2}(E_{Fs}, n_{z}) F\left(\frac{\pi}{2}, l(E_{Fs}, n_{z})\right) - \left[ a^{2}(E_{Fs}, n_{z}) - b^{2}(E_{Fs}, n_{z}) \right] \right]$$

$$- b^{2}(E_{Fs}, n_{z}) \left[ e^{2}(E_{Fs}, n_{z}) \right]$$

$$+ \sqrt{R_{1}(E_{Fs}, n_{z})} \left[ a^{2}(E_{Fs}, n_{z}) + b^{2}(E_{Fs}, n_{z}) \right]^{-1/2}$$

$$\times \left[ a(E_{Fs}, n_{z}) (a(E_{Fs}, n_{z}))' + b(E_{Fs}, n_{z}) (b(E_{Fs}, n_{z}))' \right]$$

$$\times \left[ a^{2}(E_{Fs}, n_{z}) F\left(\frac{\pi}{2}, l(E_{Fs}, n_{z})\right) - \left[ a^{2}(E_{Fs}, n_{z}) - b^{2}(E_{Fs}, n_{z}) \right] \right]$$

$$- b^{2}(E_{Fs}, n_{z}) \left[ e^{2}(E_{Fs}, n_{z}) + b^{2}(E_{Fs}, n_{z}) \right]^{1/2}$$

$$\times \left[ 2a(E_{Fs}, n_{z}) (a(E_{Fs}, n_{z}))' F\left(\frac{\pi}{2}, l(E_{Fs}, n_{z})\right) + a^{2}(E_{Fs}, n_{z}) \left( e^{2}(E_{Fs}, n_{z}) \right)' \right]$$

$$- 2b(E_{Fs}, n_{z}) (b(E_{Fs}, n_{z}))' \left[ e^{2}(E_{Fs}, n_{z}) \right] \left( e^{2}(E_{Fs}, n_{z}) \right)$$

$$- \left[ a^{2}(E_{Fs}, n_{z}) - b^{2}(E_{Fs}, n_{z}) \right] \left( e^{2}(E_{Fs}, n_{z}) \right) \right]'$$

Thus, the EEM in this case is a function of both the Fermi energy and the size quantum number due to the presence of band nonparabolicity only.

The total 2D DOS function can be written following (1.52), as

The total 2D DOS function can be written following (1.53), as

$$N_{2DT}(E) = \left(\frac{2g_{\nu}}{3\pi^2 \sqrt{p_1}}\right) \sum_{n=1}^{n_{z_{max}}} R_3(E, n_z) H(E - E_{n_{z6}})$$
 (1.55)

where, the subband energies  $E_{n_{76}}$  assume the form

$$E_{n_{z6}}(1 + \alpha E_{n_{z6}}) = \frac{\hbar^2}{2m_3} \left(\frac{n_2 \pi}{d_z}\right)'$$
 (1.56)

Combining (1.55) with the Fermi-Dirac occupation probability factor, the 2D electron statistics in UFs of Bi in accordance with the McClure and Choi model can be expressed as

$$n_{2D} = \left(\frac{2g_{\nu}}{3\pi^2 \sqrt{p_1}}\right) \sum_{n_z=1}^{n_{zmax}} [\theta_1(E_{Fs}, n_z) + \theta_2(E_{Fs}, n_z)]$$
 (1.57)

where,

$$\theta_{1}(E_{Fs}, n_{z}) \equiv \left\{ \sqrt{R_{1}(E_{Fs}, n_{z})} [a^{2}(E_{Fs}, n_{z}) + b^{2}(E_{Fs}, n_{z})]^{1/2} \right.$$

$$\times \left[ a^{2}(E_{Fs}, n_{z}) F\left(\frac{\pi}{2}, l(E_{Fs}, n_{z})\right) - [a^{2}(E_{Fs}, n_{z}) - b^{2}(E_{Fs}, n_{z})] F\left(\frac{\pi}{2}, l(E_{Fs}, n_{z})\right) \right] \right\}$$

and 
$$\theta_2(E_{Fs}, n_z) \equiv \sum_{r=1}^{s} L(r)[\theta_1(E_{Fs}, n_z)].$$

#### (b) The Hybrid Model

The dispersion relation of the carriers in bulk specimens of Bi in accordance with the Hybrid model can be represented as [152]

$$E(1+\alpha E) = \frac{\theta_0(E)(\hbar k_y^2)}{2M_2} + \frac{\alpha \gamma_0 \hbar^4 k_y^4}{4M_2^2} + \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_z^2}{2m_3}$$
(1.58)

in which  $\theta_0(E) \equiv [1 + \alpha E(1 - \gamma_0) + \overline{\delta}_0]$ ,  $\gamma_0 \equiv \frac{M_2}{m_2}$ ,  $\overline{\delta}_0 \equiv \frac{M_2}{M_2'}$  and the other notations are defined in [152].

In the presence of size quantization along *y*-direction, the 2D electron dispersion relation can be written as

$$\frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_z^2}{2m_3} = E(1 + \alpha E) - \frac{\theta_0(E)\hbar^2}{2M_2} \left(\frac{\pi n_y}{d_y}\right)^2 - \frac{\alpha \gamma_0 \hbar^4}{4M_2^2} \left(\frac{\pi n_y}{d_y}\right)^4 \tag{1.59}$$

The 2D area is given by

$$A(E, n_y) = \frac{2\pi \sqrt{m_1 m_3}}{\hbar_2} t_{29}(E, n_y)$$
 (1.60)

$$t_{29}(E,n_y) = \left[ E(1+\alpha E) - \frac{\theta_0(E)\hbar^2}{2M_2} \left( \frac{\pi n_y}{d_y} \right)^2 - \frac{\alpha \gamma_0 \hbar^4}{4M_2^4} \left( \frac{\pi n_y}{d_y} \right)^4 \right]$$

The effective mass in the X–Z plane can be written as

$$m^*(E_{Fs}, n_y) = [\sqrt{m_1 m_3}]t'_{29}(E_{Fs}, n_y)$$
 (1.61)

Therefore, the effective mass in UFs of Bi in accordance with Hybrid model is a function of Fermi energy and the size quantum number due to the presence of band nonparabolicity only.

The subband energy are given as

$$E_{n_y}(1 + \alpha E) - \frac{\theta_0(E_{n_y})\hbar^2}{2M_2} \left(\frac{\pi n_y}{d_y}\right)^2 - \frac{\alpha \gamma_0 \hbar^4}{4M_2^2} \left(\frac{\pi n_y}{d_y}\right)^4 = 0$$
 (1.62)

The total DOS function in this case can be written as

$$N_{2DT}(E) = \frac{g_v \sqrt{m_1 m_3}}{\pi \hbar^2} \sum_{n_v=1}^{n_{ymax}} \left\{ t_{29}(E, n_y) \right\}' H(E - E_{n_y})$$
 (1.63)

The use of (1.63) leads to the 2D electron statistics in UFs of Bi in this case as

$$N_{2D} = \frac{g_v \sqrt{m_1 m_3}}{\pi \hbar^2} \sum_{n_v=1}^{n_{ymax}} \left[ t_{29}(E_{Fs}, n_y) + t_{30}(E_{Fs}, n_y) \right]$$
(1.64)

in which 
$$t_{30}(E_{Fs}, n_y) = \sum_{r=1}^{s_o} L(r)[t_{29}(E_{Fs}, n_y)]$$

#### (c) The Cohen model

In accordance with the Cohen model [151], the dispersion law of the carriers in Bi is given by

$$E(1+\alpha E) = \frac{p_x^2}{2m_1} + \frac{p_z^2}{2m_3} - \frac{\alpha E p_y^2}{2m_2'} + \frac{p_y^2 (1+\alpha E)}{2m_2} + \frac{\alpha p_y^4}{4m_2 m_2'}$$
(1.65)

The 2D electron dispersion law in UFs of Bi in accordance with this model can be written following (1.65) as

$$E(1+\alpha E) = \frac{p_x^2}{2m_1} + \frac{\hbar^2}{2m_3} \left(\frac{n_z \pi}{d_z}\right)^2 - \frac{\alpha E p_y^2}{2m_2'} + \left(\frac{\alpha p_y^4}{4m_2 m_2'}\right) + \frac{p_y^2}{2m_2} (1+\alpha E) \quad (1.66)$$

The (1.66) can be written as

$$\gamma_1(E, n_z) = p_1 k_x^z + q_2(E) k_y^2 + R_2 k_y^4$$
 (1.67)

where, 
$$q_2(E) \equiv \left[\frac{\hbar^2}{2m_2}(1 + \alpha E) - \frac{\alpha E \hbar^2}{2m_2'}\right]$$
 and  $R_2 \equiv \left(\frac{\alpha \hbar^4}{4m_2m_2'}\right)$ .

The EEM in this case can be written as

$$m^*(E_{Fs}, n_z) = \left(\frac{2\hbar^2}{3\pi\sqrt{p_1}}\right) \left[R_4(E, n_z)\right]|_{E=E_{Fs}}$$
(1.68)

in which,

$$\begin{split} R_4(E_{Fs},n_z) & \equiv \sqrt{R_2}[a_1^2(E_{Fs},n_z) + b^2(E_{Fs},n_z)]^{-1/2}[a_1(E_{Fs},n_z)(a_1(E_{Fs},n_z))' \\ & + b_1(E_{Fs},n_z)(b_1(E_{Fs},n_z))'] \left[ a_1^2(E_{Fs},n_z) F\left(\frac{\pi}{2},l(E_{Fs},n_z)\right) \right. \\ & - \left[ a_1^2(E_{Fs},n_z) - b_1^2(E_{Fs},n_z) \right] E\left(\frac{\pi}{2},l_1(E_{Fs},n_z)\right) \right] \\ & + \sqrt{R_2} \left[ a_1^2(E_{Fs},n_z) + b_1^2(E_{Fs},n_z) \right]^{1/2} \left[ 2a_1(E_{Fs},n_z)(a_1(E_{Fs},n_z))' \right. \\ & \times F\left(\frac{\pi}{2},l_1(E_{Fs},n_z)\right) + a_1^2(E_{Fs},n_z) \left\{ F\left(\frac{\pi}{2},l_1(E_{Fs},n_z)\right) \right\}' \\ & \times \left[ 2a_1(E_{Fs},n_z)(a_1(E_{Fs},n_z))' - 2b_1(E_{Fs},n_z)(b_1(E_{Fs},n_z))' \right] E\left(\frac{\pi}{2},l_1(E_{Fs},n_z)\right) \\ & - \left[ a_1^2(E_{Fs},n_z) - b_1^2(E_{Fs},n_z) \right] \left( E\left(\frac{\pi}{2},l_1(E_{Fs},n_z)\right) \right)' \right] \right], \end{split}$$

$$a_1^2(E_{Fs}, n_z) \equiv \frac{q_2(E_{Fs})}{2R_2} + \frac{1}{2} \left[ \frac{q_2^2(E_{Fs})}{R_2^2} + \frac{4\gamma_1(E_{FS}, n_z)}{R_2} \right]^{1/2},$$

$$b_1^2(E_{Fs}, n_z) \equiv \frac{1}{2} \left[ \frac{q_2^2(E_{Fs})}{R_2^2} + \frac{4\gamma_1(E_{Fs}, n_z)}{R_2} \right]^{1/2} - \left( \frac{q_2(E_{Fs})}{2R_2} \right)$$
and  $l_1(E_{Fs}, n_z) \equiv \frac{b_1(E_{Fs}, n_z)}{\sqrt{a_1^2(E_{Fs}, n_z) + b_1^2(E_{Fs}, n_z)}}.$ 

which shows that the EEM in this present case is again a function of both the size quantum number and the Fermi energy due to the presence of the band nonparabolicity only.

The total DOS is given by

$$N_{2DT}(E) = \left(\frac{2g_v}{3\pi^2 \sqrt{p_1}}\right) \sum_{n_z=1}^{n_{zmax}} R_4(E, n_z) H(E - E_{nz7})$$
 (1.69a)

where,  $E_{n_{z_7}}$  is the lowest positive root of the equation

$$\gamma_1\left(E_{n_{z_7}}, n_z\right) = 0 \tag{1.69b}$$

Combining (1.69a) with the Fermi-Dirac occupation probability factor, the 2D electron statistics in UFs of Bi in accordance with the Cohen model can be written as

$$n_{2D} = \left(\frac{2g_{\nu}}{3\pi^2 \sqrt{p_1}}\right) \sum_{n_z=1}^{n_{zmax}} \left[\theta_3(E_{Fs}, n_z) + \theta_4(E_{Fs}, n_z)\right]$$
(1.70)

where.

$$\begin{split} \theta_3(E_{Fs},n_z) &\equiv \left\{ \sqrt{R_2} \left[ a_1^2(E_{Fs},n_z) - b_1^2(E_{Fs},n_z) \right]^{1/2} \left[ a_1^2(E_{Fs},n_z) F\left(\frac{\pi}{2},l_1(E_{Fs},n_z)\right) \right. \\ &\left. - \left[ a_1^2(E_{Fs},n_z) - b_1^2(E_{Fs},n_z) \right] F\left(\frac{\pi}{2},l_1(E_{Fs},n_z)\right) \right], \end{split}$$

and 
$$\theta_4(E_{Fs}, n_z) \equiv \sum_{r=1}^s L(r) \left[ \theta_3(E_{Fs}, n_z) \right].$$

### (d) The Lax model

The electron energy spectra in bulk specimens of Bi in accordance with the Lax model can be written as [147]

$$E(1 + \alpha E) = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{p_z^2}{2m_3}$$
 (1.71)

The 2D electron dispersion law in this case can be written as

$$E(1 + \alpha E) = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y}{2m_2} + \frac{\hbar^2}{2m_3} \left(\frac{n_z \pi}{d_z}\right)^2$$
 (1.72)

The EEM in this case assumes the form

$$m^*(E_{Fs}) = \sqrt{m_1 m_2} (1 + 2\alpha E_{Fs}) \tag{1.73}$$

Thus, we see that the EEM for the Lax model is a function of the Fermi energy alone due to the band nonparabolicity.

The subband energy, the total DOS function and the 2D electron statistics for this model can, respectively, be expressed as

$$E_{n_{z8}}(1 + \alpha E_{n_{z8}}) = \frac{\hbar^2}{2m_3} (n_z \pi / d_z)^2$$
 (1.74)

$$N_{2DT}(E) = \frac{g_v \sqrt{m_1 m_2}}{\pi \hbar^2} \sum_{n_*=1}^{n_{zmax}} (1 + 2\alpha E) H(E - E_{n_z 8})$$
 (1.75)

$$n_{2D} = \frac{g_v \sqrt{m_1 m_2} k_B T}{\pi \hbar^2} \sum_{n_z=1}^{n_{zmax}} \left[ (1 + 2\alpha E_{n_{z8}}) F_0(\eta_{y2}) + 2\alpha k_B T F_1(\eta_{y2}) \right]$$
(1.76)

where, 
$$\eta_{y_2} = \frac{E_{Fs} - E_{n_{z8}}}{k_B T}$$
.

### (e) The ellipsoidal parabolic model

The 2D dispersion relation, the EEM, the subband energy  $(E_{n_{29}})$ , the total DOS,

and the 2D electron statistics for this model can respectively be written as

$$E = \left(\frac{\hbar^2 k_x^2}{2m_1}\right) + \left(\frac{\hbar^2 k_y^2}{2m_2}\right) + \left(\frac{\hbar^2}{2m_3}\right) \left(\frac{n_z \pi}{d_z}\right)^2 \tag{1.77}$$

$$m^*(E_{Fs}) = (\sqrt{m_1 m_2})$$
 (1.78)

$$N_{2DT}(E) = \frac{g_{\nu}\sqrt{m_1m_2}}{\pi\hbar^2} \sum_{n_{\nu}=1}^{n_{zmax}} H(E - E_{n_{z9}})$$
 (1.79)

$$E_{n_{z9}} = \left(\frac{\hbar^2}{2m_3}\right) \left(\frac{n_z \pi}{d_z}\right)^2 \tag{1.80}$$

$$N_{2D} = \left[\frac{k_B T g_v \sqrt{m_1 m_2}}{\pi \hbar^2}\right] \sum_{n_\tau = 1}^{n_{zmax}} F_0(\eta_{y_3})$$
 (1.81)

where,  $\eta_{y3} \equiv (k_B T)^{-1} \left[ E_{Fs} - E_{n_{z9}} \right]$ 

## 1.2.5 The EEM in UFs of IV-VI Semiconductors

The dispersion relation of the conduction electrons in IV-VI semiconductors can be expressed in accordance with Dimmock [221] as

$$\left[\overline{\varepsilon} - \frac{E_{g0}}{2} - \frac{\hbar^2 k_s^2}{2m_t^-} - \frac{\hbar^2 k_z^2}{2m_l^-}\right] \left[\overline{\varepsilon} + \frac{E_{g0}}{2} + \frac{\hbar^2 k_s^2}{2m_t^-} + \frac{\hbar^2 k_z^2}{2m_l^-}\right] = P_{\perp}^2 k_s^2 + P_{\parallel}^2 k_z^2$$
(1.82)

where  $\overline{\varepsilon}$  is the energy as measured from the center of the band gap  $E_{g0}$ ,  $m_t^{\pm}$  and  $m_l^{\pm}$  represent the contributions to the transverse and longitudinal effective masses of the external  $L_6^+$  and  $L_6^-$  bands arising from the  $\vec{k}.\vec{p}$  perturbations with the other bands taken to the second order. Using  $\varepsilon = E + \left(E_{g0}/2\right)$ ,  $P_{\perp}^2 = \frac{\hbar^2 E_{g0}}{2m_t^*}$ ,  $P_{\parallel}^2 = \frac{\hbar^2 E_{g0}}{2m_l^*}$  ( $m_l^*$  and  $m_l^*$  are the transverse and longitudinal effective electron masses at k=0) in (1.82), we can write

$$\left[E - \frac{\hbar^2 k_s^2}{2m_t^-} - \frac{\hbar^2 k_z^2}{2m_l^-}\right] \left[1 + \alpha E + \alpha + \frac{\hbar^2 k_s^2}{2m_t^+} + \alpha + \frac{\hbar^2 k_z^2}{2m_l^+}\right] = \frac{\hbar^2 k_s^2}{2m_t^*} + \frac{\hbar^2 k_z^2}{2m_l^*} \tag{1.83}$$

The 2D dispersion relation of the conduction electrons in IV-VI materials in UFs for the dimensional quantization along z direction can be expressed as

$$\begin{split} E(1+\alpha E) + \alpha E \left(\frac{\hbar^2 k_x^2}{2x_4} + \frac{\hbar^2 k_y^2}{2x_5}\right) + \alpha E \frac{\hbar^2}{2x_6} \left(\frac{n_z \pi}{d_z}\right)^2 - (1+\alpha E) \left(\frac{\hbar^2 k_x^2}{2x_1} + \frac{\hbar^2 k_y^2}{2x_2}\right) \\ - \alpha \left(\frac{\hbar^2 k_x^2}{2x_1} + \frac{\hbar^2 k_y^2}{2x_2}\right) \left(\frac{\hbar^2 k_x^2}{2x_4} + \frac{\hbar^2 k_y^2}{2x_5}\right) - \alpha \left(\frac{\hbar^2 k_x^2}{2x_1} + \frac{\hbar^2 k_y^2}{2x_2}\right) \frac{\hbar^2}{2x_6} \left(\frac{n_z \pi}{d_z}\right)^2 \\ - (1+\alpha E) \frac{\hbar^2}{2x_3} \left(\frac{n_z \pi}{d_z}\right)^2 - \alpha \frac{\hbar^2}{2x_3} \left(\frac{n_z \pi}{d_z}\right)^2 \left(\frac{\hbar^2 k_x^2}{2x_4} + \frac{\hbar^2 k_y^2}{2x_5}\right) - \alpha \frac{\hbar^2}{2x_3} \left(\frac{n_z \pi}{d_z}\right)^2 \frac{\hbar^2}{2x_6} \left(\frac{n_z \pi}{d_z}\right)^2 \\ = \frac{\hbar^2 k_x^2}{2m_1} + \frac{\hbar^2 k_y^2}{2m_2} + \frac{\hbar^2}{2m_3} \left(\frac{n_z \pi}{d_z}\right)^2 \end{split} \tag{1.84}$$

where

$$x_4 = m_t^+, x_5 = \frac{m_t^+ + 2m_l^+}{3}, x_6 = \frac{3m_t^+ m_l^+}{2m_l^+ + m_t^+}, x_1 = m_t^-, x_2 = \frac{m_t^- + 2m_l^-}{3},$$
$$x_3 = \frac{3m_t^- m_l^-}{2m_l^- + m_t^-}, m_1 = m_t^*, m_2 = \frac{m_t^+ + 2m_l^*}{3} \text{ and } m_3 = \frac{3m_l^* m_t^*}{m_t^* + 2m_l^*}.$$

Substituting  $k_x = r \text{Cos}\theta$  and  $k_y = r \text{Sin}\theta$  (where r and  $\theta$  are 2D polar coordinates in 2D wave vector space) in (1.84), we can write

$$\begin{split} & r_{4} \left[ \alpha \frac{1}{4} \left( \frac{\hbar^{2} Cos^{2} \theta}{x_{1}} + \frac{\hbar^{2} Sin^{2} \theta}{x_{2}} \right) \left( \frac{\hbar^{2} Cos^{2} \theta}{x_{4}} + \frac{\hbar^{2} Sin^{2} \theta}{x_{5}} \right) \right] + r^{2} \frac{1}{2} \left[ \left( \frac{\hbar^{2} Cos^{2} \theta}{m_{1}} + \frac{\hbar^{2} Sin^{2} \theta}{m_{2}} \right) \right. \\ & + \alpha \frac{\hbar^{2}}{2x_{3}} \left( \frac{n_{z} \pi}{d_{z}} \right)^{2} \left( \frac{\hbar^{2} Cos^{2} \theta}{x_{4}} + \frac{\hbar^{2} Sin^{2} \theta}{x_{5}} \right) + \alpha \left( \frac{\hbar^{2} Cos^{2} \theta}{x_{1}} + \frac{\hbar^{2} Sin^{2} \theta}{x_{2}} \right) \frac{\hbar^{2}}{2x_{6}} \left( \frac{n_{z} \pi}{d_{z}} \right)^{2} \\ & + \hbar^{2} (1 + \alpha E) \left( \frac{Cos^{2} \theta}{x_{1}} + \frac{Sin^{2} \theta}{x_{2}} \right) - \hbar^{2} \alpha E \left( \frac{Cos^{2} \theta}{x_{4}} + \frac{Sin^{2} \theta}{x_{5}} \right) \right] - \left[ E(1 + \alpha E) \right. \\ & + \alpha E \frac{\hbar^{2}}{2x_{6}} \left( \frac{n_{z} \pi}{d_{z}} \right)^{2} - \left( 1 + \alpha E \right) \frac{\hbar^{2}}{2x_{3}} \left( \frac{n_{z} \pi}{d_{z}} \right)^{2} - \alpha \left( \frac{\hbar^{4}}{4x_{3}x_{6}} \left( \frac{n_{z} \pi}{d_{z}} \right) \right) \right] = 0 \end{split} \tag{1.85}$$

The area  $A(E, n_z)$  of the 2D wave vector space can be expressed as

$$A(E, n_z) = \overline{J}_1 - \overline{J}_2 \tag{1.86}$$

where

$$\overline{J}_1 \equiv 2 \int_0^{\pi/2} \frac{c}{b} d\theta \tag{1.87}$$

and

$$\overline{J}_2 \equiv 2 \int_0^{\pi/2} \frac{ac^2}{b^3} d\theta \tag{1.88}$$

in which

$$\alpha \equiv \left[\alpha \left(\frac{\hbar^4}{4}\right) \left(\frac{Cos^2\theta}{x_1} + \frac{Sin^2\theta}{x_2}\right) \left(\frac{Cos^2\theta}{x_4} + \frac{Sin^2\theta}{x_3}\right)\right],$$

$$\begin{split} b &\equiv \left(\frac{\hbar^2}{2}\right) \left[ \left(\frac{Cos^2\theta}{m_1} + \frac{Sin^2\theta}{m_2}\right) + \alpha \left(\frac{\hbar^2}{2x_3}\right) \left(\frac{n_2\pi}{d_z}\right)^2 \left(\frac{Cos^2\theta}{x_4} + \frac{Sin^2\theta}{x_5}\right) \right. \\ &\quad + \alpha \left(\frac{\hbar^2}{2x_6}\right) \left(\frac{n_2\pi}{d_z}\right)^2 \left(\frac{Cos^2\theta}{m_1} + \frac{Sin^2\theta}{m_2}\right) + (1 + \alpha E) \left(\frac{Cos^2\theta}{x_1} + \frac{Sin^2\theta}{x_2}\right) \\ &\quad - \alpha E \left(\frac{Cos^2\theta}{x_4} + \frac{Sin^2\theta}{x_5}\right) \right] \end{split}$$

and

$$\begin{split} c &\equiv \left[ E(1+\alpha E) + \alpha E \left(\frac{\hbar^2}{2x_6}\right) \left(\frac{n_z \pi}{d_z}\right)^2 - (1+\alpha E) \left(\frac{\hbar^2}{2x_3}\right) \left(\frac{n_z \pi}{d_z}\right)^2 \right. \\ &\left. - \alpha \left(\frac{\hbar^4}{4x_3x_6}\right) \left(\frac{n_z \pi}{d_z}\right) \right] \end{split}$$

(1.87) can be expressed as  $\overline{J}_1 = 2 \int_0^{\pi/2} \frac{t_3(E, n_z)d\theta}{A_1(E, n_z)Cos^2\theta + B_1(E, n_z)Sin^2\theta}$  where,  $t_3(E, n_z) \equiv c$ ,  $A_1(E, n_z) \equiv \frac{\hbar^2}{2m_1}t_1(E, n_z)$ ,

$$t_1(E, n_z) \equiv \left[ 1 + m_1 \left[ \frac{1}{x_4} \frac{\alpha \hbar^2}{2x_3} \left( \frac{n_z \pi}{d_z} \right)^2 + \frac{\alpha \hbar^2}{2x_1 x_6} \left( \frac{n_z \pi}{d_z} \right)^2 + \frac{1 + \alpha E}{x_1} - \frac{\alpha E}{x_4} \right] \right]$$

$$\begin{split} B_1(E,n_z) &\equiv \frac{\hbar^2}{2m_2} t_2(E,n_z) \text{ and} \\ t_2(E,n_z) &\equiv \left[1 + m_2 \left[\frac{\alpha \hbar^2}{2x_3 x_5} \left(\frac{n_z \pi}{d_z}\right)^2 + \frac{\alpha \hbar^2}{2x_2 x_6} \left(\frac{n_z \pi}{d_z}\right)^2 + \frac{1 + \alpha E}{d_z} - \frac{\alpha E}{x_5}\right]\right]. \end{split}$$

Performing the integration, we get

$$\overline{J}_1 = \pi t_3(E, n_z) [A_1(E, n_z) B_1(E, n_z)]^{-1/2}$$
(1.89)

From (1.88) we can write

$$\overline{J}_2 = \frac{\alpha t_3^2(E, n_z)\hbar^4}{2B_1^3(E, n_z)}I\tag{1.90}$$

where

$$I \equiv \int_{0}^{\infty} \frac{(a_1 + a_2 z^2)(a_3 + a_4 z^2)dz}{[(\overline{a})^2 + z^2]^3}$$
 (1.91)

in which  $a_1 \equiv \frac{1}{x_1}$ ,  $a_2 \equiv \frac{1}{x_2}$ ,  $z = \tan\theta$ ,  $\theta$  is a new variable,  $a_3 \equiv \frac{1}{x_4}$ ,  $a_4 \equiv \frac{1}{x_5}$  and  $(\overline{a})^2 \equiv \left(\frac{A_1(E,n_z)}{B_1(E,n_z)}\right)$ . The use of the Residue theorem leads to the evaluation of the integral in (1.91) as

$$I \equiv \frac{\pi}{4\overline{a}}[a_1a_4 + 3a_2a_4] \tag{1.92}$$

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

$$A(E, n_z) = \frac{\pi t_3(E, n_z)}{\sqrt{A_1(E, n_z)B_1(E, n_z)}} \left[ 1 - \frac{1}{x_5} \left( \frac{1}{x_1} + \frac{3}{x_2} \right) \frac{\alpha t_3(E, n_z)\hbar^4}{8B_1^2(E, n_z)} \right]$$
(1.93)

The EEM for the UFs of IV-VI materials can thus be written as

$$m^*(E, n_z) = \frac{\hbar^2}{2} [\theta_5(E, n_z)] \Big|_{E=E_{Ez}}$$
 (1.94)

where,

$$\begin{split} \theta_5(E,n_z) &\equiv \left[1 - \frac{1}{x_5} \left(\frac{1}{x_1} + \frac{3}{x_2}\right) \frac{\alpha t_3(E,n_z)\hbar^4}{8[B_1(E,n_z)]^2}\right] [A_1(E,n_z)B_1(E,n_z)]^{-1} \\ &\times \left[\sqrt{A_1(E,n_z)B_1(E,n_z)} \{t_3(E,n_z)\}' - t_3(E,n_z)\right. \\ &\times \left[\frac{1}{2} \{A_1(E,n_z)\}' \left[\frac{B_1(E,n_z)}{A_1(E,n_z)}\right]^{-1/2} + \frac{1}{2} \{B_1(E,n_z)\}' \left[\frac{A_1(E,n_z)}{B_1(E,n_z)}\right]^{-1/2}\right\}\right] \\ &- \frac{1}{8} \frac{t_3(E,n_z)\alpha\hbar^4}{\sqrt{A_1(E,n_z)B_1(E,n_z)}} \frac{1}{x_5} \left(\frac{1}{x_1} + \frac{3}{x_2}\right) [B_1(E,n_z)]^{-4} \\ &\times \left[\{B_1(E,n_z)\}^2 \{t_3(E,n_z)\}' - 2B_1(E,n_z)\{B_1(E,n_z)\}' t_3(E,n_z)\right] \end{split}$$

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

$$N_{2DT}(E) = \left(\frac{g_{\nu}}{2\pi}\right) \sum_{n_{z}=1}^{n_{zmax}} \theta_{5}(E, n_{z}) H(E - E_{n_{z10}})$$
 (1.95)

where the subband energy  $(E_{n_{z10}})$  in this case can be written as

$$E_{n_{z10}}\left(1 + \alpha E_{n_{z10}}\right) + \alpha E_{n_{z10}} \frac{\hbar^2}{2x_6} \left(\frac{n_z \pi}{d_z}\right)^2 - (1 + \alpha E_{n_{z10}}) \frac{\hbar^2}{2x_3} \left(\frac{n_z \pi}{d_z}\right)^2 - \alpha \frac{\hbar^2}{2x_3} \left(\frac{n_z \pi}{d_z}\right)^2 \frac{\hbar^2}{2x_6} \left(\frac{n_z \pi}{d_z}\right)^2 - \left[\frac{\hbar^2}{2m_3} \left(\frac{n_z \pi}{d_z}\right)^2\right] = 0$$
(1.96)

The use of (1.95) leads to the expression of 2D electron statistics as

$$n_{2D} = \frac{g_v}{2\pi} \sum_{n_z=1}^{n_{z_{max}}} [T_{59}(E_{Fs}, n_z) + T_{60}(E_{Fs}, n_z)]$$
 (1.97)

where 
$$T_{59}(E_{Fs}, n_z) \equiv \frac{A(E_{Fs}, n_z)}{\pi}$$
 and  $T_{60}(E_{Fs}, n_z) \equiv \sum_{r=1}^{s} L(r)T_{59}(E_{Fs}, n_z)$ .

### 1.2.6 The EEM in UFs of Stressed Semiconductors

The electron energy spectrum in stressed Kane-type semiconductors can be written [222–225] as

$$\left(\frac{k_x}{\overline{a}_0(E)}\right)^2 + \left(\frac{k_y}{\overline{b}_0(E)}\right)^2 + \left(\frac{k_z}{\overline{c}_0(E)}\right)^2 = 1 \tag{1.98}$$

where

$$[\overline{a}_{0}(E)]^{2} \equiv \frac{\overline{K}_{0}(E)}{\overline{A}_{0}(E) + \frac{1}{2}\overline{D}_{0}(E)}, \overline{K}_{0}(E) \equiv \left[E - C_{1}\varepsilon - \frac{2C_{2}^{2}\varepsilon_{xy}^{2}}{3E_{g}'}\right] \left(\frac{3E_{g}'}{2B_{2}^{2}}\right),$$

 $C_1$  is the conduction band deformation potential,  $\varepsilon$  is the trace of the strain tensor  $\hat{\varepsilon}$  which can be written as  $\hat{\varepsilon} = \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{xy} & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{bmatrix}$ ,  $C_2$  is a constant which describes the strain interaction between the conduction and valance bands,  $E_g' \equiv E_g + E - C_1 \varepsilon$ ,  $B_2$  is the momentum matrix element,

$$\overline{A}_0(E) \equiv \left[ 1 - \frac{(\overline{a}_0 + C_1)}{E_g'} + \frac{3\overline{b}_0 \varepsilon_{xx}}{2E_g'} - \frac{\overline{b}_0 \varepsilon}{2E_g'} \right],$$

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

 $\overline{l}, \overline{m}, \overline{n}$  are the matrix elements of the strain perturbation operator,  $\overline{D}_0(E) \equiv (\overline{d}_0\sqrt{3})\frac{\varepsilon_{xy}}{E_o'}$ ,

$$\begin{split} & [\bar{b}_0(E)]^2 \equiv \frac{\overline{K}_0(E)}{\overline{A}_0(E) - \frac{1}{2}\overline{D}_0(E)}, \quad [\bar{c}_0(E)]^2 \equiv \frac{\overline{K}_0(E)}{\overline{L}_0(E)}, \\ & \text{and } \overline{L}_0(E) \equiv \left[1 - \frac{(\bar{a}_0 + C_1)}{E_g'} + \frac{3\bar{b}_0\varepsilon_{zz}}{E_g'} - \frac{\bar{b}_0\varepsilon}{2E_g'}\right] \end{split}$$

The 2D electron energy spectrum in UFs of stressed materials assumes the form

$$\frac{K_x^2}{[\bar{a}_0(E)]^2} + \frac{K_y^2}{[\bar{b}_0(E)]^2} + \frac{1}{[\bar{c}_0(E)]^2} (n_z \pi / d_z) = 1$$
 (1.99)

The area of 2D wave vector space enclosed by (1.99) can be written as

$$A(E, n_z) = \pi P^2(E, n_z)\bar{a}_0(E)\bar{b}_0(E)$$
 (1.100)

where  $P^2(E, n_z) = [1 - [n_z \pi / d_z \bar{c}_0(E)]^2].$ 

The expression of the surface EEM in this case can be written as

$$m^*(E_{Fs}, n_z) = \frac{\hbar^2}{2} [\theta_6(E, n_z)] \bigg|_{E=E_F}$$
 (1.101)

in which,

$$\theta_{6}(E, n_{z}) = \left[2P(E, n_{z})\{P(E, n_{z})\}'\bar{a}_{0}(E)\bar{b}_{0}(E) + \{P(E, n_{z})\}^{2}\{\bar{a}_{0}(E)\}'\bar{b}_{0}(E) + \{P(E, n_{z})\}^{2}\{\bar{b}_{0}(E)\}'\bar{a}_{0}(E)\right]$$

The EEM in this case is the function of Fermi energy and the size quantization number due to the presence of stress only.

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

$$N_{2DT}(E) = \left(\frac{g_{\nu}}{2\pi}\right) \sum_{n_{\tau}=1}^{n_{z,max}} \theta_{6}(E, n_{z}) H(E - E_{n_{z11}})$$
 (1.102)

The subband energies  $(E_{n_{z11}})$  are given by

$$\bar{c}_0(E_{n_{z11}}) = n_z \pi / d_z \tag{1.103}$$

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

$$n_{2D} = \frac{g_v}{2\pi} \sum_{n_z=1}^{n_{z_{max}}} [T_{61}(E_{Fs}, n_z) + T_{62}(E_{Fs}, n_z)]$$
 (1.104)

where

$$T_{61}(E_{Fs}, n_z) \equiv [P^2(E_{Fs}, n_z)\bar{a}_0(E_{Fs})\bar{b}_0(E_{Fs})]$$
  
and  $T_{62}(E_{Fs}, n_z) \equiv \sum_{r=1}^s L(r)T_{61}(E_{Fs}, n_z).$ 

In the absence of stress together with the substitution,  $B_2^2 \equiv 3\hbar^2 (E_g/4m_c)$ , (1.98) assumes the same form as given by (1.16).

## 1.2.7 The EEM in UFs of Tellurium

The dispersion relation of the conduction electrons in Te can be expressed as [226]

$$E = \psi_1 k_z^2 + \psi_2 k_s^2 \pm [\psi_3^2 k_s^2 + \psi_2^4 k_s^2]^{1/2}$$
 (1.105)

where,  $\psi_1 = 6.7 \times 10^{-16} \text{ mev.m}^2$ ,  $\psi_2 = 4.2 \times 10^{-16} \text{ mev.m}^2$ ,  $\psi_3 = 6 \times 10^{-8}$ , mev.m and  $\psi_4 = 3.6 \times 10^{-8} \text{ mev.m}$ 

The 2D electron energy spectrum in ultrathin films of Te assumes the form

$$k_s^2 = \psi_5(E) - \psi_6 \left(\frac{\pi n_z}{d_z}\right)^2 \pm \psi_7 \left[\psi_8^2(E) - \left(\frac{\pi n_z}{d_z}\right)^2\right]^{\frac{1}{2}}$$
(1.106)

where, 
$$\psi_5(E) = \left[\frac{E}{\psi_2} + \frac{\psi_4^2}{2\psi_2^2}\right], \psi_6 = \frac{\psi_1}{\psi_2}, \psi_7 = \frac{\psi_4\sqrt{\psi_1}}{\psi_2^{\frac{3}{2}}}, \psi_8^2(E) = \frac{\psi_4^4 + 4E\psi_2\psi_4^2 + 4\psi_2^2\psi_3^2}{4\psi_1\psi_2\psi_4^2}$$

The EEM in this case is given by

$$m^*(E_{Fs}, n_z) = \frac{\hbar^2}{2} \left[ t'_{40}(E, n_z) \right]_{E=E_{Fs}}$$
 (1.107)

where, 
$$t_{40}(E, n_z) = \left[ \psi_5(E) - \psi_6 \left( \frac{\pi n_z}{d_z} \right)^2 \pm \psi_7 \left[ \psi_8^2(E) - \left( \frac{\pi n_z}{d_z} \right)^2 \right]^{1/2} \right]^{1/2}$$

It appears that the EEM in UFs of Te is a function of Fermi energy and size quantum number which are the characteristics of such systems.

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

$$N_{2DT}(E) = \left(\frac{g_{\nu}}{\pi}\right) \sum_{n_z=1}^{n_{z_{max}}} t'_{40}(E, n_2) H(E - E_{n_{z12}})$$
 (1.108)

The subband energies  $(E_{n_{z12}})$  are given by

$$E_{n_{z12}} = \psi_1 (n_z \pi / d_z)^2 \pm \psi_3 (n_z \pi / d_z)$$
 (1.109)

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

$$n_{2D} = \frac{g_v}{\pi} \sum_{n_z=1}^{n_{z_{max}}} [t_{40}(E_{Fs}, n_2) + t_{41}(E_{Fs}, n_2)]$$
 (1.110)

where 
$$t_{41}(E_{Fs}, n_2) \equiv \sum_{r=1}^{s} L(r)t_{40}(E_{Fs}, n_z)$$
.

## 1.2.8 The EEM in UFs of Gallium Phosphide

The energy spectrum of the conduction electrons in n-GaP can be written as [227]

$$E = \frac{\hbar^2 k_s^2}{2m_{\perp}^*} + \frac{\hbar^2}{2m_{||}^*} [\overline{A}' k_s^2 + k_z^2] - \left[ \frac{\hbar^4 k_0^2}{m_{||}^{*2}} (k_s^2 + k_z^2) + |V_G|^2 \right]^{1/2} + |V_G| \quad (1.111)$$

where,  $K_0$  and  $|V_G|$  are constants of the energy spectrum and  $\overline{A}' = 1$ .

The 2D electron dispersion relation in size quantized n-GaP can be expressed as

$$E = ak_s^2 + C(n_z \pi/d_z)^2 + |V_G| - \left[Dk_s^2 + |V_G|^2 + D(n_z \pi/d_z)^2\right]^{1/2}$$
 (1.112)

in which,  $a\equiv {\hbar^2\over 2m_\parallel^*}+{\hbar^2\over 2m_\parallel^*},$   $C\equiv {\hbar^2\over 2m_\parallel^*}$  and  $D\equiv (\hbar^2k_0/m_\parallel^*)^2$ 

The subband energy  $(E_{n_{z13}})$  are given by

$$E_{n_{z13}} = C(\pi n_z/d_z)^2 + |V_G| - \left[|V_G|^2 + D(\pi n_z/d_z)^2\right]^{1/2}$$
(1.113)

Equation (1.112) can be expressed as

$$k_s^2 = t_{42}(E, n_z) (1.114)$$

in which,  $t_{42}(E, n_z) \equiv [\{2a(E - t_1) + D\} - \{[2a(E - t_1) + D]^2 - 4a^2[(E - t_1)^2 - t_2]\}^{1/2}], t_1 \equiv |V_G| + C(\pi n_z/d_z)^2$  and  $t_2 \equiv |V_G|^2 + D(\pi n_z/d_z)^2$ 

The EEM can be expressed from (1.114) as

$$m^*(E_{Fs}, n_z) = \frac{\hbar^2}{2} t'_{42}(E_{Fs}, n_z)$$
 (1.115)

It appears that the EEM in UFs of GaP is a function of Fermi energy and size quantum number due to the presence of the system constant  $k_0$ .

The total DOS function is given by

$$N_{2DT}(E) = \frac{g_v}{4\pi a^2} \sum_{n_z=1}^{n_{z_{max}}} \left[ t'_{42}(E, n_z) \right] H(E - E_{n_{z_{13}}})$$
 (1.116)

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

$$n_{2D} = \frac{g_v}{4\pi a^2} \sum_{n_z=1}^{n_{z,max}} \left[ t_{42}(E_{Fs}, n_z) + t_{43}(E_{Fs}, n_z) \right]$$
 (1.117)

where, 
$$t_{43}(E_{Fs}, n_z) \equiv \sum_{r=1}^{s} L(r) \left[ t_{42}(E_{Fs}, n_z) \right]$$

# 1.2.9 The EEM in UFs of Platinum Antimonide

The dispersion relation for the n-type PtSb<sub>2</sub> can be written as [228]

$$\left(E + \lambda_0 \frac{(\bar{a})^2}{4} k^2 - l k_s^2 \frac{(\bar{a})^2}{4}\right) \left(E + \delta_0 - \nu \frac{(\bar{a})^2}{4} k^2 - \bar{n} \frac{(\bar{a})^2}{4} k_s^2\right) = I \frac{(\bar{a})^4}{16} k^4$$
 (1.118) where  $\omega_1 \equiv \left(\lambda_0 \frac{(\bar{a})^2}{4} - l \frac{(\bar{a})^2}{4}\right)$ ,  $\omega_2 \equiv \lambda_0 \frac{(\bar{a})^2}{4}$ ,  $\omega_3 \equiv \left((\bar{n}) \frac{(\bar{a})^2}{4} + \nu \frac{(\bar{a})^2}{4}\right)$ ,  $\omega_4 \equiv \nu \frac{(\bar{a})^2}{4}$ ,  $I_1 \equiv I \left(\frac{(\bar{a})^2}{4}\right)^2$ ,  $\lambda_0$ ,  $l$ ,  $\delta_0$ ,  $\nu$  and  $\bar{n}$  are the band constants and  $\bar{a}$  is the lattice constant.

The (1.118) can be expressed as

$$\[E + \omega_1 k_s^2 + \omega_2 k_z^2\] \[E + \delta_0 - \omega_3 k_s^2 - \omega_4 k_z^2\] = I_1 (k_z^2 + k_s^2)^2 \tag{1.119}$$

The use of (1.119) leads to the expression of the 2D dispersion law in UFs of  $n-PtSb_2$  as

$$k_s^2 = t_{44}(E, n_z) (1.120)$$

where,

$$t_{44}(E, n_z) = [2A_9]^{-1} \left[ -A_{10}(E, n_z) + \sqrt{A_{10}^2(E, n_z) + 4A_9A_{11}(E, n_z)} \right]$$
(1.121)

$$A_9 = [I_1 + \omega_1 \omega_3], A_{10}(E, n_z)$$

$$= \left[\omega_3 E + \omega_1 \left\{ E + \delta_0 - \omega_4 \left(\frac{\pi n_z}{d_z}\right)^2 \right\} + \omega_2 \omega_3 \left(\frac{\pi n_z}{d_z}\right)^2 + 2I_1 \left(\frac{\pi n_z}{d_z}\right)^2 \right]$$

and

$$\begin{split} A_{11}(E,n_z) &\equiv \left[ E \left[ E + \delta_0 - \omega_4 \left( \frac{\pi n_z}{d_z} \right)^2 \right] \right. \\ &+ \omega_2 \left( \frac{\pi n_z}{d_z} \right)^2 \left[ E + \delta_0 - \omega_4 \left( \frac{\pi n_z}{d_z} \right)^2 \right] - I_1 \left( \frac{\pi n_z}{d_z} \right)^4 \right] \end{split}$$

The area of  $k_s$  space can be expressed as

$$A(E, n_z) = \frac{\pi}{2A_0} t_{44}(E, n_z)$$
 (1.122)

The EEM can be written as

$$m^*(E_{Fs}, n_z) = \frac{\hbar^2}{4A_9} t'_{44}(E_{Fs}, n_z)$$
 (1.123)

It appears that the EEM in UFs of  $PtSb_2$  is a function of Fermi energy and size quantum number which is the characteristic features of such systems.

The total DOS function assumes the form

$$N_{2DT}(E) = \frac{g_v}{4\pi A_9} \sum_{n_z=1}^{n_{z_{max}}} [t'_{44}(E, n_z)] H(E - E_{n_{z_{14}}})$$
 (1.124)

where the quantized levels  $E_{n_{z14}}$  can be expressed through the equation

$$E_{n_{z_{1}4}} = (2)^{-1} \left[ -\left[ \omega_{2} \left( \frac{\pi n_{z}}{d_{z}} \right)^{2} + \delta_{0} - \omega_{4} \left( \frac{\pi n_{z}}{d_{z}} \right)^{2} \right] + \left\{ \left[ \omega_{2} \left( \frac{\pi n_{z}}{d_{z}} \right)^{2} + \delta_{0} - \omega_{4} \left( \frac{\pi n_{z}}{d_{z}} \right)^{2} \right]^{2} + 4 \left[ I_{1} \left( \frac{\pi n_{z}}{d_{z}} \right)^{4} + \omega_{2} \omega_{4} \left( \frac{\pi n_{z}}{d_{z}} \right)^{4} - \omega_{2} \delta_{0} \left( \frac{\pi n_{z}}{d_{z}} \right)^{2} \right]^{1/2} \right]$$

$$(1.125)$$

The electron statistics can be written as