

Kamakhya Prasad Ghatak
Sitangshu Bhattacharya

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Thermoelectric Power in Nanostructured Materials

Strong Magnetic Fields



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Kamakhya Prasad Ghatak
Sitangshu Bhattacharya

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Strong Magnetic Fields

With 174 Figures

 Springer

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Dedicated to the Sweet Memories of Late Professor Sushil Chandra Dasgupta, D. Sc., Formerly Head of the Department of Mathematics of the then Bengal Engineering College (Presently Bengal Engineering and Science University), Shibpur, West Bengal, India, Late Professor Biswaranjan Nag, D. Sc., Formerly Head of the Departments of Radiophysics and Electronics and Electronic Science, University of Calcutta, Kolkata, West Bengal, India, and Late Professor Sankar Sebak Baral, D. Sc., Formerly Founding Head of the Department of Electronics and Telecommunication Engineering of the then Bengal Engineering College (Presently Bengal Engineering and Science University), Shibpur, West Bengal, India, for their pioneering contributions in research and teaching of Applied Mathematics, Semiconductor Science, And Applied Electronics, respectively, to which the first author remains ever grateful as a student and research worker

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 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, etc.) spawns not only useful quantum effect devices but also unearth new concepts in the realm of nanostructured materials science and related disciplines. It is worth remarking that these semiconductor nanostructures occupy a paramount position in the entire arena of low-dimensional science 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, heterojunction field-effect, quantum well and quantum wire 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, thin film transistors, intermediate-band solar cells, microoptical systems, high-performance infrared imaging systems, bandpass filters, thermal sensors, optical modulators, optical switching systems, single electron/molecule electronics, nanotube based diodes, and other nanoelectronic devices. 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].

With the advent of Seebeck effect in 1821 [3–6], it is evident that the investigations regarding the thermoelectric materials, the subset of the generalized set materials science have unfathomable proportions with respect to accumulated knowledge and new research in multidimensional aspects of thermoelectrics in general [7–17]. The timeline of thermoelectric and related research during the 200 years spanning from 1800 to 2000 is given in [18], and with great dismay, we admit that the citation of even pertinent references in this context is placed permanently in the gallery of impossibility theorems. It is rather amazing to observe from the detailed survey of

almost the whole spectrum of the literature in this particular aspect that the available monographs, hand books, and review articles on thermoelectrics and related topics have not included any detailed investigations on the thermoelectric power in nanostructured materials under strong magnetic field (TPSM).

It is well known that the TPSM is a very important quantity [19], since the change in entropy (a vital concept in thermodynamics) can be known from this relation by determining the experimental values of the change of electron concentration. The analysis of TPSM generates information regarding the effective mass of the carriers in materials, which occupies a central position in the whole field of materials science in general [20]. The classical TPSM (G_0) equation is valid only under the nondegenerate carrier concentration, and the magnitude of the TPSM is given by ($G_0 = (\pi^2 k_B / 3e)$ (k_B and e are Boltzmann's constant and the magnitude of the carrier charge, respectively; [21]). From this equation, it is readily inferred that this conventional form is a function of three fundamental constants only, being independent of the signature of the charge carriers in materials. The significant work of Zawadzki [22–24] reflects the fact that the TPSM 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 nano thickness 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.

This monograph, which is based on our 20 years of continuous and ongoing research, is divided into four parts. The first part deals with the thermoelectric power under large magnetic field in quantum-confined materials and it contains four chapters. In Chap. 1, we have investigated the TPSM for quantum dots of nonlinear optical, III–V, II–VI, n-GaP, n-Ge, Te, Graphite, PtSb₂, zerogap, II–V, Gallium Antimonide, stressed materials, Bismuth, IV–VI, lead germanium telluride, Zinc and Cadmium diphosphides, Bi₂Te₃, and Antimony on the basis of respective carrier energy spectrum. In Chap. 2, the TPSM in ultrathin films and quantum wires of nonlinear optical, Kane type III–V, II–VI, Bismuth, IV–VI, stressed materials, and carbon nanotubes (a very important quantum material) have been investigated. In Chap. 3, the TPSM in quantum dot III–V, II–VI, IV–VI, HgTe/CdTe superlattices with graded interfaces and quantum dot effective mass superlattices of the aforementioned materials have been investigated. In Chap. 4, the TPSM in quantum wire superlattices of the said materials have been studied.

The second part of this monograph deals with the thermoelectric power under magnetic quantization in macro and micro electronic materials. In Chap. 5, the thermoelectric power in nonlinear optical, Kane type III–V, II–VI, Bismuth, IV–VI, and stressed materials has been investigated in the presence of quantizing magnetic field. In Chap. 6, the thermoelectric power under magnetic quantization in III–V, II–VI, IV–VI, HgTe/CdTe superlattices with graded interfaces and effective mass superlattices of the aforementioned materials together with the quantum wells of said

superlattices have been investigated. In Chap. 7, the thermoelectric power under magnetic quantization in ultrathin films of nonlinear optical, Kane type III–V, II–VI, Bismuth, IV–VI, and stressed materials has been investigated.

The third part deals with the thermoelectric power under large magnetic field in quantum-confined optoelectronic materials in the presence of light waves. In Chap. 8, the influence of light on the thermoelectric power under large magnetic field in ultrathin films and quantum wires of optoelectronic materials has been investigated. In Chap. 9, the thermoelectric power under large magnetic field in quantum dots of optoelectronic materials has been studied in the presence of external light waves. In Chap. 10, the same has been studied for III–V quantum wire and quantum dot superlattices with graded interfaces and III–V quantum wire and quantum dot effective mass superlattices, respectively.

The last part of this monograph deals with thermoelectric power under magnetic quantization in macro and micro optoelectronic materials in the presence of light waves. In Chap. 11, the optothermoelectric power in macro optoelectronic materials under magnetic quantization has been investigated. In Chap. 12, the optothermoelectric power in ultrathin films of optoelectronic materials under magnetic quantization has been studied. In Chap. 13, the magneto thermo power in III–V quantum well superlattices with graded interfaces and III–V quantum well effective mass superlattices have been studied. Chapter 14 discusses eight applications of our results in the realm of quantum effect devices and also discusses very briefly the experimental results, and additionally, we have proposed a single multidimensional open research problem for experimentalists regarding the thermoelectric power in nanostructured materials having various carrier energy spectra under different physical conditions. Chapter 15 contains the conclusion and scope of future research. Appendix A contains the TPSM for bulk specimens of few technologically important materials. Each chapter except the last two contains a table highlighting the basic results pertaining to it in a summarized form.

It is well known that the errorless first edition of any book is virtually impossible from the perspective of academic reality and the same stands very true for this monograph in spite of the Herculean joint effort of not only the authors but also the seasoned Editorial team of Springer. Naturally, we are open to accept constructive criticisms for the purpose of their inclusion in the future edition. From Chap. 1 till end, this monograph presents to its esteemed readers 150 open research problems, which will be useful in the real sense of the term for the researchers in the fields of solid state sciences, materials science, computational and theoretical nanoscience and technology, nanostructured thermodynamics and condensed matter physics in general in addition to the graduate courses on modern thermoelectric materials in various academic departments of many institutes and universities. We strongly hope that the 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 will also generate new research problems, both theoretical and experimental and, thereby, transforming this monograph into a monumental superstructure.

It is needless to say that this monograph exposes only the tip of the iceberg, the rest of which will be worked upon by the researchers of the appropriate fields whom we would like to believe are creatively superior to us. It is an amazing fact to observe that the experimental investigations of the thermoelectric power under strong magnetic field in nanostructured materials have been relatively less investigated in the literature, although such studies will throw light on the understanding of the band structures of nanostructured materials, which, in turn, control the transport phenomena in such low-dimensional quantized systems. Various mathematical analyses and few chapters of this monograph are appearing for the first time in printed form. We hope that our esteemed readers will enjoy the investigations of TPSM in a wide range of nanostructured materials having different energy-wave vector dispersion relation of the carriers under various physical conditions as presented in this book. Since a monograph on the thermoelectric power in nanostructured materials under strong magnetic field is really nonexistent to the best of our knowledge even in the field of nanostructured thermoelectric materials, we earnestly hope our continuous effort of 20 years will be transformed into a standard reference source for creatively enthusiastic readers and researchers engaged either in theoretical or applied research in connection with low-dimensional thermal electronics in general to probe into the in-depth investigation of this extremely potential and promising research area of materials science.

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Kolkata
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K.P. Ghatak
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List of Symbols

α	Band nonparabolicity parameter
α_{11}, α_{12}	Energy-band constants
$\bar{\alpha}_{11}, \alpha_{22}, \alpha_{33}, \alpha_{23}$	Spectrum constants
$\bar{\alpha}_{11}, \bar{\alpha}_{22}, \bar{\alpha}_{33}, \bar{\alpha}_{23}$	Spectrum constants
$\beta_1, \beta_2, \beta_4, \beta_5$	System constants
γ_{11}, γ_{12}	Energy-band constants
$\beta_{11}, \beta_{12}, \gamma_1, \gamma_5$	Energy-band constants
δ	Crystal field splitting constant
δ'	Dirac's delta function
δ_0	Band constant
$\Delta_{ }$	Spin-orbit splitting constant parallel to the C-axis
Δ_{\perp}	Spin-orbit splitting constant perpendicular to the C-axis
Δ	Isotropic spin-orbit splitting constant
Δ_0	Interface width in superlattices
Δ_1	Energy-band constant
Δ'_c, Δ''_c	Spectrum constants
λ	Wavelength
λ_0	Band constant
$\hat{\epsilon}$	Strain tensor
ϵ	Trace of the strain tensor
$\bar{\epsilon}$	Energy as measured from the center of the band gap E_{g_0}
ϵ_{sc}	Semiconductor permittivity
ϵ_0	Permittivity of vacuum
$\zeta(2r)$	Zeta function of order $2r$
ζ_0	Constant of the spectrum
$\Gamma(j+1)$	Complete Gamma function
ω_0	Cyclotron resonance frequency
ν	Frequency
$\theta_1(k)$	Warping of the Fermi surface
$\theta_2(k)$	Inversion asymmetry splitting of the conduction band
Γ_i	Broadening parameter
Ω	Thermodynamic potential
\bar{a}	Constant of the spectrum

\bar{a}	Lattice constant
a_c	Nearest neighbor C–C bonding distance
a_{13}	Nonparabolicity constant
a_{15}	Warping parameter
a_0	The width of the barrier for superlattice structures
\bar{A}	Spectrum constant
A_i	Energy band constants
b_0	The width of the well for superlattice structures
B	Quantizing magnetic field
B_2	Momentum matrix element
c	Velocity of light
\bar{c}	Constant of the spectrum
C_0	Splitting of the two-spin states by the spin orbit coupling and the crystalline field
C_1	Conduction band deformation potential
C_2	Strain interaction between the conduction and valance bands
d_x, d_y, d_z	Nano thickness along the x , y , and z -directions
e	Magnitude of electron charge
E	Total energy of the carrier
E'	Sub-band energy
\bar{E}	Energy of the hole as measured from the top of the valance band in the vertically downward direction
E_F	Fermi energy
E_{F1}	Fermi energy as measured from the mid of the band gap in the vertically upward direction in connection with nanotubes
E_{FB}	Fermi energy in the presence of magnetic field
\bar{E}_i	Energy-band constant
E_{n_z}	Energy of the n th sub-band
E_{FQD}	Fermi energy in the presence of 3D quantization as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
E_{F1D}	Fermi energy in the presence of two-dimensional quantization as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
E_{F2D}	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
$E_{FQDSLGI}$	Fermi energy in quantum dot superlattices with graded interfaces as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
$E_{FQDSLEM}$	Fermi energy in quantum dot effective mass superlattices as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization

E_{FQWSLGI}	Fermi energy in quantum wire superlattices with graded interfaces as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
E_{FQWSLEM}	Fermi energy in quantum wire effective mass superlattices as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
E_{FQWSLEML}	Fermi energy in quantum wire effective mass superlattices in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
E_{FQDSLEML}	Fermi energy in quantum dot effective mass superlattices in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
$E_{\text{g}0}$	Band gap in the absence of any field
E_{B}	Bohr electron energy
E_{QD}	Totally quantized energy
E_{FQD}	Fermi energy in quantum dots as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
$E_{\text{F}2\text{DL}}$	Fermi energy in ultrathin films in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
$E_{\text{F}0\text{DL}}$	Fermi energy in quantum dots in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
E_{FBL}	Fermi energy under quantizing magnetic field in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
$E_{\text{F}2\text{DBL}}$	Fermi energy in ultrathin films under quantizing magnetic field in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
$E_{\text{FBQWSLEML}}$	Fermi energy in quantum well effective mass superlattices under magnetic quantization in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
E_{FBQWSLGI}	Fermi energy in quantum well superlattices with graded interfaces under magnetic quantization in the presence of light waves as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization
$E_{n_x}, E_{n_y}, E_{n_z}$	The quantized energy levels due to infinity deep potential well along the x , y and z -directions
$f(E)$	Fermi–Dirac occupation probability factor

$F_j(\eta)$	One parameter Fermi–Dirac integral of order j
$F_0(\eta_{n_z})$	Special case of the one parameter Fermi–Dirac integral of order j
$F_1(\eta_{n_z})$	Special case of the one parameter Fermi–Dirac integral of order j
g_v	Valley degeneracy
G_0	Thermoelectric power under strong magnetic field
h	Planck’s constant
\hbar	Dirac’s constant ($\equiv h/(2\pi)$)
H	Heaviside step function
i	Integer
I_0	Light intensity
k_0	Constant of the energy spectrum
\bar{k}_0	Inverse Bohr radius
k_B	Boltzmann’s constant
k	Electron wave vector
l_x	Sample length along x direction
$\bar{l}, \bar{m}, \bar{n}$	Matrix elements of the strain perturbation operator
l	Band constant
L_0	Period of the superlattices
m_0	Free electron mass
m^*	Isotropic effective electron mass at the edge of the conduction band
$m_{ }^*$	Longitudinal effective electron mass at the edge of the conduction band
m_{\perp}^*	Transverse effective electron mass at the edge of the conduction band
m_1	Effective carrier mass at the band-edge along x direction
m_2	Effective carrier mass at the band-edge along y direction
m_3	The effective carrier mass 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_t^*	The transverse effective mass at $k = 0$
m_l^*	The longitudinal effective mass at $k = 0$
$m_{\perp,1}^*, m_{ ,1}^*$	Transverse and longitudinal effective electron mass 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 valence band in the absence of any field
m_v^*	Effective mass of the holes at the top of the valence band
m_t^{\pm}	Contributions to the transverse effective mass of the external L_6^+ and L_6^- bands arising from the $\vec{k} \cdot \vec{p}$ perturbations with the other bands taken to the second order

m_l^\pm	Contributions to the longitudinal effective mass of the external L_6^+ and L_6^- bands arising from the $\vec{k} \cdot \vec{p}$ perturbations with the other bands taken to the second order
m_{tc}	Transverse effective electron mass of the conduction electrons at the edge of the conduction band
m_{lc}	Longitudinal effective electron mass of the conduction electrons at the edge of the conduction band
m_{tv}	Transverse effective hole mass of the holes at the edge of the valence band
m_{lv}	Longitudinal effective hole mass of the holes at the edge of the valence band
n_x, n_y, n_z	Size quantum numbers along the x , y , and z -directions
n_0	Carrier degeneracy
n	Landau quantum number/chiral indices
\bar{n}	Band constant
$N(E)$	Density of states in bulk specimens
N_c	Effective number of states in the conduction band
$N_{2D}(E)$	2D density-of-states function per sub-band
$N_{2DT}(E)$	Total 2D density-of-states function
P_0	Momentum matrix element
(\bar{P})	Energy-band constant
P_{\parallel}, P_{\perp}	Momentum matrix elements parallel and perpendicular to the direction of C-axis
\bar{Q}, \bar{R}	Spectrum constants
r_0	Radius of the nanotube
\bar{s}	Spectrum constant
s_0	Upper limit of the summation
\bar{S}_0	Entropy per unit volume
t_c	Tight binding parameter
t_i	Energy band constants
T	Temperature
v	Band constant
\bar{v}_0, \bar{w}_0	Constants of the spectrum
V_0	Potential barrier
$ V_G $	Constants of the energy spectrum
x, y	Alloy compositions

Part I
Thermoelectric Power Under
Large Magnetic Field in Quantum
Confined Materials

Chapter 1

Thermoelectric Power in Quantum Dots Under Large Magnetic Field

1.1 Introduction

In recent years, with the advent of Quantum Hall Effect (QHE) [1,2], there has been considerable interest in studying the thermoelectric power under strong magnetic field (TPSM) in various types of nanostructured materials having quantum confinement of their charge carriers in one, two, and three dimensions of the respective wave-vector space leading to different carrier energy spectra [3–38]. The classical TPSM equation as mentioned in the preface is valid only under the condition of carrier nondegeneracy, is being independent of carrier concentration, and reflects the fact that the signature of the band structure of any material is totally absent in the same.

Zawadzki [8] demonstrated that the TPSM for electronic materials having degenerate electron concentration is essentially determined by their respective energy band structures. It has, therefore, different values in different materials and changes with the doping; with the magnitude of the reciprocal quantizing magnetic field under magnetic quantization, quantizing electric field as in inversion layers, and nanothickness as in quantum wells, wires, and dots; and with the superlattice period as in quantum-confined semiconductor superlattices with graded interfaces having various carrier energy spectra and also in other types of field-assisted nanostructured materials. Some of the significant features that have emerged from these studies are:

- (a) The TPSM decreases with the increase in carrier concentration.
- (b) The TPSM decreases with increasing doping in heavily doped semiconductors forming band tails.
- (c) The nature of variations is significantly influenced by the spectrum constants of various materials having different band structures.
- (d) The TPSM exhibits oscillatory dependence with inverse quantizing magnetic field because of the Shubnikov–de Haas effect.
- (e) The TPSM decreases with the magnitude of the quantizing electric field in inversion layers.
- (f) The TPSM exhibits composite oscillations with significantly different values in superlattices and various other quantized field aided structures.

In this chapter, an attempt is made to investigate the TPSM in quantum dots of nonlinear optical, III–V, II–VI, GaP, Ge, Te, Graphite, PtSb₂, zerogap, II–V, GaSb, stressed materials, Bismuth, IV–VI, Lead Germanium Telluride, Zinc and Cadmium diphosphides, Bi₂Te₃, and Antimony from Sects. 1.2.1 to 1.2.18, respectively. In this context, it may be noted that with the advent of fine line lithography [39], molecular beam epitaxy [40, 41], organometallic vapor-phase epitaxy [42], and other experimental techniques, low-dimensional structures [43–55] having quantum confinement of the charge carriers in one, two, and three dimensions [such as ultrathin films (UFs), nipi structures, inversion and accumulation layers, quantum well superlattices, carbon nanotubes, quantum wires (QWs), quantum wire superlattices, quantum dots (QDs), magnetoinversion and accumulation layers, quantum dot superlattices, etc.] have, in the last few years, created tremendous passion among the interdisciplinary researchers not only for the potential of these quantized structures in uncovering new phenomena in nanostructured science but also for their new diverse technological applications. As the dimension of the UFs increases from one dimension to three dimension, the degree of freedom of the free carriers decreases drastically and the density-of-states function changes from the Heaviside step function in UFs to the Dirac's delta function in QDs [56, 57].

The QDs can be used for visualizing and tracking molecular processes in cells using standard fluorescence microscopy [58–61]. They display minimal photobleaching [62], thus allowing molecular tracking over prolonged periods, and consequently, single molecule can be tracked by using optical fluorescence microscopy [63, 64]. The salient features of quantum dot lasers [65–67] include lower threshold currents, higher power, and greater stability compared with that of the conventional one, and the QDs find extensive applications in nanorobotics [68–71], neural networks [72–74], and high density memory or storage media [75]. The QDs are also used in nanophotonics [76] because of their theoretically high quantum yield and have been suggested as implementations of qubits for quantum information processing [77]. The QDs also find applications in diode lasers [78], amplifiers [79, 80], and optical sensors [81, 82]. High-quality QDs are well suited for optical encoding [83, 84] because of their broad excitation profiles and narrow emission spectra. The new generations of QDs 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 [85, 86]. The QD nanotechnology is one of the most promising candidates for use in solid-state quantum computation [87, 88]. It may also be noted that the QDs are being used in single electron transistors [89, 90], photovoltaic devices [91, 92], photoelectrics [93], ultrafast all-optical switches and logic gates [94–97], organic dyes [98–100], and in other types of nanodevices.

Section 1.2.1 investigates the TPSM in QDs of nonlinear optical materials (taking n-CdGeAs₂ as an example), which find applications in nonlinear optics and light-emitting diodes [101]. The quasicubic 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 [102]. Including the anisotropic crystal potential in the Hamiltonian and the special features of the nonlinear optical compounds, Kildal [103]

formulated the electron dispersion law under the assumptions of isotropic momentum matrix 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 [104–106].

In this context, it may be noted that the III–V compounds find potential applications in infrared detectors [107], quantum dot light-emitting diodes [108], quantum cascade lasers [109], quantum well wires [110], optoelectronic sensors [111], high electron mobility transistors [112], etc. The III–V, ternary and quaternary materials are called the Kane-type compounds, since their electron energy spectra are being defined by the three-band model of Kane [113]. In Sect. 1.2.2, the TPSM from QDs of III–V materials has been studied, and the simplified results for two-band model of Kane and that of wide gap materials have further been demonstrated as special cases. Besides Kane, the conduction electrons of III–V materials also obey another six different types of electron dispersion laws as given in the literature. The TPSM has also been investigated for all the cases for the purpose of complete presentation and relative assessment among the energy band models of III–V compounds.

The II–VI compounds are being extensively used in nanoribbons, blue green diode lasers, photosensitive thin films, infrared detectors, ultrahigh-speed bipolar transistors, fiber-optic communications, microwave devices, photovoltaic and solar cells, semiconductor gamma-ray detector arrays, and semiconductor detector gamma camera and allow for a greater density of data storage on optically addressed compact discs [114–121]. The carrier energy spectra in II–VI materials are defined by the Hopfield model [122], 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 TPSM in QDs of II–VI compounds, taking p-CdS as an example.

The n-Gallium Phosphide (n-GaP) is being used in quantum dot light-emitting diode [123], high-efficiency yellow solid state lamps, light sources, and 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 [124–126]. In Sect. 1.2.4, the TPSM in QDs of n-GaP is studied. The importance of Germanium is already well known since the inception of transistor technology, and in recent years, memory circuits, single photon detectors, single photon avalanche diode, ultrafast all-optical switch, THz lasers, and THz spectrometers [127–130] are made of Ge. In Sect. 1.2.5, the TPSM has been studied in QDs of Ge.

Tellurium (Te) is also an elemental semiconductor which has been used as the semiconductor layer in thin-film transistors (TFT) [131]. Te also finds extensive applications in CO₂ laser detectors [132], electronic imaging, strain sensitive devices [133, 134], and multichannel Bragg cell [135]. Section 1.2.6 contains the investigation of TPSM in QDs of Tellurium. The importance of graphite is already well known in the whole spectrum of materials science, and the low-dimensional graphite is used instead of carbon wire in many practical applications. Graphite intercalation compounds are often used as suitable model for investigation of low-dimensional systems and, in particular, for investigation of phase transition in such systems [136–139]. In Sect. 1.2.7, the TPSM in QDs of graphite has

been explored. Platinum Antimonide (PtSb_2) finds applications in device miniaturization, colloidal nanoparticle synthesis, sensors and detector materials, and thermo-photovoltaic devices [140–142]. The TPSM in QDs of p- PtSb_2 has been investigated in Sect. 1.2.8.

Zerogap compounds are used in optical waveguide switch or modulators that can be fabricated by using the electro-optic and thermo-optic effects for facilitating optical communications and signal processing. The gapless materials also find extensive applications in infrared detectors and night vision cameras [143–147]. Section 1.2.9 contains the study of TPSM in QDs of the same taking p-HgTe as an example.

The II–V materials are used in photovoltaic cells constructed of single crystal materials in contact with electrolyte solutions. Cadmium selenide shows an open-circuit voltage of 0.8 V and power conservation coefficients of nearly 6% for 720-nm light [148]. They are also used in ultrasonic amplification [149]. The thin film transistor using cadmium selenide as the semiconductor has been developed [150, 151]. In Sect. 1.2.10, the TPSM in QDs of II–V materials has been studied taking CdSb as an example. Gallium antimonide (GaSb) finds applications in the fiber-optic transmission window, heterojunctions, and quantum wells. A complementary heterojunction field effect transistor (CHFET) 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 [152–157]. In Sect. 1.2.11, the TPSM in QDs of GaSb has been studied.

It may be noted that the stressed materials are being widely investigated for strained silicon transistors, quantum cascade lasers, semiconductor strain gages, thermal detectors, and strained-layer structures [158–161]. The TPSM in QDs of stressed materials (taking stressed n-InSb as an example) has been investigated in Sect. 1.2.12. In recent years, Bismuth (Bi) nanolines are fabricated, and Bi also finds use in array of antennas which leads to the interaction of electromagnetic waves with such Bi nanowires [162, 163]. Several dispersion relations of the carriers have been proposed for Bi. Shoenberg [164, 165] 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 [166]. The experimental investigations on the magneto-optical [167] and the ultrasonic quantum oscillations [168] support the Lax ellipsoidal nonparabolic model [166]. Kao [169], Dinger and Lawson [170], and Koch and Jensen [171] demonstrated that the Cohen model [172] 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 [173]. McClure and Choi [174] devised 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. 1.2.13, we have formulated the TPSM in QDs of Bi in accordance with the aforementioned energy band models for the purpose of relative assessment.

Lead chalcogenides (PbTe, PbSe, and PbS) are IV–VI compounds whose studies over several decades have been motivated by their importance in infrared IR detectors, lasers, light-emitting devices, photovoltaics, and high-temperature thermoelectric [175–179]. PbTe, in particular, is the end compound of several ternary

and quaternary high-performance high-temperature thermoelectric materials [180–184]. It has been used not only as bulk but also as films [185–188], quantum wells [189], superlattices [190, 191], nanowires [192], and colloidal and embedded nanocrystals [193–196]. PbTe films doped with various impurities have also been investigated [197–200]. These studies revealed some of the interesting features that have been observed in bulk PbTe, such as Fermi level pinning, and in the case of superconductivity [201]. In Sects. 1.2.14 and 1.2.15, the TPSM in QDs of IV–VI materials $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$ has been studied.

The diphosphides find prominent role in biochemistry where the folding and structural stabilization of many important extracellular peptide and protein molecules, including hormones, enzymes, growth factors, toxins, and immunoglobulin, are concerned [202–204]. Besides, artificial introduction of extra diphosphides into peptides or proteins can improve biological activity [205, 206] or confer thermostability [207]. 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 spectrophotometric titration of the released 3-nitro-2-pyridinethiol [208, 209]. In Sect. 1.2.16, the TPSM in QDs of zinc and cadmium diphosphides has been investigated.

Bismuth telluride (Bi_2Te_3) was first identified as a material for thermoelectric refrigeration in 1954 [210] and its physical properties were later improved by the addition of bismuth selenide and antimony telluride to form solid solutions [211–215]. The alloys of Bi_2Te_3 are very important compounds for the thermoelectric industry and have extensively been investigated in the literature [211–215]. In Sect. 1.2.17, the TPSM in QDs of Bi_2Te_3 has been considered. In recent years, antimony has emerged to be very promising, since glasses made from antimony are being extensively used in near infrared spectral range for third- or second-order nonlinear processes. The chalcogenide glasses are in general associated with high nonlinear properties for their Infrared transmission from 0.5–1 μm to 12–18 μm [216–221]. Alloys of Sb are used as ultrahigh-frequency indicators and in thin-film thermocouple [216–221]. In Sect. 1.2.18, the TPSM in QDs of Sb has been studied. Section 1.3 contains results and discussion for this chapter. Section 1.4 contains the open research problems pertinent to this chapter.

1.2 Theoretical Background

1.2.1 *Magnetothermopower in Quantum Dots of Nonlinear Optical Materials*

The form of $\mathbf{k}\cdot\mathbf{p}$ matrix for nonlinear optical compounds can be expressed extending Bodnar [222] as

$$H = \begin{bmatrix} H_1 & H_2 \\ H_2^+ & H_1 \end{bmatrix}, \quad (1.1)$$

where

$$H_1 \equiv \begin{bmatrix} E_{g_0} & 0 & P_{\parallel} k_z & 0 \\ 0 & (-2\Delta_{\parallel}/3) & (\sqrt{2}\Delta_{\perp}/3) & 0 \\ P_{\parallel} k_z & (\sqrt{2}\Delta_{\perp}/3) & -(\delta + \frac{1}{3}\Delta_{\parallel}) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and

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

in which E_{g_0} is the band gap in the absence of any field; P_{\parallel} and P_{\perp} the momentum matrix elements parallel and perpendicular to the direction of crystal axis, respectively; δ the crystal field splitting constant; and Δ_{\parallel} and Δ_{\perp} are the spin-orbit splitting constants parallel and perpendicular to the C -axis, respectively, $f_{,\pm} \equiv (P_{\perp}/\sqrt{2})(k_x \pm ik_y)$ 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 compounds [223] as

$$\gamma(E) = f_1(E)k_s^2 + f_2(E)k_z^2, \quad (1.2)$$

where

$$\begin{aligned} \gamma(E) &\equiv E(E + E_{g_0}) \left[(E + E_{g_0})(E + E_{g_0} + \Delta_{\parallel}) \right. \\ &\quad \left. + \delta \left(E + E_{g_0} + \frac{2}{3}\Delta_{\parallel} \right) + \frac{2}{9}(\Delta_{\parallel}^2 - \Delta_{\perp}^2) \right], \quad k_s^2 = k_x^2 + k_y^2, \\ f_1(E) &\equiv \frac{\hbar^2 E_{g_0} (E_{g_0} + \Delta_{\perp})}{[2m_{\perp}^* (E_{g_0} + \frac{2}{3}\Delta_{\perp})]} \left[\delta \left(E + E_{g_0} + \frac{1}{3}\Delta_{\parallel} \right) \right. \\ &\quad \left. + (E + E_{g_0}) \left(E + E_{g_0} + \frac{2}{3}\Delta_{\parallel} \right) + \frac{1}{9}(\Delta_{\parallel}^2 - \Delta_{\perp}^2) \right], \\ f_2(E) &\equiv \frac{\hbar^2 E_{g_0} (E_{g_0} + \Delta_{\parallel})}{[2m_{\parallel}^* (E_{g_0} + \frac{2}{3}\Delta_{\parallel})]} \left[(E + E_{g_0}) \left(E + E_{g_0} + \frac{2}{3}\Delta_{\parallel} \right) \right] \end{aligned}$$

and m_{\parallel}^* and m_{\perp}^* are the longitudinal and transverse effective electron masses at the edge of the conduction band, respectively.

Let E_{n_i} ($i = x, y$ and z) be the quantized energy levels due to infinitely deep potential well along i th axis with $n_i = 1, 2, 3 \dots$ as the size quantum numbers. Therefore, from (1.2), one can write

$$\gamma(E_{n_x}) = f_1(E_{n_x}) \left(\frac{\pi n_x}{d_x} \right)^2 \quad (1.3)$$

$$\gamma(E_{n_y}) = f_1(E_{n_y}) \left(\frac{\pi n_y}{d_y} \right)^2 \quad (1.4)$$

$$\gamma(E_{n_z}) = f_2(E_{n_z}) \left(\frac{\pi n_z}{d_z} \right)^2 \quad (1.5)$$

From (1.2), the totally quantized energy (E_{QD1}) in this case can be expressed as

$$\gamma(E_{\text{QD1}}) = f_1(E_{\text{QD1}}) \left[\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 \right] + f_2(E_{\text{QD1}}) \left[\left(\frac{\pi n_z}{d_z} \right)^2 \right] \quad (1.6)$$

The total electron concentration per unit volume in this case assumes the form

$$n_0 = \frac{2g_v}{d_x d_y d_z} \sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{L_{11}}{M_{11}}, \quad (1.7)$$

where g_v is the valley degeneracy,

$$L_{11} = [1 + A_1 \cos H_1] \quad (1.8)$$

$$M_{11} = 1 + A_1^2 + 2A_1 \cos H_1 \quad (1.9)$$

in which

$$A_1 = \exp \left[\frac{E_{\text{QD1}} - E_{\text{FQD}}}{k_B T} \right],$$

E_{FQD} is the Fermi energy in the presence of three-dimensional quantization as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization; T the temperature; $H_1 = \Gamma_1/k_B T$; and Γ_1 is the broadening parameter in this case.

The TPSM (G_0) can, in general, be expressed as [3]

$$G_0 = \frac{1}{e} \left(\frac{\partial \overline{S}_0}{\partial n_0} \right)_{E_F, T}, \quad (1.10)$$

where E_F is the Fermi energy corresponding to the electron concentration n_0 and \overline{S}_0 is the entropy per unit volume which can be written as

$$\overline{S}_0 = - \left. \frac{\partial \Omega}{\partial T} \right|_{E=E_F} \quad (1.11)$$

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

$$\Omega = -k_B T \sum \ln \left| 1 + \exp \left[\frac{E_F - E_{\delta_0}}{k_B T} \right] \right|, \quad (1.12)$$

where the summation is carried out over all the possible δ_0 states.

Thus, combining (1.10)–(1.12), the magnitude of the TPSM can be written in a simplified form as [10]

$$G_0 = (\pi^2 k_B^2 T / 3en_0) \left(\frac{\partial n_0}{\partial E_F} \right) \quad (1.13)$$

It should be noted that being a thermodynamic relation and temperature-induced phenomena, the TPSM as expressed by (1.13), 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, (1.13) 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, magnetoinversion and accumulation layers, quantum dot superlattices, magneto nipsis, quantum well superlattices under magnetic quantization, ultrathin films under magnetic quantization, etc.). The formulation of G_0 requires the relation between the 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, magnetoinversion and accumulation layers, magneto nipsis, quantum well superlattices under magnetic quantization and magnetosize 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.

The TPSM in this case using (1.7) and (1.13) can be written as

$$G_0 = \frac{\pi^2 k_B}{3e} \left[\sum_{n_x=1}^{n_{x_{\max}}} \sum_{n_y=1}^{n_{y_{\max}}} \sum_{n_z=1}^{n_{z_{\max}}} \frac{L_{11}}{M_{11}} \right]^{-1} \left[\sum_{n_x=1}^{n_{x_{\max}}} \sum_{n_y=1}^{n_{y_{\max}}} \sum_{n_z=1}^{n_{z_{\max}}} \frac{Q_{11}}{(M_{11})^2} \right], \quad (1.14)$$

where

$$Q_{11} = A_1 [(1 + A_1^2) \cos H_1 + 2A_1]. \quad (1.15)$$

1.2.2 Magnetothermopower in Quantum Dots of 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) [224, 225], Stillman et al. [226], Newson and Kurobe [227], Rossler [228], Palik et al. [229], Johnson and Dickey [230], and Agafonov et al. [231], respectively. For the purpose of complete and coherent presentation, the TPSM in QDs of III–V compounds has also been investigated in accordance with the aforementioned different dispersion relations for the purpose of relative comparison as follows.

1.2.2.1 The Three Band Model of Kane

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

$$\frac{\hbar^2 k^2}{2m^*} = I(E), \quad I(E) \equiv \frac{E(E + E_{g0})(E + E_{g0} + \Delta)(E_{g0} + \frac{2}{3}\Delta)}{E_{g0}(E_{g0} + \Delta)(E + E_{g0} + \frac{2}{3}\Delta)} \quad (1.16)$$

which is known as the three band model of Kane [224, 225] and is often used to study the electronic properties of III–V materials.

The totally quantized energy (E_{QD2}) in this case assumes the form

$$I(E_{\text{QD2}}) = \frac{\hbar^2 \pi^2}{2m^*} \left[\left(\frac{n_x}{d_x} \right)^2 + \left(\frac{n_y}{d_y} \right)^2 + \left(\frac{n_z}{d_z} \right)^2 \right]. \quad (1.17)$$

The electron concentration is given by

$$n_0 = \frac{2g_v}{d_x d_y d_z} \sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{L_{12}}{M_{12}}, \quad (1.18)$$

where $L_{12} = [1 + A_2 \cos H_2]$, $A_2 = \exp[E_{\text{QD2}} - E_{\text{FQD}}/k_B T]$, $H_2 = \Gamma_2/k_B T$, Γ_2 is the broadening parameter in this case, and $M_{12} = 1 + A_2^2 + 2A_2 \cos H_2$.

The TPSM in this case, using (1.13) and (1.18), can be expressed as

$$G_0 = \frac{\pi^2 k_B}{3e} \left[\sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{L_{12}}{M_{12}} \right]^{-1} \left[\sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{Q_{12}}{(M_{12})^2} \right], \quad (1.19)$$

where $Q_{12} = A_2 [(1 + A_2^2) \cos H_2 + 2A_2]$.

1.2.2.2 The Two Band Model of Kane

Under the inequalities $\Delta \gg E_{g0}$ or $\Delta \ll E_{g0}$, (1.16) assumes the form

$$E(1 + \alpha E) = (\hbar^2 k^2 / 2m^*), \quad \alpha \equiv 1/E_{g0}. \quad (1.20)$$

Equation (1.20) is known as the two-band model of Kane and should be as such for studying the electronic properties of the materials whose band structures obey the above inequalities [224, 225].

The totally quantized energy E_{QD3} in this case is given by

$$E_{QD3} (1 + \alpha E_{QD3}) = \frac{\hbar^2 \pi^2}{2m^*} \left[\left(\frac{n_x}{d_x} \right)^2 + \left(\frac{n_y}{d_y} \right)^2 + \left(\frac{n_z}{d_z} \right)^2 \right]. \quad (1.21)$$

The electron concentration can be written as

$$n_0 = \frac{2g_v}{d_x d_y d_z} \sum_{n_x=1}^{n_{x\max}} \sum_{n_y=1}^{n_{y\max}} \sum_{n_z=1}^{n_{z\max}} \frac{L_{13}}{M_{13}}, \quad (1.22)$$

where $L_{13} = [1 + A_3 \cos H_3]$, $A_3 = \exp[E_{QD3} - E_{FQD}/k_B T]$, $H_3 = \Gamma_3/k_B T$, Γ_3 is the broadening parameter in this case, and $M_{13} = 1 + A_3^2 + 2A_3 \cos H_3$.

The TPSM in this case, using (1.13) and (1.22), can be expressed as

$$G_0 = \frac{\pi^2 k_B}{3e} \left[\sum_{n_x=1}^{n_{x\max}} \sum_{n_y=1}^{n_{y\max}} \sum_{n_z=1}^{n_{z\max}} \frac{L_{13}}{M_{13}} \right]^{-1} \left[\sum_{n_x=1}^{n_{x\max}} \sum_{n_y=1}^{n_{y\max}} \sum_{n_z=1}^{n_{z\max}} \frac{Q_{13}}{(M_{13})^2} \right], \quad (1.23)$$

where $Q_{13} = A_3 [(1 + A_3^2) \cos H_3 + 2A_3]$.

1.2.2.3 The Model of Stillman et al.

In accordance with the model of Stillman et al. [226], the electron dispersion law of III–V materials assumes the form

$$E = t_{11} k^2 - t_{12} k^4 \quad (1.24)$$

where $t_{11} \equiv \hbar^2/2m^*$ and

$$t_{12} \equiv \left(1 - \frac{m^*}{m_0} \right)^2 \left(\frac{\hbar^2}{2m^*} \right)^2 \times \left[\left(3E_{g0} + 4\Delta + \frac{2\Delta^2}{E_{g0}} \right) \cdot \{ (E_{g0} + \Delta) (2\Delta + 3E_{g0}) \}^{-1} \right]$$

Equation (1.24) can be expressed as

$$\frac{\hbar^2 k^2}{2m^*} = I_{11}(E), \quad (1.25)$$

where

$$I_{11}(E) \equiv a_{11} \left[1 - (1 - a_{12}E)^{1/2} \right],$$

$$a_{11} \equiv \left(\frac{\hbar^2 t_{11}}{4m^* t_{12}} \right), a_{12} \equiv \frac{4t_{12}}{t_{11}^2}.$$

The E_{QD4} in this case can be defined as

$$I_{11}(E_{\text{QD4}}) = \frac{\hbar^2 \pi^2}{2m^*} \left[\left(\frac{n_x}{d_x} \right)^2 + \left(\frac{n_y}{d_y} \right)^2 + \left(\frac{n_z}{d_z} \right)^2 \right]. \quad (1.26)$$

The electron concentration is given by

$$n_0 = \frac{2g_v}{d_x d_y d_z} \sum_{n_x=1}^{n_{x\max}} \sum_{n_y=1}^{n_{y\max}} \sum_{n_z=1}^{n_{z\max}} \frac{L_{14}}{M_{14}}, \quad (1.27)$$

where $L_{14} = [1 + A_4 \cos H_4]$, $A_4 = \exp[E_{\text{QD4}} - E_{\text{FQD}}/k_B T]$, $H_4 = \Gamma_4/k_B T$, Γ_4 is the broadening parameter in this case, and $M_{14} = 1 + A_4^2 + 2A_4 \cos H_4$.

The TPSM in this case, using (1.13) and (1.27), can be expressed as

$$G_0 = \frac{\pi^2 k_B}{3e} \left[\sum_{n_x=1}^{n_{x\max}} \sum_{n_y=1}^{n_{y\max}} \sum_{n_z=1}^{n_{z\max}} \frac{L_{14}}{M_{14}} \right]^{-1} \left[\sum_{n_x=1}^{n_{x\max}} \sum_{n_y=1}^{n_{y\max}} \sum_{n_z=1}^{n_{z\max}} \frac{Q_{14}}{(M_{14})^2} \right], \quad (1.28)$$

where $Q_{14} = A_4 [(1 + A_4^2) \cos H_4 + 2A_4]$.

1.2.2.4 The Model of Newson and Kurobe

In accordance with the model of Newson and Kurobe, the electron dispersion law in this case assumes the form as [227]

$$E = a_{13} k_z^4 + \left[\frac{\hbar^2}{2m^*} + a_{14} k_s^2 \right] k_z^2 + \frac{\hbar^2}{2m^*} k_s^2 + a_{14} k_x^2 k_y^2 + a_{13} (k_x^4 + k_y^4), \quad (1.29)$$

where a_{13} is the nonparabolicity constant, $a_{14} (\equiv 2a_{13} + a_{15})$ and a_{15} is known as the warping parameter.

The totally quantized energy E_{QD5} in this case can be written as

$$\begin{aligned}
 E_{\text{QD5}} = & a_{13} \left(\frac{\pi n_z}{d_z} \right)^4 + \left[\frac{\hbar^2}{2m^*} + a_{14} \left(\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 \right) \right] \cdot \left(\frac{\pi n_z}{d_z} \right)^2 \\
 & + \frac{\hbar^2}{2m^*} \left[\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 \right] + a_{14} \pi^4 \left(\frac{n_x n_y}{d_x d_y} \right)^2 \\
 & + a_{13} \pi^4 \left[\left(\frac{n_x}{d_x} \right)^4 + \left(\frac{n_y}{d_y} \right)^4 \right]. \tag{1.30}
 \end{aligned}$$

The electron concentration is given by

$$n_0 = \frac{2g_v}{d_x d_y d_z} \sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{L_{15}}{M_{15}}, \tag{1.31}$$

where $L_{15} = [1 + A_5 \cos H_5]$, $A_5 = \exp[E_{\text{QD5}} - E_{\text{FQD}}/k_B T]$, $H_5 = \Gamma_5/k_B T$, Γ_5 is the broadening parameter in this case, and $M_{15} = 1 + A_5^2 + 2A_5 \cos H_5$.

The TPSM in this case, using (1.13) and (1.31), can be expressed as

$$G_0 = \frac{\pi^2 k_B}{3e} \left[\sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{L_{15}}{M_{15}} \right]^{-1} \left[\sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{Q_{15}}{(M_{15})^2} \right], \tag{1.32}$$

where $Q_{15} = A_5 [(1 + A_5^2) \cos H_5 + 2A_5]$.

1.2.2.5 The Model of Rossler

The dispersion relation of the conduction electrons in accordance with the model of Rossler can be written as [228]

$$\begin{aligned}
 E = & \frac{\hbar^2 k^2}{2m^*} + [\alpha_{11} + \alpha_{12}k] k^4 + (\beta_{11} + \beta_{12}k) [k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2] \\
 & \pm [\gamma_{11} + \gamma_{12}k] [k^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2) - 9k_x^2 k_y^2 k_z^2]^{1/2}, \tag{1.33}
 \end{aligned}$$

where α_{11} , α_{12} , β_{11} , β_{12} , γ_{11} , and γ_{12} are energy-band constants.

$E_{\text{QD6},\pm}$ in this case assumes the form

$$\begin{aligned}
E_{\text{QD6},\pm} \equiv & \frac{\hbar^2 \pi^2}{2m^*} \left[\left(\frac{n_x}{d_x} \right)^2 + \left(\frac{n_y}{d_y} \right)^2 + \left(\frac{n_z}{d_z} \right)^2 \right] \\
& + \left[\alpha_{11} + \alpha_{12} \left[\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 + \left(\frac{\pi n_z}{d_z} \right)^2 \right]^{1/2} \right] \\
& \times \left[\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 + \left(\frac{\pi n_z}{d_z} \right)^2 \right]^2 \\
& + \left[\beta_{11} + \beta_{12} \left[\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 + \left(\frac{\pi n_z}{d_z} \right)^2 \right]^{1/2} \right] \\
& \times \left[\pi^4 \left(\frac{n_x n_y}{d_x d_y} \right)^2 + \pi^4 \left(\frac{n_y n_z}{d_y d_z} \right)^2 + \pi^4 \left(\frac{n_z n_x}{d_z d_x} \right)^2 \right] \\
& \pm \left[\gamma_{11} + \gamma_{12} \left[\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 + \left(\frac{\pi n_z}{d_z} \right)^2 \right]^{1/2} \right] \\
& \times \left[\left[\left(\frac{\pi n_x}{d_x} \right)^2 + \left(\frac{\pi n_y}{d_y} \right)^2 + \left(\frac{\pi n_z}{d_z} \right)^2 \right] \right] \\
& \times \left[\pi^4 \left(\frac{n_x n_y}{d_x d_y} \right)^2 + \pi^4 \left(\frac{n_y n_z}{d_y d_z} \right)^2 + \pi^4 \left(\frac{n_z n_x}{d_z d_x} \right)^2 \right] \\
& - 9\pi^6 (n_x n_y n_z / d_x d_y d_z)^6 \Big] \tag{1.34}
\end{aligned}$$

The electron concentration is given by

$$n_0 = \frac{g_v}{d_x d_y d_z} \sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{L_{16,\pm}}{M_{16,\pm}}, \tag{1.35}$$

where $L_{16,\pm} = [1 + A_{6,\pm} \cos H_6]$, $A_{6,\pm} = \exp[E_{\text{QD6},\pm} - E_{\text{FQD}}/k_B T]$, $H_6 = \Gamma_6/k_B T$, Γ_6 is the broadening parameter in this case, and $M_{16,\pm} = 1 + A_{6,\pm}^2 + 2A_{6,\pm} \cos H_6$.

The TPSM in this case, using (1.13) and (1.35), can be expressed as

$$G_0 = \frac{\pi^2 k_B}{3e} \left[\sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{L_{16,\pm}}{M_{16,\pm}} \right]^{-1} \left[\sum_{n_x=1}^{n_x^{\max}} \sum_{n_y=1}^{n_y^{\max}} \sum_{n_z=1}^{n_z^{\max}} \frac{Q_{16,\pm}}{(M_{16,\pm})^2} \right], \tag{1.36}$$

where $Q_{16,\pm} = A_{6,\pm} \left[(1 + A_{6,\pm}^2) \cos H_6 + 2A_{6,\pm} \right]$.