

Preface

The combination of the concept of asymmetry of the wave-vector space of charge carriers in semiconductors with modern techniques of fabricating nanostructured materials such as MBE, MOCVD and FLL in one, two and three dimensions (such as quantum wells (QWs), doping superlattices, accumulation and inversion layers, quantum well superlattices, carbon nanotubes, quantum wires, quantum wire superlattices, magnetic quantization, magneto size quantization, quantum dots, magneto accumulation and inversion layers, magneto NIPs, magneto quantum well superlattices, quantum dot superlattices and other field aided low-dimensional systems) spawns not only useful quantum effect devices but also unearths new concepts in the realm of low-dimensional solid-state science and related disciplines. These semiconductor nanostructures occupy a central position in the entire arena of condensed matter science in general, by their own right and find extensive applications in quantum registers, quantum switches, quantum sensors, quantum logic gates, quantum well and quantum wire transistors, quantum cascade lasers, heterojunction field-effect transistors, high-speed digital networks, high-frequency microwave circuits, high-resolution terahertz spectroscopy, superlattice photo-oscillator, advanced integrated circuits, superlattice photocathodes, resonant tunneling diodes and transistors, thermoelectric devices, superlattice coolers, thin film transistors, intermediate-band solar cells, micro-optical systems, high performance infrared imaging systems, band-pass filters, thermal sensors, optical modulators, optical switching systems, single electron electronics, molecular electronics, nanotube-based diodes and other nanoelectronic devices. Knowledge regarding these quantized structures may be gained from original research contributions in scientific journals, various patents, personal communications, proceedings of the conferences/seminars, review articles and different research monographs [1] respectively. In this context, it may be noted that the available reports on the said areas cannot afford to cover even an entire chapter regarding the Einstein Relation (ER) for the diffusivity-mobility ratio of carriers in heavily doped (HD) two-dimensional (2D) quantized structures and the single first book on ER [2] does not contain even a paragraph regarding this important specialized topic of research and, after 30 years of continuous effort, we see that the complete investigations of the ER comprising the whole set of materials and allied sciences is really a sea and is a permanent member of the domain of impossibility theorems.

It is well known that the ER occupies a central position in the whole field of solid-state device electronics and the related sciences since the diffusion constant (a quantity very useful for device analysis where exact experimental determination is rather difficult) can be obtained from this ratio by knowing the experimental values of the mobility. The classical value of the ER is equal to $(k_B T / |e|)$, (k_B , T and $|e|$ are Boltzmann's constant, temperature and the magnitude of the carrier charge respectively). This relation in this form was first introduced by Einstein to study the diffusion of gas particles and is known as the Einstein relation [2, 3]. It appears that the ER increases linearly with increasing T and is independent of electron concentration. This relation is applicable for both types of charge carriers only under nondegenerate carrier concentration although its validity has been suggested erroneously for degenerate materials [4]. Landsberg first pointed out that the ER for degenerate semiconductors is essentially determined by their energy band structures [5, 6]. This relation is useful for semiconductor homostructures [7, 8], semiconductor–semiconductor heterostructures [9, 10], metals–semiconductor heterostructures [11–19] and insulator–semiconductor heterostructures [20–23]. The nature of the variations of the ER under different physical conditions has been studied in the literature [1–3, 5, 6, 24–49]. Incidentally, A. N. Chakravarti (a recognized leading expert of ER in general) and his research group are still contributing significantly under his able leadership regarding this pinpointed research topic on ER from 1972 [2, 24, 25–28, 34, 39–49] and some of the significant features, which have emerged from these studies, are:

- (a) The ER increases monotonically with increasing carrier concentration in bulk semiconductors and the nature of these variations is significantly influenced by the band structures of different materials.
- (b) The ER increases with the increasing quantizing electric field as in inversion layers.
- (c) The ER oscillates with the inverse quantizing magnetic field under magnetic quantization due to the Shubnikov-de Haas effect.
- (d) The ER shows composite oscillations with the various controlled quantities of semiconductor superlattices.
- (e) In ultrathin films, quantum wires and other field assisted low-dimensional systems, the value of the ER changes appreciably with the external variables depending on the nature of quantum confinements of different materials.

The ER depends on the density-of-states (DOS) function, which, in turn, is significantly affected by the different carrier energy spectra of different semiconductors having various band structures. In recent years, various energy wave-vector dispersion relations of carriers of different materials have been proposed [50], which have created interest in studying the ER in HD 2D-quantized structures. It is well known that heavy doping and carrier degeneracy are the keys to unlock the important properties of semiconductors and they are especially instrumental in dictating the characteristics of Ohmic and Schottky contacts respectively [11–19, 51]. It is an amazing fact that although heavily doped semiconductors (HDS) have been investigated in the literature the study of carrier

transport in such materials through proper formulation of the Boltzmann transport equation which needs, in turn, *the corresponding HD carrier energy spectra is still one of the open research problems.*

It is well known that band tails are being formed in the forbidden zone of the HDS and can be explained by the overlapping of the impurity band with the conduction and valence bands [52]. Kane [53] and Bonch Bruevich [54] have independently derived the theory of band tailing for semiconductors having unperturbed parabolic energy bands. Kane's model [53] was used to explain the experimental results on tunneling [55] and the optical absorption edges [56, 57] in this context. Halperin and Lax [58] developed a model for band tailing applicable only to the deep tailing states. Although Kane's concept is often used in the literature for the investigation of band tailing [59, 60], it may be noted that this model [53, 61] suffers from serious assumptions in the sense that the local impurity potential is assumed to be small and slowly varying in space coordinates [60]. In this respect, the local impurity potential may be assumed to be a constant. In order to avoid these approximations, we have developed in this book, the electron energy spectra for HDS for studying the ER based on the concept of the variation of the kinetic energy [52, 60] of the electron with the local point in space coordinates. This kinetic energy is then averaged over the entire region of variation using a Gaussian-type potential energy. On the basis of the E - k dispersion relation, we have obtained the electron statistics for different HDS for the purpose of numerical computation of the respective ERs. It may be noted that a more general treatment of many-body theory for the DOS of HDS merges with one-electron theory under macroscopic conditions [52]. Also, the experimental results for the Fermi energy and others are the average effect of this macroscopic case. So, the present treatment of the one-electron system is more applicable to the experimental point of view and it is also easy to understand the overall effect in such a case [62]. In a HDS, each impurity atom is surrounded by electrons, assuming a regular distribution of atoms and it is screened independently [59, 61, 63]. The interaction energy between electrons and impurities is known as the impurity screening potential. This energy is determined by the inter-impurity distance and the screening radius (popularly known as the Debye screening length). The screening length changes with the band structure. Furthermore, these entities are important for HDS in characterizing the semiconductor properties [64, 65] and the modern electronic devices [59, 66]. The works on Fermi energy and the screening length in an n-type GaAs have already been initiated in the literature [67], based on Kane's model. Incidentally, the limitations of Kane's model [53, 60], as mentioned above, are also present in their studies.

At this point, it may be noted that many band tail models are proposed using Gaussian distribution of the impurity potential variation [53, 60]. From the very start, we have used Gaussian band tails to obtain the *exact E - k dispersion relations* for HD nonlinear optical, III-V, II-VI, IV-VI, stressed Kane-type semiconductors, Te, GaP, PtSb₂, Bi₂Te₃, Ge and GaSb respectively. Our method is not related with the DOS technique as used in the aforementioned works. From the electron energy spectrum, one can obtain the DOS but the DOS technique, as used in the literature

cannot provide the E - k dispersion relation. *Therefore, our study is more fundamental than those in the existing literature, because the Boltzmann transport equation, which controls the study of the charge transport properties of the semiconductor devices, can be solved if and only if the E - k dispersion relation is known.* We wish to note that many authors have used the Gaussian function for the impurity potential distribution. It has been widely used since 1963 when Kane first proposed it and we will use the Gaussian distribution for the present study.

This book contains ten chapters where the Appendices A to E are placed chronologically in chapters five to ten respectively, is partially based on our ongoing researches on the ER of HDS from 1990, and an attempt has been made to present a cross section of the ER for wide range of HDS and their quantized-structures with varying carrier energy spectra under various physical conditions. The first chapter deals with the influence of quantum confinement on the ER in non-parabolic HDS. First, we study the ER in QWs of HD nonlinear optical materials on the basis of a generalized electron dispersion law introducing the anisotropies of the effective masses and the spin orbit splitting constants, respectively, together with the inclusion of the crystal field splitting within the framework of the $k.p$ formalism. *We observe that the appearance of the complex electron dispersion law in HDS instead of real one occurs from the existence of the poles in the finite complex plane of the corresponding electron energy spectrum in the absence of band tails.* It may be noted that the complex band structures have already been studied for bulk semiconductors and superlattices without heavy doping [69] and bears no relationship to the complex electron dispersion law as formulated in this book. The physical picture behind the existence of the complex energy spectrum in HD nonlinear optical semiconductors is the interaction of the impurity atoms in the tails with the splitting constants of the valance bands. The more the interaction, the more the prominence of the complex part than the other case. In the absence of band tails, there is no interaction of impurity atoms in the tails with the spin orbit constants and, consequently, the complex part vanishes. Besides, the complex spectra are not related to same evanescent modes in the band tails and the conduction bands. In this context it is worth remarking that the concept of effective electron mass (EEM) is one of the basic pillars in the whole set of materials science in general [68]. One important consequence of the HDS forming band tails is that *the EEM exists in the forbidden zone, which is impossible without the effect of band tailing. In the absence of band tails, the effective mass in the band gap of semiconductors is infinity. Besides, depending on the type of the unperturbed carrier energy spectrum, the new forbidden zone will appear within the normal energy band gap for HDS.* The results of HD III–V (e.g., InAs, InSb, GaAs etc.), ternary (e.g., $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, etc.), quaternary (e.g., $\text{In}_{1-x}\text{Ga}_x\text{As}_{1-y}\text{P}_y$ lattice matched to InP, etc.) compounds form a special case of our generalized analysis under certain limiting conditions. The ER in HD QWs of II–VI, IV–VI, stressed Kane-type semiconductors, Te, GaP, PtSb_2 , Bi_2Te_3 , Ge and GaSb has been investigated by formulating the respective appropriate HD energy band structure. The importance of the aforementioned semiconductors has been described in the same chapter. As a collateral study we shall observe that the EEM

in such QWs becomes a function of size quantum number, the Fermi energy, the scattering potential and other constants of the system which is the intrinsic property of such 2D electrons.

With the advent of modern experimental techniques of fabricating nanomaterials, it is possible to grow semiconductor superlattices (SLs) composed of alternative layers of two different degenerate layers with controlled thickness [70]. These structures have found wide applications in many new devices such as photodiodes [71], photo-resistors [72], transistors [73], light emitters [74], tunneling devices [75], etc. [76–87]. The investigations of the physical properties of narrow gap SLs have increased extensively since they are important for optoelectronic devices and because of the quality of heterostructures involving narrow gap materials have been improved. It may be noted in this context that the doping superlattices are crystals with a periodic sequence of ultrathin film layers [88, 89] of the same semiconductor with the intrinsic layer in-between together with the opposite sign of doping. All the donors are positively charged and all the acceptors negatively. This periodic space charge causes a periodic space charge potential which quantizes the motions of the carriers in the z -direction together with the formation of the subband energies. The electronic structures of the doping superlattices differ radically from the corresponding bulk semiconductors as stated below:

- (a) Each band is split into mini-bands;
- (b) The magnitude and the spacing of these mini-bands may be designed by the choice of the superlattices parameters; and
- (c) The electron energy spectrum of the nippy crystal becomes two-dimensional leading to the step functional dependence of the DOS function.

In the second chapter, the ER in doping superlattices of HD nonlinear optical, III–V, II–VI, IV–VI and stressed Kane-type semiconductors has been investigated. In this case we note that the EEM in such doping superlattices becomes a function of nipi subband index, surface electron concentration, Fermi energy, the scattering potential and other constants of the system which is the intrinsic property of such 2D-quantized systems.

In 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 in the direction perpendicular to it leading to the formation of electric subbands [90]. Although considerable work has already been done regarding the various physical properties of different types of inversion layers having various band structures, nevertheless, it appears from the literature that there lies scopes in the investigations made while the interest for studying different other features of accumulation layers is becoming increasingly important. In the third chapter, the ER in accumulation layers of HD nonlinear optical, III–V, II–VI, IV–VI, stressed Kane-type

semiconductors and Ge, have been investigated. For the purpose of relative comparisons, we have also studied the ER in inversion layers of the aforementioned materials. *It is interesting to note that the EEM in such layers is a function of electric subband index, surface electric field, Fermi energy, the scattering potential and other constants of the system which is the intrinsic property of such 2D electrons.*

Chapter four suggests the experimental determinations of 2D and 3D ERs for HDS and contains six related applications of the content of this book. Our suggestion for the experimental determination of the ERs and the theoretical formula for degenerate tetragonal compounds (e.g., Cd_3As_2) based on our generalized analysis incorporating all types of anisotropies of the energy band structure agree well with each other and are discussed in this chapter. Chapter five contains the conclusion and the scope for future research.

It may be noted that the effects of quantizing magnetic field (B) on the band structures of compound semiconductors are more striking than 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 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 [91] of various materials having different carrier dispersion relations [92]. The ER in the presence of magnetic quantization is a tensor quantity and we take that particular element of the ER which is in the direction of magnetic field only $(D/\mu)_{zz}$. *Appendix A studies the ER in HD nonlinear optical, III–V, IV–VI, stressed compounds, n-Te, n-GaP, PtSb₂, n-Ge, II–V semiconductors and Lead Germanium Telluride under magnetic quantization respectively. In this appendix we observe that the EEM depends on Landau quantum number in addition to Fermi energy and the other system constants due to the specific band structures of the HD materials together with the fact that EEM exists in the band gap due to the presence of finite scattering potential as noted already.*

It is well known that Keldysh [93] first suggested the fundamental concept of a superlattice (SL), although it was successfully experimentally realized by Esaki and Tsu [94]. The importance of SLs in the field of nanoelectronics has already been described in [95–97]. The most extensively studied III–V SL is that consisting of alternate layers of GaAs and $\text{Ga}_{1-x}\text{Al}_x\text{As}$ owing to the relative ease of fabrication. The GaAs layers form quantum wells and $\text{Ga}_{1-x}\text{Al}_x\text{As}$ form potential barriers. The III–V SLs are attractive for the realization of high speed electronic and optoelectronic devices [98]. In addition to SLs with usual structure, SLs with more complex structures such as II–VI [99], IV–VI [100] and HgTe/CdTe [101] SLs have also been proposed. The IV–VI SLs exhibit quite different properties compared to the III–V SL due to the peculiar band structure of the constituent materials [102]. The epitaxial growth of II–VI SL is a relatively recent development and the primary motivation for studying the mentioned SLs made of materials with large

band gap is in their potential for optoelectronic operation in the blue [102]. HgTe/CdTe SLs have aroused a great deal of attention since 1979 as promising new materials for long wavelength infrared detectors and other electro-optical applications [103]. Interest in Hg-based SLs has been further increased as new properties with potential device applications were revealed [103, 104]. These features arise from the unique zero band gap material HgTe [105] and the direct band gap semiconductor CdTe that can be described by the three-band mode of Kane [106]. The combination of the aforementioned materials with specified dispersion relation makes HgTe/CdTe SL very attractive, especially because of the possibility to tailor the material properties for various applications by varying the energy band constants of the SLs. In addition, for effective mass SLs, the electronic subbands appear continually in real space [107].

We note that all the aforementioned SLs have been proposed with the assumption that the interfaces between the layers are sharply defined, of zero thickness, i.e., devoid of any interface effects. The SL potential distribution may be then considered as a one-dimensional array of rectangular potential wells. The aforementioned advanced experimental techniques may produce SLs with physical interfaces between the two materials crystallographically abrupt; adjoining their interface will change at least on an atomic scale. As the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the electrons. The influence of finite thickness of the interfaces on the electron dispersion law is very important, since the electron energy spectrum governs the electron transport in SLs.

In Appendix B, we study the ER under magnetic quantization in III–V, II–VI, IV–VI, HgTe/CdTe and strained layer HD SLs with graded interfaces. We also investigate the ER in III–V, II–VI, IV–VI, HgTe/CdTe and strained layer effective mass HD SLs in the presence of quantizing magnetic field respectively. *This appendix explores the fact that the EEM becomes a function of the Fermi energy, Landau quantum number, scattering potential and the magnetic field in all the cases which are the characteristic features of such superlattices. We present a simplified analysis of the ER in superlattices of HD nonparabolic semiconductors under magnetic quantization, which is a huge topic of research by its own right.*

It is worth remarking that the influence of crossed electric and quantizing magnetic fields on the transport properties of semiconductors having various band structures are relatively less investigated compared with the corresponding magnetic quantization, although the crossfields 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 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 effective electron mass along y-axis tends to infinity which indicates the fact that the electron motion along y-axis is forbidden. The effective electron mass of the isotropic, bulk semiconductors having parabolic energy bands exhibits mass anisotropy in the presence of crossfields and

this anisotropy depends on the electron energy, the magnetic quantum number, the electric and the magnetic fields, respectively, although the effective electron mass along z -axis is a constant quantity. In 1966, Zawadzki and Lax [108] formulated the electron dispersion law for III–V semiconductors in accordance with the two-band model of Kane under crossfields configuration which generates the interest to study this particular topic of solid-state science in general [109]. *Appendix C investigates the ER under crossfield configuration in HD nonlinear optical, III–V, II–VI, IV–VI, stressed Kane-type semiconductors and their ultrathin films counterparts. This appendix tells us that the EEM in all the cases is a function of the size quantum number, the finite scattering potential, the magnetic quantum number and the Fermi energy even for HD semiconductors whose bulk electrons in the absence of band tails are defined by the parabolic energy bands.*

With the advent of nano-devices, the build-in electric field becomes so large that the electron energy spectrum changes fundamentally instead of being invariant and Appendix D investigates the ER under intense electric field in bulk specimens of HD III–V, ternary and quaternary semiconductors. This appendix also explores the influence of electric field on the ER based on HD new dispersion law under magnetic quantization, size quantization, accumulation layers, HD doping superlattices and effective mass HD superlattices under magnetic quantization. It is interesting to note that the EEM depends on the strong electric field (which is not observed elsewhere) together with the fact that the EEM in accumulation layers, HD doping superlattices and effective mass HD superlattices depend on the respective quantum numbers in addition to the Fermi energy, the scattering potential and other system constants which are the characteristics features of such heterostructures.

With the advent of nano-photonics, there has been considerable interest in studying the optical processes in semiconductors and their nanostructures in the presence of intense light waves [110]. *It appears from the literature that investigations in the presence of external intense photo-excitation have been carried out on the assumption that the carrier energy spectra are invariant quantities under strong external light waves, which is not fundamentally true.* The physical properties of semiconductors in the presence of strong light waves which alter the basic dispersion relations have relatively been much less investigated in [111, 112] as compared with the cases of other external fields needed for the characterization of low-dimensional semiconductors. Appendix E of this book studies the influence of light waves on the ER in HD opto-electronic semiconductors by formulating new electron dispersion relation within the framework of $k.p$ formalism. The same appendix explores the opto ER for HD opto-electronic materials under magnetic quantization, crossfields configuration, size quantization, doping superlattices and effective mass superlattices respectively. It is interesting to note that the EEM is a function of incident light intensity and wave length (not observed elsewhere) together with the fact that the EEM in superlattices and crossfields configuration depend on quantum numbers, Fermi energy, scattering potential and other system constants which are the characteristic features in this case. In these appendices, no graphs together with results and discussions are presented since we strongly feel

that the readers should not lose a chance to enjoy the complex computer algorithm to investigate the ER in the respective cases generating new physics and thereby transforming each Appendix into a monograph by considering various materials having different dispersion relations.

It is needless to say that this monograph is based on the ‘iceberg principle’ [113] and the rest of which will be explored by researchers from different appropriate fields. Since there is no existing report devoted solely to the study of ER for HD 2D-quantized structures 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 solid-state and allied sciences in general. Since the production of an error-free first edition of any book from every point of view is a permanent member in the domain of impossibility theorems, therefore in spite of our joint concentrated efforts for a couple of years together with the seasoned team of Springer, the same stands very true for this monograph also. Various expressions and a few chapters of this book appear for the first time in printed form. Suggestions from readers for the development of the book will be highly appreciated for the purpose of inclusion in future editions, if any. In this book, from chapter one till the end, we have presented *200 open research problems* for graduate students, Ph.D. aspirants, researchers and engineers in this pinpointed research topic. We strongly hope that alert readers of this monograph will not only solve the said problems by removing all the mathematical approximations and establishing the appropriate uniqueness conditions, but will also generate new research problems both theoretical and experimental and, thereby, transform this bried monograph into a solid book. Incidentally, our readers after reading this book will easily understand how little is presented and how much more is yet to be investigated in this exciting topic which is the signature of coexistence of new physics, advanced mathematics combined with the inner fire for performing creative research in this context from young scientists, since like Kikoin [114] we feel that *A young scientist is no good if his teacher learns nothing from him and gives his teacher nothing to be proud of*. We emphatically stress that the problems presented here form an integral part of this book and will be useful for readers to initiate their own contributions on the ER in HDS and their quantized counterparts, since like Sakurai [115] we firmly believe *The reader who has read the book but cannot do the exercise has learned nothing*. It is nice to note that if we assign the alphabets A to Z, the positive integers from 1 to 26, chronologically, then the word *ATTITUDE* receives the perfect score 100 and is the vital quality needed from the readers since *attitude* is the ladder on which all the other virtues mount.

In this monograph, we have investigated various dispersion relations of different HD quantized structures and the corresponding carrier statistics to study the concentration dependence of the ER in HD quantum confined materials. *Besides, the expressions of effective electron mass and the subband energy have been formulated throughout this monograph as a collateral study, for the purpose of in-depth investigations of the said important pinpointed research topics*. Thus, in this book, readers will get much information regarding the influence of quantization in HD low-dimensional materials having different band structures. For the

enhancement of the materials aspect, we have considered various materials having the same dispersion relation to study the influence of energy band constants of the different HDS on ER. Although the name of the book is extremely specific, from the content one can easily infer that it should be useful in graduate courses on condensed matter physics, materials science, modern physics of materials, solid-state electronics, nano-science and technology and solid-state sciences and devices in many universities and institutions in addition to both Ph.D. students and researchers in the aforementioned fields. *Last but not the least, we do hope that our humble effort will kindle the desire to delve deeper into this fascinating and deep topic by anyone engaged in materials research and device development either in academics or in industry.*

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