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ELECTRON ENERGY SPECTRA IN QUANTIZED STRUCTURES

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Abstract

In this paper we study the Electron Energy Spectra (EES) in quantum wells (QWs) of heavily doped (HD) non-linear optical, III-V, II-VI, IV-VI and stressed Kane type compounds by formulating HDEES in each case respectively considering all the specialties of the energy band constants of the said materials . It is noted that the complex EES in many cases in HDS, instead of real one, occurs from the existence of the essential poles in the corresponding EES in the absence of band tails. *The EES in QWs is Quantized 2D closed surfaces.* As a collateral study we have also investigated the effective mass (EM), Density-of-states (DOS) function and the electron statistics in this context for the purpose of comprehensive understanding. The EM exists in the forbidden zone, which is impossible without the effect of band tailing. In the absence of band tails, the EM in the band gap of semiconductors is infinity. Besides, depending on the type of unperturbed carrier energy spectrum, the new forbidden zone will appear within the normal energy band gap for HDS. Under certain limiting conditions all the results for all the models get simplified the well-known results of an isotropic parabolic energy bands which exhibit the mathematical compatibility of our present generalized analysis.

Keywords*: Electron Energy Spectra, Heavy Doping, Quantum Wells, Effective Mass, Density-of-States Function (DOS)*

1. INTRODUCTION:

The concept of the Electron Energy Spectra (EES) of the carriers in electronic materials and their nano-structures occupies a singular position in the whole arena of Nano Science and related disciplines in general and its importance [1-22] has already been established since the inception of the theory of band structure of Solid State Physics. The concept of EES is of fundamental importance for not only the characterization of nano-structures but also the study of the carrier transport in electronic materials and their quantized counter parts through the proper formulation of the Boltzmann Transport equation which, in turn, needs the corresponding EES of the heavily doped materials. **It is important to note that six important transport quantities namely, the effective mass (EM), density-of-states (DOS) function, the sub-band energy and the measurement of band-gap in the presence of strong light waves, intense electric field and heavy doping are in disguise in the very important concept of EES. Besides, the acoustic mobility limited momentum relaxation time is inversely proportional to the respective DOS function of a particular semiconductor and integral over the DOS function leads to carrier statistics under the condition of extreme carrier degeneracy which, in turn, is connected to the twenty five important transport topics of quantum effect devices namely** *the Landau Dia and Pauli's Para Magnetic Susceptibilities [23], the Einstein's Photoemission [24], the Einstein Relation [25], the Debye Screening Length[26], the Generalized Raman gain [27], the Normalized Hall coefficient[28], the Fowler-Nordheim Field Emission [29], the Thermoelectric Power [30-31], the Plasma Frequency [32],the Magneto-Thermal effect in Quantized Structures [33], the Activity coefficient [34], the Reflection coefficient [35], the Heat Capacity [36], the Faraday rotation [37], the Optical Effective Mass [38], the Carrier contribution to the elastic constants [39], the Diffusion coefficient of the minority carriers [40], the Nonlinear optical response [41], the Third order nonlinear optical susceptibility [42], the Righi-Leduc coefficient [43], the Electric Susceptibility [44], the Electric Susceptibility Mass [45], the Electron Diffusion Thermo-power [46] and the Hydrostatic Piezo-resistance Coefficient [47] respectively.*

It is well known that the constant energy 3D wave-vector space of bulk materials becomes 2D wave-vector surface in QWs due to dimensional quantization. Thus, the concept of reduction of symmetry of the wave-vector space and its consequence can unlock the physics of low-dimensional structures. In this Paper, we study the EES in QWs of Heavily Doped (HD) non-parabolic materials having different band structures in the presence of Gaussian band tails. At first we shall investigate the EES in Quantum Wells (QWs) of HD nonlinear optical compounds which are being used in nonlinear optics and light emitting diodes [48]. The quasi-cubic model can be used to investigate the symmetric properties of both the bands at the zone center of wave vector space of the same compound. Including the anisotropic crystal potential in the Hamiltonian, and special features of the nonlinear optical compounds, Kildal [49] 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 [50–52]. In section 2.2.1, the EES in QWs of HD nonlinear optical materials has been investigated on the basis of newly formulated HD EES of the said compound by considering the combined influence of the anisotropies of the said energy band constants together with the inclusion of the crystal field splitting respectively within the framework of $\vec{k}.\vec{p}$ formalism. As a collateral study we have also investigated the effective mass (EM), Density-of-states (DOS) function and the electron statistics in this context for the purpose of comprehensive understanding.

In section 2.2.2, the EES in QWs of HD III-V, ternary and quaternary materials has been studied in accordance with the corresponding HD formulation of the band structure and the simplified results for wide gap materials having parabolic energy bands under certain limiting conditions have further been demonstrated as a special case in the absence of band-tails and thus confirming the compatibility test. The II-VI materials are being used in nano-ribbons, blue green diode lasers, photosensitive thin films, infrared detectors, ultra-high-speed bipolar transistors, fiber optic communications, microwave devices, solar cells, semiconductor gamma-ray detector arrays, semiconductor detector gamma camera and allow for a greater density of data storage on optically addressed compact discs [53–60]. The carrier energy spectra in II-VI compounds are defined by the Hopfield model [110] where the splitting of the two-spin states by the spin-orbit coupling and the crystalline field has been taken into account. The section 2.2.3 contains the investigation of the EES in QWs of HD II-VI compounds.

Lead Chalcogenides (PbTe, PbSe, and PbS) are IV-VI non-parabolic materials whose studies over several decades have been motivated by their importance in infrared IR detectors, lasers, light-emitting devices, photo-voltaic, and high temperature thermo-electrics [68-72]. PbTe, in particular, is the end compound of several ternary and quaternary high performance high temperature thermoelectric materials [73-77]. It has been used not only as bulk but also as films [78-81], QWs [82] super-lattices [83, 84] nanowires [85] and colloidal and embedded nano-crystals [86–89], and PbTe films doped with various impurities have also been investigated [90-97] 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 [98]. In section 2.2.4, the 2D EES in QWs of HD IV-VI materials has been studied taking PbTe, PbSe, and PbS as examples. The stressed materials are being investigated for strained silicon transistors, quantum cascade lasers, semiconductor strain gages, thermal detectors, and strained-layer structures [99-102]. The EES in QWs of HD stressed compounds (taking stressed n-InSb as an example) has been investigated in section 2.2.5. Section 3 contains the result and discussion pertaining to this Paper.

2. THEORETICAL BACKGROUND

2.1 The EES in Quantum Wells (QWs) of HD nonlinear optical materials

The form of **k. p** matrix for nonlinear optical compounds can be expressed extending Bodnar [74] as

$$H = \begin{bmatrix} H_1 & H_2 \\ H_2^+ & H_1 \end{bmatrix} \tag{1}$$

$$where,\ H_1 = \begin{bmatrix} E_{g_0} & 0 & P_{\parallel} k_z & 0 \\ 0 & (-2\Delta_{\parallel}/3) & (\sqrt{2}\Delta_{\perp}/3) & 0 \\ P_{\parallel} k_z & (\sqrt{2}\Delta_{\perp}/3) & -\left(\delta + \frac{1}{3}\Delta_{\parallel}\right) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, H = \begin{bmatrix} 0 & -f_{,+} & 0 & f_{,-} \\ f_{,+} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ f_{,+} & 0 & 0 & 0 \end{bmatrix}$$

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, δ 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, $f_{,\pm} \equiv (P_{\perp} / \sqrt{2})(k_x \pm ik_y)$ 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 materials as

$$\gamma(E) = f_1(E)k_s^2 + f_2(E)k_z^2 \qquad (2)$$

where E

$$\gamma(E) = E(E+E_{g_0})[(E+E_{g_0})(E+E_{g_0}+\Delta_{\parallel}) + \delta(E+E_{g_0}+\frac{2}{3}\Delta_{\parallel}) + \frac{2}{3}(\Delta_{\parallel}^2 - \Delta_{\perp}^2)],$$

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

$$f_1(E) = \hbar^2 E_{g_0}(E_{g_0}+\Delta_{\perp})[\delta(E+E_{g_0}+\frac{1}{3}\Delta_{\parallel}) + (E+E_{g_0})(E+E_{g_0}+\frac{2}{3}\Delta_{\parallel}) + \frac{1}{9}(\Delta_{\parallel}^2 - \Delta_{\perp}^2)][2m_{\perp}^*(E_{g_0}+\frac{2}{3}\Delta_{\perp})]^{-1},$$

$$f_2(E) = \hbar^2 E_{g_0}(E_{g_0}+\Delta_{\parallel})[(E+E_{g_0})(E+E_{g_0}+\frac{2}{3}\Delta_{\parallel})][2m_{\parallel}^*(E_{g_0}+\frac{2}{3}\Delta_{\parallel})]^{-1}, \ \hbar = \frac{h}{2\pi}$$

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.

Thus the generalized unperturbed electron energy spectrum for the bulk specimens of the nonlinear optical materials in the absence of band tails can be expressed following (2) as

$$\frac{\hbar^2 k_z^2}{2m_{\parallel}^*} + (\frac{b_{\parallel}}{b_{\perp}}\frac{c_{\perp}}{c_{\parallel}})\frac{\hbar^2 k_s^2}{2m_{\perp}^*} = \{\frac{E(\alpha E+1)(b_{\parallel}E+1)}{(c_{\parallel}E+1)} + \frac{\alpha b_{\parallel}}{c_{\parallel}}[\delta E + \frac{2}{9}(\Delta_{\parallel}^2 - \Delta_{\perp}^2)] - (\frac{2}{9})\frac{\alpha b_{\parallel}}{c_{\parallel}}\frac{(\Delta_{\parallel}^2 - \Delta_{\perp}^2)}{(c_{\parallel}E+1)}\}$$

$$-(\frac{\hbar^2 k_s^2}{2m_{\perp}^*})\{(\frac{b_{\parallel}}{b_{\perp}}\frac{c_{\perp}}{c_{\parallel}})[(\frac{\delta}{2} + \frac{\Delta_{\parallel}^2 - \Delta_{\perp}^2}{6\Delta_{\parallel}})\frac{\alpha_{\parallel}}{\alpha_{\parallel}E+1} + (\frac{\delta}{2} - \{\frac{\Delta_{\parallel}^2 - \Delta_{\perp}^2}{6\Delta_{\parallel}}\})\frac{c_{\parallel}}{c_{\parallel}E+1}]\} \qquad (3)$$

where, $b_{\parallel} \equiv (E_g + \Delta_{\parallel})^{-1}, c_{\perp} \equiv (E_g + \frac{2}{3}\Delta_{\perp})^{-1}, b_{\perp} \equiv (E_g + \Delta_{\perp})^{-1}, c_{\parallel} = (E_g + \frac{2}{3}\Delta_{\parallel})^{-1}$ *and* $\alpha = (E_g)^{-1}$

The Gaussian distribution *F(V)* of the impurity potential is given by [103]

$$F(V) = (\pi\eta_g^2)^{1/2}\exp(-V^2/\eta_g^2) \qquad (4)$$

where, η_g is the impurity screening potential. It appears from (4) that the variance parameter η_g is not equal to zero, but the mean value is zero. Further, the impurities are assumed to be uncorrelated and the band mixing effect has been neglected in this simplified theoretical formalism.

We have to average the kinetic energy in the order to obtain the EES in nonlinear optical materials in the presence of band tails. Using the (3) and (4), we get

$$[\frac{\hbar^2 k_z^2}{2m_{\|}^*}\int_{-\infty}^{E} F(V)dV]+[(\frac{b_{\|}}{b_{\perp}}\frac{c_1}{c_{\|}})\frac{\hbar^2 k_s^2}{2m_{\perp}^*}\int_{-\infty}^{E} F(V)dV]=\{\int_{-\infty}^{E} \frac{(E-V)[\alpha(E-V)+1][b_{\|}(E-V)+1}{[c_{\|}(E-V)+1]}F(V)dV$$

$$+\frac{\alpha b_{\|}}{c_{\|}}[\delta\int_{-\infty}^{E} (E-V)F(V)dV+\frac{2}{9}(\Delta_{\|}^2-\Delta_{\perp}^2)\int_{-\infty}^{E} F(V)dV]-(\frac{2}{9})\frac{\alpha b_{\|}}{c_{\|}}(\Delta_{\|}^2-\Delta_{\perp}^2)\int_{-\infty}^{E} \frac{F(V)dV}{[c_{\|}(E-V)+1]}\}$$

$$-(\frac{\hbar^2 k_s^2}{2m_{\perp}^*})\{(\frac{b_{\|}}{b_{\perp}}\frac{c_{\perp}}{c_{\|}})[(\frac{\delta}{2}+\frac{\Delta_{\|}^2-\Delta_{\perp}^2}{6\Delta_{\|}})\alpha\int_{-\infty}^{E} \frac{F(V)dV}{[\alpha(E-V)+1]}+(\frac{\delta}{2}-\frac{\Delta_{\|}^2-\Delta_{\perp}^2}{6\Delta_{\|}})c_{\|}\int_{-\infty}^{E} \frac{F(V)dV}{[c_{\|}(E-V)+1]}]\} \quad (5)$$

The (5) can be rewritten as

$$\frac{\hbar^2 k_z^2}{2m_{\|}^*}I(1)+(\frac{b_{\|}}{b_{\perp}}\frac{c_{\perp}}{c_{\|}})\frac{\hbar^2 k_s^2}{2m_{\perp}^*}I(1)==\{I_3(c_{\|})+\frac{\alpha b_{\|}}{c_{\|}}[\delta I(4)+\frac{2}{9}(\Delta_{\|}^2-\Delta_{\perp}^2)I(1)]-(\frac{2}{9})\frac{\alpha b_{\|}}{c_{\|}}(\Delta_{\|}^2-\Delta_{\perp}^2)I_6(c_{\|})\}-$$

$$(\frac{\hbar^2 k_s^2}{2m_{\perp}^*})\{(\frac{b_{\|}}{b_{\perp}}\frac{c_{\perp}}{c_{\|}})[(\frac{\delta}{2}+\frac{\Delta_{\|}^2-\Delta_{\perp}^2}{6\Delta_{\|}})\alpha I(\alpha)+(\frac{\delta}{2}\{\frac{\Delta_{\|}^2-\Delta_{\perp}^2}{6\Delta_{\|}}\})c_{\|}I(c_{\|})]\} \quad (6)$$

$$where,\ I(1)=\int_{-\infty}^{E} F(V)dV \quad (7)$$

$$I_3(c_{\|})=\int_{-\infty}^{E} \frac{(E-V)[\alpha(E-V)+1][b_{\|}(E-V)+1]}{[c_{\|}(E-V)+1]}F(V)dV$$

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$$I_3(c_{\|})=\int_{-\infty}^{E} \frac{(E-V)[\alpha(E-V)+1][b_{\|}(E-V)+1]}{[c_{\|}(E-V)+1]}F(V)dV \quad (8)$$

$$I(4)=\int_{-\infty}^{E} (E-V)F(V)dV \quad (9)$$

$$I(\alpha)=\int_{-\infty}^{E} \frac{F(V)dV}{[\alpha(E-V)+1]} \quad (10)$$

Substituting $E-V\equiv x$ and, $\frac{x}{\eta_g}\equiv t_0$ we get from (7)

$$I(1)=(\exp(-\frac{E^2}{\eta_g^2}/\sqrt{\pi}))\int_0^{\infty} \exp[-t_0^2+(\frac{2Et_0}{\eta_g})]dt_0$$

Thus,

$$I(1)=[\frac{1+Erf(E/\eta_g)}{2}] \quad (11)$$

where, $Erf(E/\eta_g)$ s the error functions of (E/η_g).

From (9), one can write

$$I(4) = (1/\eta_g\sqrt{\pi})\int_{-\infty}^{E} (E-V)\exp(-V^2/\eta_g^2)dV = \frac{E}{2}[1+Erf(E\eta_g)] - \{\frac{1}{\sqrt{\pi\eta_g^2}}\int_{-\infty}^{E} V\exp(-V^2/\eta_g^2)dV\}) \quad (12)$$

After computing this simple integration, one obtains

Thus,

$$I(4) = \eta_g \exp(-E^2/\eta_g^2)(2\sqrt{\pi}) + \frac{E}{2}(1+Erf(E/\eta_g)) = \gamma_0(E,\eta_g) \quad (13)$$

From (10), we can write

$$I(\alpha) = \frac{1}{\sqrt{\pi\eta_g^2}}\int_{-\infty}^{E} \frac{\exp(-V^2/\eta_g^2)dV}{[\alpha(E-V)+1]} \quad (14)$$

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

Thus (14) can be expressed as

$$I(\alpha) = (1/\alpha\eta_g\sqrt{\pi})\int_{-\infty}^{\infty} \exp(-t^2)(u-t)^{-1}dt \quad (15)$$

$where,\ \frac{V}{\eta_g} = t$ and $u \equiv (\frac{1+\alpha E}{\alpha\eta})$

It is well known that [104, 105]

$$W(Z) = (i/\pi)\int_{-\infty}^{\infty} (Z-t)^{-1}\exp(-t^2)dt \quad (16)$$

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

We also know [104, 105],

$$W(Z) = \exp(-Z^2)Erfc(-iZ) \quad (17)$$

where, $Erfc(Z) \equiv 1 - Erf(Z)$.

Thus, $Erfc(-iu) = 1 - Erf(-iu)$

Since, $Erf(-iu) = -Erf(iu)$

Therefore,.

Thus,

$$I(\alpha) = [-i\sqrt{\pi}/\alpha\eta_g]\exp(-u^2)[1+Erf(iu)] \quad (18)$$

We also know that [104, 105]

$$Erf\,(x+iy)=Erf\,(x)+(\frac{e^{-x^2}}{2\pi x})[(1-\cos(2xy))+i\sin(2xy)+\frac{2}{\pi}e^{-x^2}\sum_{p=1}^{\infty}\frac{\exp(-p^2/4)}{(p^2+4x^2)}]$$

$$[f_p(x,y)+ig_p(x,y)+\varepsilon(x,\mathrm{y})] \qquad (19)$$

$$where,\ f_p(x,y)=[2x-2x\cosh(py)\cos(2xy)+p\sinh(py)\sin(2xy)],$$

$$g_p(x,y)\equiv[2x\cosh(py)\sin(2xy)+p\sinh(py)\cos(2xy)]\left|\varepsilon(x,y)\right|\approx 10^{-15}\left|Erf\,(x+iy)\right|$$

Substituting $x=0$ and $y=u$ in (19), one obtains,

$$Erf\,(iu)=(\frac{2i}{\pi})\sum_{p=1}^{\infty}\{\frac{\exp(-p^2/4)}{p}\sinh(pu)\} \qquad (20)$$

Therefore, one can write

$$I(\alpha)=C_{21}(\alpha,E,\eta_g)-iD_{21}(\alpha,E,\eta_g) \qquad (21)$$

where,

$$C_{21}(\alpha,E,\eta_g)=[\frac{2}{\alpha\eta_g\sqrt{\pi}}]\exp(-u^2)[\sum_{p=1}^{\infty}\{\frac{\exp(-p^2/4)}{p}\sinh(pu)\}]\text{ and }D_{21}(\alpha,\mathrm{E},\eta_g)=[\frac{\sqrt{\pi}}{\alpha\eta_g}\exp(-u^2)]$$

The (21) consists of both real and imaginary parts and therefore, $I(\alpha)$ is complex, which can also be proved by using the method of analytic continuation of Complex Analysis.

The integral $I_3(c_{\|})$ in (8) can be written as

$$I_3(c_{\|})=(\frac{\alpha b_{\|}}{c_{\|}})I(5)+(\frac{\alpha c_{\|}+b_{\|}c_{\|}-\alpha b_{\|}}{c_{\|}^2})I(4)+\frac{1}{c_{\|}}(1-\frac{\alpha}{c_{\|}})(1-\frac{b_{\|}}{c_{\|}})I(1)-\{\frac{1}{c_{\|}}(1-\frac{\alpha}{c_{\|}})(1-\frac{b_{\|}}{c_{\|}})I(c_{\|})\} \qquad (22)$$

where

$$I(5)=\int_{-\infty}^{E}(E-V)^2F(V)dV \qquad (23)$$

From (23) one can write

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

The evaluations of the component integrals lead us to write

$$I(5)=\frac{\eta_g E}{2\sqrt{\pi}}\exp(\frac{-E^2}{\eta_g^2})+\frac{1}{4}(\eta_g^2+2E^2)[1+Erf\,(\frac{E}{\eta_g})]=\theta_0(E,\eta_g) \qquad (24)$$

Thus combining the aforementioned equations, $I_3(c_{\|})$ can be expressed as

$$I_3(c_{\|}) = A_{21}(E,\eta_g) + iB_{21}(E,\eta_g) \tag{25}$$

where,

$$A_{21}(E,\eta) = [\frac{\alpha b_{\|}}{c_{\|}}[\frac{\eta_g E}{2\sqrt{\pi}}\exp(\frac{-E^2}{\eta_g^2}) - \frac{1}{4}(\eta_g^2 + 2E^2)\{1 + Erf(\frac{E}{\eta_g})\}]$$

$$+[\frac{\alpha c_{\|} + b_{\|}c_{\|} - \alpha b_{\|}}{c_{\|}^2}]\{\frac{E}{2}[1 + Erf(E/\eta)] + \frac{\eta\exp(-E^2/\eta_g^2)}{2\sqrt{\pi}}\}$$

$$+\frac{1}{c_{\|}}(1-\frac{\alpha}{c_{\|}})(1-\frac{b_{\|}}{c_{\|}})\frac{1}{2}[1 + Erf(E/\eta)] - \{\frac{2}{c_{\|}^2\eta_g\sqrt{\pi}}(1-\frac{\alpha}{c_{\|}})(1-\frac{b_{\|}}{c_{\|}})\exp(-u_1^2)\}[\sum_{p=1}^{\infty}\{\frac{\exp(-p^2/4)}{p}\sinh(pu_1)\}]$$

$$u_1 \equiv [\frac{1 + c_{\|}E}{c_{\|}\eta_g}] \, and \; B_{21}(E,\eta_g) \equiv \frac{\sqrt{\pi}}{c_{\|}^2\eta_g}(1-\frac{\alpha}{c_{\|}})(1-\frac{b_{\|}}{c_{\|}})\exp(-u_1^2)$$

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

$$\frac{\mathrm{h}^2 k_z^2}{2m_{\|}^{*}T_{21}(E,h_g)} + \frac{\mathrm{h}^2 k_s^2}{2m_{\wedge}^{*}T_{22}(E,h_g)} = 1 \tag{26}$$

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

$$T_{21}(E,h_g) = [T_{27}(E,h_g) + iT_{28}(E,h_g)], \; T_{27}(E,h_g) = [\frac{T_{23}(E,h_g)}{T_5(E,h_g)}]$$

$$T_{23}(E,h_g) \,º\, [A_{21}(E,h_g) + \frac{ab_{\|}}{c_{\|}}[dg_0(E,h_g) + \frac{1}{9}(\mathrm{D}_{\|}^2 - \mathrm{D}_{\wedge}^2)[1 + Erf(E/h_g)]]$$

$$- \{\frac{2}{9}(\frac{ab_{\|}}{c_{\|}})(\mathrm{D}_{\|}^2 - \mathrm{D}_{\wedge}^2)G_{21}(c_{\|},E,h_g)\}],$$

$$G_{21}(E,h_g) \equiv \frac{2}{c_{\|} h_g \sqrt{\pi}} \exp(-u_1^2) \sum_{p=1}^{\infty} \{\frac{\exp(-p^2/4)}{p} \sinh(p u_1)\}, T_5(E,h_g) \equiv \frac{1}{2}[1+Erf(E/h_g)]$$

$$T_{28}(E,h_g) \equiv [\frac{T_{24}(E,h_g)}{T_5(E,h_g)}], T_{24}(E,h_g) \equiv [B_{21}(E,h_g) + \frac{2}{9}\frac{a b_{\|}}{c_{\|}}(\Delta_{\|}^2 - \Delta_{\perp}^2) H_{21}(c_{\|},E,h_g)]$$

$$H_{21}(c_{\|},E,h_g) \equiv [\frac{\sqrt{\pi}}{h_g c_{\|}} \exp(-u_1^2)], T_{22}(E,h_g) \equiv [T_{29}(E,h_g) + i T_{30}(E,h_g)],$$

$$T_{29}(E,h_g) \equiv \frac{T_3(E,h_g) T_{25}(E,h_g) - T_{24}(E,h_g) T_{26}(E,h_g)}{[(T_{25}(E,h_g))^2 + (T_{26}(E,h_g))^2]},$$

$$T_{25}(E,h_g) \equiv [(\frac{b_{\|}}{b_{\perp}}\frac{c_{\perp}}{c_{\|}})\frac{1}{2}[1+Erf(\frac{E}{h_g})] + (\frac{b_{\|}}{b_{\perp}}\frac{c_{\|}}{c_{\perp}})(\frac{d}{2} + [\frac{\Delta_{\|}^2 - \Delta_{\perp}^2}{6\Delta_{\|}}]) a_{\|} C_{21}(a_{\|},E,h_g)$$
$$+ (\frac{b_{\|} c_{\perp}}{b_{\perp}})(\frac{d}{2} - [\frac{\Delta_{\|}^2 - \Delta_{\perp}^2}{6\Delta_{\|}}]) G_{21}(a_{\|},E,h_g)],$$

$$C_{21}(a,E,h_g) \equiv [\frac{2}{a\sqrt{\pi} h_g} \exp(-u^2)[\sum_{p=1}^{\infty} \frac{\exp(-p^2/4)}{p} \sinh(pu)]]$$

$$T_{26}(E,h_g) \equiv (\frac{b_{\|}}{b_{\perp}}\frac{c_{\perp}}{c_{\|}})(\frac{d}{2} - \frac{\Delta_{\|}^2 - \Delta_{\perp}^2}{6\Delta_{\|}}) a D_{21}(a,E,h_g) + \frac{b_{\|} c_{\perp}}{b_{\perp}}(\frac{d}{2} - \frac{\Delta_{\|}^2 - \Delta_{\perp}^2}{6\Delta_{\|}}) H_{21}(c_{\|},E,h_g)$$

and

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

From (26), it appears that the energy spectrum in HD nonlinear optical materials is complex. **The complex nature of the electron dispersion law in HD materials occurs from the existence of the essential poles in the corresponding electron energy spectrum in the absence of band tails.** It may be noted that the complex band structures have already been studied for bulk materials and super lattices without heavy dopingand bears no relationship with the complex electron dispersion law as indicated by (26). The physical picture behind the formulation of the complex energy spectrum in HDS is the interaction of the impurity atoms in the tails with the splitting constants of the valance bands. More is the interaction; more is the prominence of the complex part than the other case. In the absence of band tails, $h_g \to 0$, and there is no interaction of the impurity atoms in the tails with the spin orbit constants. As a result, there exist no complex energy spectrum and (26) gets converted into (2) when $h_g \to 0$. Besides, the complex spectra are not related to same evanescent modes in the band tails and the conduction bands.

The transverse and the longitudinal EMs at the Fermi energy E_{F_h} of HD nonlinear optical materials can, respectively, be expressed as

$$m_{\perp}^{*} = (E_{F_{n,}} \eta_g) = m_{\perp}^{*}\{T_{29}(E,\eta_g) \qquad (27)$$

and

$$m_{\parallel}^{*} = (E_{F_n},\eta_g) = m_{\parallel}^{*}\{T_{27}(E,\eta_g)\}'\Big|_{E=E_{F_n}} \qquad (28)$$

where E_{F_h} is the Fermi energy of HDS in the presence of band tails as measured from the edge of the conduction band in the vertically upward direction in the absence of band tails and the primes denote the differentiations of the differentiable functions with respect to Fermi energy in the appropriate case.

In the absence of band tails h_g ® 0 and we get

$$m_{\perp}^{*}(E_F,O) = \frac{\hbar^2}{2}\left[\frac{\psi_2(E)\{\psi_1(E)\}' - \psi_1(E)\{\psi_2(E)\}'}{\{\psi_2(E)\}}\right]_{E=E_F} \qquad (29)$$

and

$$m_{\parallel}^{*}(E_F,O) = \frac{\hbar^2}{2}\left[\frac{\psi_3(E)\{\psi_1(E)\}' - \{\psi_1(E)\}\{\psi_3(E)\}'}{\{\psi_3(E)\}}\right]_{E=E_F} \qquad (30)$$

where E_F is the Fermi energy as measured from the edge of the conduction band in the vertically upward direction in the absence of any perturbation, $\psi_1(E) = \gamma(E), \psi_2(E) = f_1(E), and\, \psi_3(E) = f_2(E),$ Comparing the aforementioned equations, one can infer that **the effective masses exist in the forbidden zone, which is impossible without the effect of band tailing. For semiconductors, in the absence of band tails the effective mass in the band gap is infinity.** The density-of-states (DOS) function is given by

$$N_{HD}(E,\eta_g) = \frac{2g_v m_{\perp}^{*}\sqrt{2m_{\parallel}^{*}}}{3\pi^2\hbar^3} R_{11}(E,\eta_g)\cos[\psi_{11}(E,\eta_g)] \qquad (31a)$$

where, g_v is the valley degeneracy,

$$R_{11}(E,\eta_g) \equiv [[\{T_{29}(E,\eta_g)\}'\sqrt{x(E,\eta_g)} + \frac{T_{29}(E,\eta_g)\{x(E,\eta_g)\}'}{2\sqrt{x(E,\eta_g)}} - \{T_{30}(E,\eta_g)\}'\sqrt{y(E,\eta_g)}\frac{T_{30}(E,\eta_g)\{y(E,\eta_g)\}'}{2\sqrt{y(E,\eta_g)}}]^2$$

$$+[\{T_{29}(E,\eta_g)\}'\sqrt{y(E,\eta_g)} + \frac{T_{29}(E,\eta_g)\{y(E,\eta_g)\}'}{2\sqrt{y(E,\eta_g)}} + \{T_{30}(E,\eta_g)\}'\sqrt{x(E,\eta_g)}\frac{T_{30}(E,\eta_g)\{x(E,\eta_g)\}'}{2\sqrt{x(E,\eta_g)}}]^2]^{1/2},$$

$$x(E,\eta_g) \equiv \frac{1}{2}[T_{27}(E,\eta_g) + \sqrt{\{T_{27}(E,\eta_g)\}^2 + \{T_{28}(E,\eta_g)\}^2}],$$

$$y(E,\eta_g) \equiv \frac{1}{2}[\sqrt{\{T_{27}(E,\eta_g)\}^2 + \{T_{28}(E,\eta_g)\}^{22}} - T_{27}(E,\eta_g)],$$

$$and\ \psi_{11}(E,\eta_g) \equiv \tan^{-1}[[\{T_{29}(E,\eta_g)\}'\sqrt{y(E,\eta_g)} + \frac{T_{29}(E,\eta_g)}{2\sqrt{y(E,\eta_g)}} + \{T_{30}(E,\eta_g)\}'\sqrt{x(E,\eta_g)} + \frac{T_{30}\{x(E,\eta_g)\}'}{2\sqrt{x(E,\eta_g)}}]$$

$$[\{\{T_{29}(E,\eta_g)\}'\}\sqrt{x(E,\eta_g)} + \frac{T_{29}(E,\eta_g)\{x(E,\eta_g)\}'}{2\sqrt{x(E,\eta_g)}} - \{T_{30}(E,\eta_g)\}'\sqrt{y(E,\eta_g)} + \frac{T_{30}\{t(E,\eta_g)\}'}{2\sqrt{y(E,\eta_g)}}]^{-1}]$$

The oscillatory nature of the DOS for HD nonlinear optical materials is apparent from (31a). For, $\psi_{11}(E,\eta_g) \geq \pi$, the cosine function becomes negative leading to the negative values of the DOS. The electrons cannot exist for the negative values of the DOS and therefore, this region is forbidden for electrons, which indicates that in the band tail, **there appears a new forbidden zone in addition to the normal band gap of the semiconductor.**

The use of (31a) leads to the expression of the electron concentration as

$$n_0 = \frac{2g_v m_\perp^* \sqrt{2m_\Box^*}}{3\pi^2\hbar^3}[I_{11}(E_{F_h},\eta_g) + \sum_{r=1}^{s} L(r)[I_{11}(E_{F_h},\eta_g)]] \qquad (31b)$$

$$where,\ I_{11}(E_{F_h},\eta_g) \equiv [T_{29}(E_{F_h},\eta_g)\sqrt{x(E_{F_h},\eta_g)} - T_{30}(E_{F_h},\eta_g)\sqrt{y(E_{F_h},\eta_g)}$$

$L(r) = 2(k_B T)^{2r}(1-2^{1-2r})\xi(2r)\frac{\partial^{2r}}{\partial E_{Fs}^{2r}}$ r is the set of real positive integers whose upper s and $\xi(2r)$ is the Zeta function of order 2r [104, 105].

For dimensional quantization along z- direction, the dispersion relation of the 2D electrons in this case can be written following (26) as

$$\frac{\hbar^2(n_z\pi/d_z)^2}{2m_\parallel^* T_{21}(E,\eta_g)} + \frac{\hbar^2 k_s^2}{2m_\perp^* T_{22}(E,\eta_g)} = 1 \qquad (32)$$

where, $n_z (=1,2,3,...)$ and d_z are the size quantum number and the nano-thickness along the z-direction respectively.

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

$$N_{2DT}(E) = \frac{m_\perp^* g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}} T_{1D}{}'(E,\eta_g,n_z)H(E-E_{n_zD_1}) \qquad (33)$$

where $A(E,n_z)$ is the area of the constant energy 2D wave vector space and in this case it is for QWs, $H(E-E_{n_z})$ is the Heaviside step function and E_{n_z} is the corresponding sub-band energy. Using (32) and (33), the expression of the $N_{2DT}(E)$ for QWs of HD nonlinear optical materials can be written as

$$N_{2DT}(E) = \frac{m_\perp^* g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}} T_{1D}{}'(E,\eta_g,n_z)H(E-E_{n_zD_1}) \qquad (34)$$

where, $T_{1D}(E,\eta_g,n_z) = [1 - \frac{\hbar^2(n_z\pi/d_z)^2}{2m_\parallel^* T_{21}(E,\eta_g)}]T_{22}(E,\eta_g)$ and the sub band energies $E_{n_zD_1}$ in this case is given by the following equation

$$\frac{kh^2(n_z\pi/d_z)^2}{2m_\parallel^* T_{21}(E_{n_zD_1},\eta_g)} = 1 \qquad (35)$$

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

The EM in this case is given by

$$m^*(E_{F_1HD},\eta_g,n_z)=m_\perp^*[\text{Real part of } T'_{1D}(E_{F_1HD,}\eta_g,n_z)] \tag{36a}$$

Although the importance of the EM is already well-known in the literature [106-107], we observe that the EM is the function of size quantum number and the Fermi energy due to the combined influence of the crystal filed splitting constant and the anisotropic spin-orbit splitting constants respectively. Besides it is a function of η_g due to which the EM exists in the band gap, which is otherwise impossible.

Combining (34) with the Fermi-Dirac occupation probability factor, integrating between $E_{n_{z_1}}$ to infinity and applying the generalized Sommerfeld's lemma [108], the 2D carrier statistics in this case assumes the form

$$n_{2D}=\frac{m_\perp^* g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{\max}}[\text{Re}\,al\ part\,of\,[T_{1D}(E_{F1HD},\eta_{g,}n_z)+T_{2D}(E_{F1HD},\eta_g,n_z)]] \tag{36b}$$

where, $T_{1D}(E_{F1HD},\eta_g,n_z)=\sum_{r=1}^{s}L(r)[T_{1D}(E_{F1HD},\eta_g,n_z)]$, E_{F1HD} is the Fermi energy in the presence of size quantization of the QWs of HD non-linear optical materials as measured from the edge of the conduction band in the vertically upward direction in the absence of any perturbation.

In the absence of band-tails, the 2D EM in the x-y plane at the Fermi level, the total 2D DOS, the sub-band energy $E_{n_{z_1}}$, of non-linear optical materials and the surface electron concentration can, respectively, be written as

$$\psi_1(E)=\psi_2(E)k_s^2+\psi_3(E)(n_z\pi/d_z)^2 \tag{37}$$

$$m^*(E_{Fs},n_z)=(\frac{\hbar^2}{2})[\psi_2(E_{Fs})]^2[\psi_2(E_{Fs})\{\{\psi_1(E_{Fs})\}'-\{\psi_3(E_{Fs})\}'(\frac{n_z\pi}{d_z})^2\}$$

$$-\{\psi_1(E_{Fs})-\psi_3(E_{Fs}(\frac{n_z\pi}{d_z})^2)\}\{\psi_2(E_{Fs})\}'] \tag{38}$$

$$\mathrm{N}_{2DT}(E)=(\frac{g_v}{2\pi})\sum_{n_z=1}^{n_{z_{\max}}}[\psi_2(E)]^2[\psi_2(E)\{\{\psi_1(\mathrm{E})\}'-\{\psi_3(E)\}'(\frac{n_z\pi}{d_z})^2\}$$

$$-\{\psi_1(E)-\psi_3(E)(\frac{n_z\pi}{d_z})^2\}\{\psi_2(E)\}']H(E-E_{n_{z_1}}) \tag{39}$$

$$\psi_1(E_{n_{z_1}})=\psi_2(E_{n_{z_1}})(n_2\pi/d_z)^2 \tag{40a}$$

where

$$\psi_1(E)=\gamma(E),\psi_2(E)=f_1(E),\psi_3(E)=f_2(E)$$

E_{FS} is the Fermi energy in the 2-D sized quantized material in the presence of size quantization and in the absence of band-tails as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization,

$$T_{51}(E_{Fs},n_z)\equiv[\frac{\psi_1(E_{Fs})-\psi_3(E_{Fs})(n_z\pi/d_z)^2}{\psi_2(E_{Fs})}]\,and\,T_{52}(E_{Fs},n_z)\equiv\sum_{r=1}^{s}L(r)[T_{51}(E_{Fs},n_z)]$$

In the absence of band-tails, the DOS for bulk specimens of non-linear optical materials is given by

$$D_0(E) = g_v(3\pi^2)^{-1}\psi_4(E) \tag{41a}$$

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

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

$$[\psi_2(E)]' \equiv [2m_\perp^*(E_g+\frac{2}{3}\Delta_\perp)]^{-1}[\hbar^2 E_g(E_g+\Delta_\perp)][\delta+2E+2E_g+\frac{2}{3}\Delta_\parallel]$$

$$and\,[\psi_3(E)]' \equiv [2m_\parallel^*(E_g+\frac{2}{3}\Delta_\parallel)]^{-1}[\hbar^2 E_g(E_g+\Delta_\parallel)][2E+2E_g+\frac{2}{3}\Delta_\parallel]$$

Combining (41a) with the Fermi-Dirac occupation probability factor and using the generalized Sommerfeld's lemma [108], the electron concentration can be written as

$$n_0 = g_v(3\pi^2)^{-1}[M(E_F)+N(E_F)] \tag{41b}$$

$$where,\ M(E_F) \equiv [\frac{[\psi_1(E_F)]^{\frac{3}{2}}}{\psi_2(E_F)\sqrt{\psi_3(E_F)}}]$$

E_F is the Fermi energy of the bulk specimen in the absence of band tails as measured from the edge of the conduction band in the vertically upward direction

$$N(E_F) \equiv \sum_{r=1}^{s} L(r)M(E_F)$$

2.2 The EES in Quantum Wells (QWs) of HD III-V materials

The EES of the conduction electrons of III-V compounds are described by the models of Kane (both three and two bands) [83,84], Stillman et. al. [85], Newson [86] and Palik.et.al.[87] respectively. For the purpose of complete and coherent presentation and relative comparison, the EMs in QWs of HD III-V materials has also been investigated.

(a) The Three Band Model of Kane

Under the conditions, $\delta = 0, \Delta_\parallel = \Delta_\perp = \Delta$ (isotropic spin orbit splitting constant) and $m_\parallel^* = m_\perp^* = m_c$ (isotropic effective electron mass at the edge of the conduction band), (2) gets simplified as

$$\frac{\hbar^2 k^2}{2m_c} = I_{11}(E), I_{11}(E) \equiv \frac{E(E+E_{g_0})(E+E_{g_0}+\Delta)(E_{g_0}+\frac{2}{3}\Delta)}{E_{g_0}(E_{g_0}+\Delta)(E+E_{g_0}+\frac{2}{3}\Delta)} \tag{42}$$

which is known as the three band model of Kane [84] and is often used to investigate the physical properties of III-V materials.

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

$$\frac{\hbar^2 k^2}{2m_c} = T_{31}(E,\eta_g) + iT_{32}(E,\eta_g) \qquad (43)$$

where,

$$T_{31}(E,\eta_g) \equiv \left(\frac{2}{1+Erf(E/\eta_g)}\right)\left[\frac{ab}{c}\theta_0(E,\eta_g) + \left[\frac{\alpha c + bc - \alpha b}{c^2}\right]\gamma_0(E,\eta_g) + \frac{1}{c}\left(1-\frac{\alpha}{c}\right)\left(1-\frac{b}{c}\right)\frac{1}{2}\left[1+Erf\left(\frac{E}{\eta_g}\right)\right]\right.$$

$$\left. -\frac{1}{c}\left(1-\frac{\alpha}{c}\right)\left(1-\frac{b}{c}\right)\frac{2}{c\eta_g\sqrt{\pi}}\exp(-u_2^2)\left[\sum_{p=1}^{\infty} \frac{\exp(-p^2/4)}{p}\sinh(pu_2)\right]\right], b \equiv (E_g+\Delta)^{-1}, c \equiv \left(E_g + \frac{2}{3}\Delta\right)^{-1}$$

$$u_2 \equiv \frac{1+cE}{c\eta_g} \text{ and } T_{32}(E,\eta_g) \equiv \left(\frac{2}{1+Erf(E/\eta_g)}\right)\frac{1}{c}\left(1-\frac{\alpha}{c}\right)\left(1-\frac{b}{c}\right)\frac{\sqrt{\pi}}{c\eta_g}\frac{\sqrt{\pi}}{c\eta_g}\exp(-u_2^2),$$

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

The EM at the Fermi level is given by

$$m^*(E_{F_s},\eta_g) = m_c\{T_{31}(E,\eta_g)\}'\Big| \qquad (44)$$

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

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

$$m^*(E_F) = m_c\{I_{11}(E_F,\eta_g)\}'\Big| \qquad (45)$$

The DOS function in this case can be written as

$$N_{HD}(E,\eta_g) = \frac{g_v}{3\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2} R_{21}(E,\eta_g)\cos[\vartheta_{21}(E,\eta_g)] \qquad (46)$$

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

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

$$T_{33}(E,\eta_g) \equiv [\{T_{31}(E,\eta_g)\}^3 - 3T_{31}(E,\eta_g)\{T_{32}(E,\eta_g)\}^2],$$

$$T_{34}(E,\eta_g) \equiv [3T_{32}(E,\eta_g)\{T_{31}(E,\eta_g)\}^2 - \{T_{32}(E,\eta_g)\}^3]$$

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

and

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

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

The electron concentration can be expressed as

$$n_0 = \frac{g_v}{3\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}[\bar{I}_{111e}(E_{Fs},\eta_s)+\sum_{r=1}^{s} l(r)[\bar{I}_{111e}(E_{Fs},\eta_s)]] \qquad (47)$$

where

$$T_{111e}(E_{Fs},\eta_g)=\{\gamma_2(E_{F_k},\eta_g)\}^{3/2}$$

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

$$\frac{\hbar^2(n_z\pi/d_z)^2}{2m_c}+\frac{\hbar^2(k_s)^2}{2m_c}=T_{31}(E,\eta_g)+iT_{32}(E,\eta_g) \qquad (48)$$

The expression of the $N_{2DT}(E)$ in this case assumes the form

$$N_{2DT}(E)=\frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z_{\max}}} T'_{5D}(E,\eta_g,n_z)H(E-E_{n_zD5}) \qquad (49)$$

$$where,\ T_{5D}(E,\eta_g,n_z)=[T_{31}(E,\eta_g)+iT_{32}(E,\eta_g)-\hbar^2(n_z\pi/d_z)^2(2m_c)^{-1}]$$

and the sub band energies E_{n_zD5} in this case given by

$$\{\hbar^2(n_z/d_z)^2\}(2m_c)^{-1}=T_{31}(E_{n_zD5},\eta_g) \qquad (50)$$

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

The EM in this case is given by

$$m^*(E_{F1HD},\eta_g,n_z)=m_c[T'_{31}(E_{F1HD},\eta_g,n_z)] \qquad (51)$$

The carrier statistics in this case can be expressed as

$$n_{2D}=\frac{m_c g_v}{\pi\hbar^2}\sum_{n_z-1}^{n_{\max}}[\text{Re}\,al\ part\,of[T_{5D}(E_{F1HD},\eta_g,n_z)+T_{6D}(E_{F1HD},\eta_g,n_z)]] \qquad (52)$$

In

$$where, T_{6D}(E_{F1HD},\eta_g,n_z)=\sum_{r=1}^{s} L(r)[T_{5D}(E_{F1HD},\eta_g,n_z)]$$

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

$$\frac{\hbar^2k_s^2}{2m_c}+\frac{\hbar^2}{2m_c}(n_z\pi/d_x)^2=I_{11}(E) \qquad (53)$$

It

$$m^*(E_{Fs})=m_c\{I_{11}(E_{Fs})\}' \qquad (54)$$

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

$$N_{2DT}(E)=\left(\frac{m_c g_v}{\pi\hbar^2}\right)\sum_{n_z=1}^{n_{z_{\max}}}\{[I_{11}(E)]'H(E-E_{n_{z_2}})\} \qquad (55)$$

where, the sub-band energies $E_{n_{z_2}}$ can be expressed as

$$I_{11}(E_{N_{Z_2}}) = \frac{\hbar^2}{2m_c}(n_z \pi / d_z)^2 \tag{56}$$

$$N_{2D}(E) = (\frac{m_c g_v}{\pi \hbar^2}) \sum_{n_z=1}^{n_{z_{\max}}} [T_{53}(E_{Fs}, n_z) + T_{54}(E_{Fs}, n_z)] \tag{57}$$

where,

$$T_{53}(E_{Fs}, n_z) \equiv [I_{11}(E_{Fs}) - \frac{\hbar^2}{2m_c}(\frac{n_z \pi}{d_z})^2], T_{54}(E_{Fs}, n_z) \equiv \sum_{r=1}^{s} L(r) T_{55}(E_{Fs}, n_z)$$

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

$$D_0(E) = 4\pi g_v (\frac{2m_c}{\hbar^2})^{3/2} \sqrt{I_{11}(E)} \left[I'_{11}(E) \right] \tag{58a}$$

$$m^*(E_F) = m_c \{I_{11}(E_F)\}' \tag{58b}$$

$$n_0 = \frac{g_v}{3\pi^2}(\frac{2m_c}{\hbar^2})^{3/2} [M_1(E_F) + N_1(E_F)] \tag{59}$$

where,

$$I_{11}'(E) \equiv I_{11}(E)[\frac{1}{E} + \frac{1}{E + E_g} + \frac{1}{E + E_g + \Delta} - \frac{1}{E + E_g + \frac{2}{3}\Delta}], M_1(E_F) \equiv [I_{11}(E)]^{3/2}$$

$$N_1(E_F) \equiv \sum_{r=1}^{s} L(r) M_1(E_F)$$

Under the inequalities $\Delta >> E_{g_0}$ or $\Delta << E_{g_0}$, (42) can be expressed as

$$E(1 + \alpha E) = \frac{\hbar^2 k^2}{2m_c} \tag{60}$$

where $\alpha \equiv (E_{g_0})^{-1}$ and is known as band non-parabolicity.

It may be noted that (60) is the well-known two band model of Kane and is used in the literature to study the physical properties of those III-V and opto-electronic materials whose energy band structures obey the aforementioned inequalities.

The dispersion relation in HD III-V, ternary and quaternary materials whose energy spectrum in the absence of band tails obeys the two band model of Kane as defined by (60), can be written as

$$\frac{\hbar^2 k^2}{2m_c} = \gamma_2(E, \eta_g) \tag{61}$$

where The

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

EM in this case can be written as

$$m^*(E_{F_h},\eta_g) = m_c\{\gamma_2(E,\eta_g)\}'\Big|_{E=E_{F_h}} \tag{62a}$$

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

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

$$m^*(E_F) = m_c\{1+2\alpha E\}\Big|_{E=E_F} \tag{62b}$$

The DOS function in this case can be written as

$$N_{HD}(E,\eta_g) = \frac{g_v}{2\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}\sqrt{\gamma_2(E,\eta_g)}\{\gamma_2(E,\eta_g)\}' \tag{62c}$$

Since, the poles of the original two band Kane model are at infinity and no finite poles with respect to energy, therefore the HD counterpart will be totally real and the complex band vanishes.

The electron concentration is given by

$$n_0 = \frac{g_v}{3\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}[\bar{I}_{111}(E_{Fs},\eta_g) + \sum_{r=1}^{s} L(r)[\bar{I}_{111}(E_{Fs},\eta_g)]] \tag{63}$$

where,

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

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (61) as

$$\frac{\hbar^2(n_z\pi/d_z)^2}{2m_c} + \frac{\hbar^2(k_s)^2}{2m_c} = \gamma_2(E,\eta_g) \tag{64}$$

The expression of the $N_{2DT}(E)$ in this case can be written as

$$N_{2DT}(E) = \frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}} T_{7D}'(E,\eta_g,n_z)H(E-E_{n_zD7}) \tag{65}$$

where, $T_{7D}(E,\eta_g,n_z) = [\gamma_2(E,\eta_g) - \hbar^2(n_z\pi/d_z)^2(2m_c)^{-1}]$

The sub-band energies E_{n_zD7} in this case given by

$$\{\hbar^2(n_z\pi/d_z)^2\}(2m_c)^{-1} = \gamma^2(E_{n_zD7},\eta_g) \tag{66}$$

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

The EM in this case is given by

$$m^*(E_{F1HD},\eta_g,n_z) = m_c[\gamma_2'(E_{F1HD},\eta_g,n_z)] \tag{67}$$

The electron statistics in this case assumes the form

$$n_{2D} = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z\max}} [T_{7D}(E_{FLHD}, \eta_g, n_z) + T_{8D}(E_{F1HD}, \eta_g, n_z)] \tag{68}$$

where,

$$T_{8D}(E_{F1HD}, \eta_g, n_z) = \sum_{r=1}^{s} L(r) T_{7D}(E_{F1HD}, \eta_g, n_z)$$

Under the inequalities $\Delta >> E_{g_0}$ or $\Delta << E_{g_0}$, (60) assumes the form

$$E(1+\alpha E) = \frac{\hbar^2 k_s^2}{2m_c} + \frac{\hbar^2}{2m_c}\left(\frac{n_z \pi}{d_z}\right)^2 \tag{69a}$$

The EM can be written from (69a) as

$$m^*(E_{Fs}) = m_c(1+2\alpha E_{Fs}) \tag{69b}$$

The total 2D DOS function assumes the form

$$N_{2DT}(E) = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z\max}} (1+2\alpha E) H(E - E_{n_{z3}}) \tag{70}$$

where, the sub-band energy $(E_{n_{z3}})$ can be expressed as

$$\frac{\hbar^2}{2m_c}(n_z \pi / d_z)^2 = E_{n_{z3}}(1+\alpha E_{n_{z3}}) \tag{71}$$

The 2D electron statistics can be written as

$$n_{2D} = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z\max}} \int_{E_{n_{z3}}}^{\infty} \frac{(1+2\alpha E)dE}{1+\exp(\frac{E-E_{Fs}}{k_B T})} = \frac{m_c k_B T g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z\max}} [(1+2\alpha E_{n_{z3}}) F_0(\eta_{n_1}) + 2\alpha k_B T F_1(\eta_{n_1}) \tag{72}$$

where,

$$\eta_{n_1} \equiv (E_{Fs} - E_{n_{z3}}) / k_B T$$

and $F_j(\eta)$ is the one parameter Fermi-Dirac integral of order j which can be written [109] as

$$F_j(n) = \left(\frac{1}{\Gamma(j+1)}\right) \int_0^{\infty} \frac{x^j dx}{1+\exp(x-\eta)}, \quad j > -1 \tag{73}$$

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

$$F_j(\eta) = \left(\frac{\Gamma(-j)}{2\pi\sqrt{-1}}\right) \int_{-\infty}^{+0} \frac{x^j dx}{1+\exp(-x-\eta)} \tag{74}$$

where η is the dimensionless quantity and x is independent variable,

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

$$D_0(E) = 4\pi g_v \left(\frac{2m_c}{\hbar^2}\right)^{3/2}, \sqrt{I_{11e}(E)}\left[I'_{11e}(E)\right] \tag{75a}$$

$$m^*(E_F) = m_c[I^{'}_{11e}(E_F)] \tag{75b}$$

$$n_0 = \frac{g_v}{3\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}[M_2(E_F) + N_2(E_F)]$$

$$where,\ I_{11e}(E) \equiv E(1+\alpha E), I'_{11e}(E) \equiv (1+2\alpha E),$$

$$M_2(E_F) \equiv [I_{11e}(E_F)]^{3/2}\ and\ N_2(E_F) \equiv \sum_{r=1}^{s} L(r) M_2(E_F)$$

(c) Under the constraints Δ □ $E_g \Delta$ □ E_g together with the inequality αE_F □ 1, the (76) assumes the forms as

$$n_0 = g_v N_c[F_{1/2}(\eta) + \left(\frac{15\alpha k_B T}{4}\right)F_{3/2}(\eta)] \tag{77}$$

where,

$$N_c \equiv 2\left(\frac{2\pi m^* k_B T}{h^2}\right)^{3/2} and \eta \equiv \frac{E_F}{k_B T}$$

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

$$\frac{\hbar^2 k^2}{2m_c} = \gamma_3(E, \eta_g) \tag{78}$$

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

Since the dispersion relation in accordance with the said model is an all zero function with no pole in the finite complex plane, therefore the HD counterpart will be totally real, which is also apparent form the expression (78).

The EM in this case can be written as

$$m^*(E_{Fh},\eta_g) = m_c\{\gamma_3(E_{Fh},\eta_g)\}' \tag{79}$$

In the absence of band tails, $n_g \to 0$ and the EM assumes the form

$$m^*(E_F) = m_c \tag{80}$$

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

The DOS function in this case can be written as

$$N_{HD}(E,\eta_g) = \frac{g_v}{2\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2}\sqrt{\gamma_3(E,\eta_g)}\{\gamma_3(E,\eta_g)\}' \tag{81}$$

The electron concentration is given by

$$n_0 = \frac{g_v}{3\pi^2}(\frac{2m_c}{\hbar^2})^{3/2}[\bar{I}_{113}(E_{F_h},\eta_g)+\sum_{r=1}^{s}L(r)[\bar{I}_{113}(E_{F_h},\eta_g)]] \qquad (82)$$

where,

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

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (78) as

$$\frac{\hbar^2(n_z z/d_z)^2}{2m_c}+\frac{\hbar^2(k_s)^2}{2m_c}=\gamma_3(E,\eta_g) \qquad (83)$$

the expression of the $N_{2DT}(E)$ in this case can be written as

$$N_{2DT}(E)=\frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}} T_{9D}{}'(E,\eta_g,n_z)H(E-E_{n_zD9}) \qquad (84)$$

where, $T_{9D}(E,\eta_g,n_z)=[\gamma_3(E,\eta_g)-\hbar^2(n_z\pi/d_z)^2(2m_c)^{-1}]$

The sub band energies E_{n_zD9} in this case given by

$$\{\hbar^2(n_z\pi/d_z)^2\}(2m_c)^{-1}=\gamma_3(E_{n_zD9},\eta_g) \qquad (85)$$

The EM in this case can be written as

$$m^*(E_{F1HD},\eta_g,n_z)=m_c[\gamma_3'(E_{F1HD},\eta_g,n_z)] \qquad (86)$$

The carrier statistics in this case assumes the form

$$n_{2D}=\frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}}[T_{9D}(E_{F1HD},\eta_g,n_z)+T_{10D}(E_{F1HD},\eta_g,n_z)] \qquad (87)$$

where, $T_{10D}(E_{F1HD},\eta_g,n_z)\sum_{r=1}^{s}L(r)[T_{9D}(E_{F1HD},\eta_g,n_z)]$

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

$$N_{2DT}(E)=\frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}}H(E-E_{n_{z_p}}) \qquad (88)$$

The sub-band energy $E_{n_{z_p}}$, the n_{2D} and the EM can, respectively, be expressed as

$$E_{n_{z_p}}=\frac{\hbar^2}{2m_c}(\frac{n_z\pi}{d_z})^2 \qquad (89)$$

$$n_{2D} = \frac{m_c k_B T g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z\max}} F_0(\eta_{n_2}) \qquad (90a)$$

$$m^*(E_F) = m_c \qquad (90b)$$

where,

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

(b) The Model of Stillman et. al.

In accordance with the model of Stillman et. al. [85], the electron dispersion law of III-V materials assumes the form

$$E = \bar{t}_{11} k^2 - \bar{t}_{12} k^4 \qquad (91)$$

$$where,\ \bar{t}_{11} \equiv \frac{\hbar^2}{2m_c};\ \bar{t}_{12} = (1 - \frac{m_c}{m_0})^2 (\frac{\hbar^2}{2m_c})^2 [(3E_{g_0} + 4\Delta + \frac{2\Delta^2}{E_{g_0}}).\{(E_{g_0} + \Delta)(2\Delta + 3E_{g_0})\}^{-1}]$$ and

m_0 is the free electron mass

In the presence of band tails, (91) gets transformed as

$$\frac{\hbar^2 k^2}{2m_c} = I_{12}(E, \eta_g) \qquad (92)$$

$$where,\ I_{12}(E,\eta_g) = a_{11}[1 - (1 - a_{12}\gamma_3(E,\eta_g))^{1/2}], a_{11} \equiv (\frac{\hbar^2 \bar{t}_{11}}{4m_c \bar{t}_{12}}) and\ a_{12} = \frac{4\bar{t}_{12}}{\bar{t}_{11}^2}$$

The EEM can be written as

$$m^*(E_{F_h}, \eta_g) = m_c \{I_{12}(E_{F_h}, \eta_g)\}' \qquad (93)$$

The DOS function in this case can be written as

$$N_{HD}(E,\eta_g) = \frac{g_v}{2\pi^2}(\frac{2m_c}{\hbar^2})^{3/2}\sqrt{I_{12}(E,\eta_g)}\{I_{12}(E,\eta_g)\}' \qquad (94)$$

The electron concentration is given by

$$n_0 = \frac{g_v}{3\pi^2}(\frac{2m_c}{\hbar^2})^{3/2}[\bar{I}_{121}(E_{F_h},\eta_g) + \sum_{r=1}^{s} L(r)[\bar{I}_{121}(E_{F_h},\eta_g)]] \qquad (95)$$

where,

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

For dimensional quantization along z- direction, the dispersion relation of the 2D electrons in this case can be written following (108) as

$$\frac{\hbar^2 (n_z \pi / d_z)^2}{2m_c} + \frac{\hbar^2 (k_s)^2}{2m_c} = I_{12}(E,\eta_g) \qquad (96)$$

The expression of the $N_{2DT}(E)$ in this case can be written as

$$N_{2DT}(E) = \frac{m_c g_v}{\pi \hbar^2} \sum_{n_z=1}^{n_{z\max}} T_{11D}{}'(E,\eta_g,n_z) H(E - E_{n_z D11}) \qquad (96)$$

$$where,\ T_{11D}((E,\eta_g,n_z) = [I_{12}(E,\eta_g) - \hbar^2 (n_z\pi/d_z)^2 (2m_c)^{-1}]$$

The sub band energies E_{n_zD11} in this case given by

$$\{\hbar^2(n_z\pi/d_z)^2\}(2m_c)^{-1} = I_{12}(E_{n_zD11},\eta_g) \qquad (98)$$

The EM in this case assumes the form

$$m^*(E_{F1HD},\eta_g,n_z) = m_c\{\mathrm{I}_{12}{}'(E_{F1HD},\eta_g,n_z)] \qquad (99)$$

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

$$n_{2D} = \frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}}[T_{11D}(E_{F1HD},\eta_g,n_z)+T_{12D}(E_{F1HD},\eta_g,n_z)] \qquad (100)$$

$$where,\ T_{12D}(E_{F1HD},\eta_g,n_z) = \sum_{r=1}^{s} L(r)[T_{11D}(E_{F1HD},\eta_g,n_z)]$$

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

$$m^*(E_{Fs}) = m_c\{\mathrm{I}_{12}(E_{Fs})\}' \qquad (101)$$

$$where,\ I_{12}(E) = a_{11}[1-(1-a_{12}(E))^{1/2}]$$

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

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

$$N_{2DT}(E) = (\frac{m_c g_v}{\pi\hbar^2})\sum_{n_z=1}^{n_{z\max}} \{[I_{12}(E)]' H(E-E_{n_{z3}})\} \qquad (102)$$

where, the sub band energies $E_{n_{z3}}$ can be expressed as

$$I_{12}(E_{n_{z3}}) = \frac{\hbar^2}{2m_c}(n_z\pi/d_z)^2 \qquad (103)$$

The 2D electron concentration assumes the form

$$N_{2D} = (\frac{m_c g_v}{\pi\hbar^2})\sum_{n_z=1}^{n_{z\max}}[T_{55}(E_{Fs},n_z)+T_{56}(E_{Fs},n_z)] \qquad (104)$$

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

The expression of electron concentration for bulk specimens of III-V semiconductors (in the absence of band tails) can be written in accordance with the model of Stillman et. al.[85] as

$$n_0 = \frac{g_v}{3\pi^2}(\frac{2m_c}{\hbar^2})^{3/2}[M_{A_{10}}(E_F) + N_{A_{10}}(E_F)] \qquad (105)$$

where,

$$M_{A_{10}}(E_F) = [I_{12}(E_F)]^{3/2}\, and\, N_{A_{10}}(E_F) = \sum_{r=1}^{s} L(r)[M_{A_{10}}(E_F)]$$

(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. [87] as

$$E=\frac{\hbar^2k^2}{2m_c}-\bar{B}_{11}k^4 \tag{106}$$

$$where,\ \bar{B}_{11}=[\frac{\hbar^4}{4E_{g_0}(m_c)^2}][\frac{1+\frac{x_{11}^2}{2}}{1+\frac{x_{11}}{2}}](1-y_{11})^2,\mathrm{x}_{11}[1+(\frac{\Delta}{E_{g_0}})]^{-1}\text{ and }y_{11}=\frac{m_c}{m_0}$$

The (116) gets simplified as

$$\frac{\hbar^2k^2}{2m_c}=I_{13}(E) \tag{107}$$

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

Under the condition of heavy doping forming Gaussian band tails, (117) assumes the form

$$\frac{\hbar^2k^2}{2m_c}=I_{13}(E,\eta_g) \tag{108}$$

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

The EM can be written as

$$m^*(E_{F_h},\eta_g)=m_c\{I_{13}(E_{F_h},\eta_g)\}' \tag{109}$$

The DOS function in this case can be expressed as

$$N_{HD}(E,\eta_g)=\frac{g_v}{2\pi^2}(\frac{2m_c}{\hbar^2})^{3/2}\sqrt{I_{13}(E,\eta_g)}\{I_{13}(E,\eta_g)\}' \tag{110}$$

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

The electron concentration is given by

$$n_0=\frac{g_v}{3\pi^2}(\frac{2m_c}{\hbar^2})^{3/2}[\bar{I}_{123}(E_{Fh},\eta_g)+\sum_{r=1}^{s}L(r)[\bar{I}_{123}(E_{Fh},\eta_g)]] \tag{111}$$

where,

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

For dimensional quantization along z-direction, the dispersion relation of the 2D electrons in this case can be written following (117) as

$$\frac{h^2(n_z\pi/d_z)^2}{2m_c}+\frac{\hbar^2(k_s)^2}{2m_c}=I_{13}(E,\eta_g) \tag{112}$$

the expression of the $N_{2DT}(E)$ in this case can be written as

$$N_{2DT}(E) = \frac{m_c g_v}{\pi\hbar^2}\sum_{n_z}^{n_{z\max}} T'_{13D}(E,\eta_g,n_z)H(E-E_{n_zD13}) \tag{113}$$

$where,\ T_{13D}(E,\eta_g,\mathrm{n}_z) = [I_{13}(E,\eta_g) - \hbar^2(n_z\pi/d_z)^2(2m_c)^{-1}]$

The sub band energies E_{n_zD13} in this case given by

$$\{\hbar(n_z\pi/d_z)^2\}(2m_c)^{-1} = I_{13}(E_{n_zD13},\eta_g) \tag{114}$$

The EM in this case can be expressed as

$$m^*(E_{F1HD},\eta_g,n_z) = m_c[I'_{13}(E_{F1HD},\eta_g,n_z)] \tag{115}$$

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

$$n_{2D} = \frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{\max}}[T_{13D}(E_{F1HD},\eta_g,n_z) + T_{14D}(E_{F1HD},\eta_g,n_z)] \tag{116}$$

$where,\ T_{14D}(E_{F1HD},\eta_g,n_z) = \sum_{r=1}^{s} L(r)[T_{13D}(E_{F1HD},\eta_g,n_z)]$

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

$$\frac{\hbar^2 k_s^2}{2m_c} + \frac{\hbar^2}{2m_c}(n_z\pi/d_z)^2 = I_{13}(E) \tag{117a}$$

The EM in this case can be written from (127a) as

$$m^*(E_{F_s}) = m_c[I_{13}(E_{F_s})] \tag{117b}$$

The total 2D DOS function can be written as

$$N_{2DT}(E) = (\frac{m_c g_v}{\pi\hbar^2})\sum_{n_z=1}^{n_{z\max}} \{[I_{13}(E)]' H(E-E_{n_{z_4}})\} \tag{118}$$

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

$$I_{13}(E_{n_{z_4}}) = \frac{\hbar^2}{2m_c}(n_z\pi/d_z)^2 \tag{119}$$

The 2D electron concentration assumes the form

$$n_{2D} = \frac{m_c g_v}{\pi\hbar^2}\sum_{n_z=1}^{n_{z\max}}[T_{57}(E_{Fs},n_z) + T_{58}(E_{Fs},n_z)] \tag{120}$$

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

The expression of electron concentration for bulk specimens of III-V semiconductors (in the absence of band tails) can be written in accordance with the model of Stillman et. al. [85] as

$$n_0 = \frac{g_v}{3\pi^2}(\frac{2m_c}{\hbar^2})^{3/2}[\bar{M}_{A_{10}}(E_F) + \bar{N}_{A_{10}}(E_F)] \tag{121}$$

$where,\ \bar{M}_{40}(E_F) = [I_{13}(E_F)]^{3/2}\ and\ \bar{N}_{A10}(E_F) = \sum_{r=1}^{s} L(r)[\bar{M}_{40}(E_F)]$

2.3. The EES in Quantum Wells (QWs) of HD II-VI materials

The carrier energy spectra in bulk specimens of II-VI compounds in accordance with Hopfield model [110] can be written as

$$E = a_0' k_s^2 + b_0' k_z^2 + \bar{\lambda}_0 k_s \tag{122}$$

where $a_0' \equiv \hbar^2 / 2m_\perp^*$, $b_0' \equiv \hbar^2 2 / m_\parallel^*$, and $\bar{\lambda}_0$ represents the splitting of the two-spin states by the spin orbit coupling and the crystalline field.

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

$$\gamma_3(E,\eta_g) = a_0' k_s^2 + b_0' k_z^2 \pm \bar{\lambda}_0 k_s \tag{123}$$

Thus, the energy spectrum in this case is real since the corresponding E-k relation in the absence of band tails as given by (123) is a no pole function in the finite complex plane.

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

$$m_\perp^*(E_{F_n},\eta_g) = m_\perp^*\{\gamma_3(E,\eta_g)\}'[1+(\frac{\bar{\lambda}_0}{\sqrt{(\bar{\lambda}_0)^2 + 4a_0'\gamma_3(E,\eta_g)}})]\Bigg|_{E-E_{F_n}} \tag{124}$$

and

$$m_\parallel^*(E_{Fn},\eta_g) = m_\parallel^*\{\gamma_3(E,\eta_g)\}'\Big|_{E-E_{Fn}} \tag{125}$$

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

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

$$m_\perp^*(E_F) = m_\perp^*[1+(\frac{\bar{\lambda}_0}{\sqrt{(\bar{\lambda}_0)^2 + 4a_0'E)}})]\Bigg|_{E-E_F} \tag{126}$$

and

$$m_\parallel^*(E_F) = m_\parallel^* \tag{127}$$

The volume in k- space as enclosed (123) can be expressed as

$$V(E,\eta_g) = \frac{4\pi}{3a_0'\sqrt{b_0'}}[\{\gamma_3(E,\eta_g)\}^{3/2} + \frac{3}{8}\frac{(\bar{\lambda}_0)^2\sqrt{\gamma_3(E,\eta_g)}}{a_0'} \pm (\frac{3}{4}\frac{\bar{\lambda}_0}{\sqrt{a_0'}})(\gamma_3(E,\eta_g) + \frac{(\bar{\lambda}_0)^2}{4a_0'})\sin^{-1}[\frac{\sqrt{\gamma_3(E,\eta_g)}}{\sqrt{\gamma_3(E,\eta_g) + \frac{(\bar{\lambda}_0)^2}{4d_0}}}]] \tag{128}$$

Therefore, the electron concentration can be written as

$$n_0 = \frac{g_v}{3\pi^2 a_0' \sqrt{b_0'}} [\bar{I}_{124}(E_{F_h}, \eta_g) + \sum_{r=1}^{s} L(r)[\bar{I}_{124}(E_{F_h}, \eta_g)]] \tag{129}$$

where,

$$\bar{I}_{124}(E_{F_h}, \eta_g) = [\{\gamma_3(E_{F_h}, \eta_g)\}^{3/2} + \frac{3}{8} \frac{(\bar{\lambda}_0)^2 \sqrt{\gamma_3(E, \eta_g)}}{a_0'}]$$

The dispersion relation of the conduction electrons of QWs of HD II-VI materials for dimensional quantization along z- direction can be written following (123) as

$$\gamma_3(E, \eta_g) = a_0' k_s^2 + b_0' (\frac{\pi n_z}{d_z})^2 \pm \bar{\lambda}_0 k_s \tag{130}$$

The EM can be expressed following (130) as

$$m^*(E_{F1HD}, n_z, \eta_g) = m_\perp^* [1 \mp \frac{(\bar{\lambda}_0)}{[(\bar{\lambda}_0)^2 - 4a_0' b_0' (\frac{n_z \pi}{d_z})^2 + 4a_0' \gamma_3(E_{F1HD}, \eta_g)]^{1/2}}] \gamma_3'(E_{F1HD}, \eta_g) \tag{131}$$

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

The sub-band energy in this case is given by

$$\gamma_3(E_{n_z D14}, \eta_g) = b_0' (\frac{\pi n_z}{d_z})^2 \tag{132}$$

The surface electron concentration at low temperatures assumes the form

$$n_{2D} = \frac{g_v m_\perp^*}{\pi \hbar^2} \sum_{n_Z=1}^{n_{z\max}} (\gamma_3(E_{F1HD}, \eta_g) - E_{n_Z D_{14}} + (\bar{\lambda})^2 m_\perp^* \hbar^{-2}) \tag{133}$$

The dispersion relation of the conduction electrons of QWs of II-VI materials for dimensional quantization along z- direction in the absence of band tails can be written following (122) as

$$E = d_0 k_s^2 + b_0' (\frac{n_z \pi}{d_z})^2 \pm \bar{\lambda}_0 k_s \tag{134}$$

Using (144), the EM in this case can be written as

$$m^*(E_{Fs}, n_z) = m_\perp^* [1 \mp \frac{(\bar{\lambda}_0)}{[(\bar{\lambda}_0)^2 - 4a_0' b_0' (\frac{n_z \pi}{d_z})^2 + 4a_0' E_{Fs}]^{1/2}}] \tag{135}$$

The sub-band energy $E_{n_{z5}}$ assumes the form

$$E_{n_{z5}} = b_0' (\frac{n_z \pi}{d_z})^2 \tag{136}$$

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

$$A_\pm(E, n_z) = [\frac{\pi}{2(a_0')^2} [(\bar{\lambda}_0)^2 + 2a_0'(E - E_{n_{z_s}}) \pm \bar{\lambda}_0 [(\bar{\lambda}_0)^2 + 4a_0'(E - E_{n_{zS}})]^{1/2}]]$$

The surface electron concentration can be expressed in this case as

$$N_{2D} = \frac{-2g_v}{2(2\pi)^2} \sum_{n_z=1}^{n_{z\max}} \int_{E_{nzS}}^{\infty} [A_+(E_{Fs,} n_z) + A_-(E_{Fs,} n_z)] \frac{\partial}{\partial E} \{f_0(E)\} dE \tag{137}$$

where $f_0(E)$ is the Fermi-Dirac occupation probability factor.

From (137) we get

$$n_{2D} = \frac{g_v m_\perp^* k_B T}{\pi \hbar^2} \sum_{n_z=1}^{n_{z\max}} F_0(\eta_{n_{zS}}) \tag{138}$$

$$where,\ \eta_{n_{zS}} = (E_{Fs} - E_{n_{zS}} + (\bar{\lambda}) m_\perp^* \hbar^{-2})(k_B T)^{-1}$$

2.4. The EES in Quantum Wells (QWs) of HD IV-VI materials

a) **The Model of Dimmock**

The dispersion relation of the conduction electrons in IV-VI semiconductors can be expressed in accordance with Dimmock [85] as

$$[\bar{\varepsilon} - \frac{E_{g_0}}{2} - \frac{\hbar^2 k_s^2}{2m_t^-} - \frac{\hbar^2 k_z^2}{2m_t^-}][\bar{\varepsilon} + \frac{E_{g_0}}{2} + \frac{\hbar^2 k_s^2}{2m_t^-} + \frac{\hbar^2 k_z^2}{2m_t^-}] = P_\perp^2 k_s^2 + P_\parallel^2 k_z^2 \tag{139}$$

where, $\bar{\varepsilon}$ is the energy as measured from the center of the band gap E_{g_0}, $m_t^\pm$ 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.

Substituting, $P_\perp^2 \equiv (\hbar^2 E_g / 2m_t^*), P_\parallel^2 \equiv (\frac{\hbar^2 E_g}{2m_l^*})$ and $\bar{\varepsilon} = [E + (\frac{E_g}{2})]$ (where, m_t^* and m_l^* are the transverse and the longitudinal effective masses at $k = 0$,(139) gets transformed as

$$[E - \frac{\hbar^2 k_s^2}{2m_t^-} - \frac{\hbar^2 k_z^2}{2m_l^-}][1 + \alpha E + \alpha \frac{\hbar^2 k_s^2}{2m_t^+} + \alpha \frac{\hbar^2 k_z^2}{2m_l^+}] = \frac{\hbar^2 k_s^2}{2m_t^*} + \frac{\hbar^2 k_z^2}{2m_l^*} \tag{140}$$

From (140), we can write

$$\frac{\alpha \hbar^4 k_s^4}{4m_t^+ m_t^-} + \hbar^2 k_s^2 [(\frac{1}{2m_t^*} - \frac{1}{2m_t^-}) + \alpha E(\frac{1}{2m_t^-} - \frac{1}{2m_t^+}) + \frac{\alpha \hbar^2 k_z^2}{4m_l^- m_t^+}]$$

$$+[(\frac{\hbar^2 k_z^2}{2m_l^*} + \frac{\hbar^2 k_z^2}{2m_l^-}) + \frac{\alpha E}{2} \hbar^2 k_z^2 (\frac{1}{m_l^-} - \frac{1}{m_l^+}) + \frac{\alpha \hbar^4 k_z^4}{4m_l^+ m_t^-} - E(1 + \alpha E)] = 0 \tag{141}$$

Using (141), the dispersion relation of the conduction electrons in HD IV-VI materials can be expressed as

$$\frac{\alpha\hbar^4 k_s^4}{4m_t^+ m_l^-} Z_0(E,\eta_g) + \hbar^2 k_s^2[\lambda_{11}(E,\eta_g)(k_z^2 + \lambda_{72}(E,\eta_g)] + [\lambda_{73}(E,\eta_g)k_z^2 + \lambda_{74}(E,\eta_g)k_z^4 - \lambda_{75}(E,\eta_g)] = 0 \quad (142)$$

$$where,\ Z_0(E,\eta_g) \equiv \frac{1}{2}[1 + Erf(\frac{E}{\eta_g})],\ \lambda_{70}(E,\eta_g) \equiv \frac{\alpha}{4m_t^+ m_t^-} Z_0(E,\eta_g),$$

$$\lambda_{71}(E,\eta_g) \equiv [\frac{\alpha\hbar^2}{4m_t^- m_l^+} Z_0(E,\eta_g) + \frac{\alpha\hbar^2}{4m_l^- m_t^+} Z_0(E,\eta_g)],$$

$$\lambda_{72}(E,\eta_g) \equiv [(\frac{1}{2m_t^*} - \frac{1}{2m_t^-})Z_0(E,\eta_g) + \alpha(\frac{1}{2m_t^-} - \frac{1}{2m_t^+})\gamma_0(E,\eta_g)],$$

$$\lambda_{73}(E,\eta_g) \equiv [(\frac{\hbar^2}{2m_l^*} + \frac{\hbar^2}{2m_l^-})Z_0(E,\eta_g) + \frac{\alpha\hbar^2}{2}(\frac{1}{m_l^-} - \frac{1}{2m_l^+})\gamma_0(E,\eta_g)],$$

$$\lambda_{74}(E,\eta_g) = \frac{\alpha\hbar^4 Z_0(E,\eta_g)}{4m_l^+ m_l^-} \text{ and } \lambda_{75}(E,\eta_g) \equiv [\gamma_0(E,\eta_g) + \alpha\theta_0(E,\eta_g)]$$

Thus, the energy spectrum in this case is real since the corresponding dispersion relation in the absence of band tails as given by (142) is a pole-less function with respect to energy axis in the finite complex plane.

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

$$m_\perp^*(E_{F_h},\eta_g) = \{2Z_0(E,\eta_g)\}^{-2} z_0(E,\eta_g)[-\{\lambda_{72}(E,\eta_g)\}' + \frac{\{\lambda_{78}(E,\eta_g)\}'}{2\sqrt{\lambda_{78}(E,\eta_g)}}]$$

$$-\{Z_0(E,\eta_g)\}'[-\lambda_{72}(E,\eta_g) + \sqrt{\lambda_{78}(E,\eta_g)}]] \ \Big|_{E_{F_h}} \quad (143)$$

$$where,\ \lambda_{78}(E,\eta_g) \equiv [4\lambda_{70}(E,\eta_g)\lambda_{75}(E,\eta_g)]$$

$$and\ \ m_\parallel^*(E_{F_h},\eta_g) = \frac{\hbar^2}{4}[-\{\lambda_{84}(E,\eta_g)\}' + \frac{\{\lambda_{84}(E,\eta_g)\}'\{\lambda_{84}(E,\eta_g)\}' + 2\{\{\lambda_{85}(E,\eta_g)\}'}{\sqrt{(\lambda_{84}(E,\eta_g))^2 + 4\lambda_{85}(E,\eta_g)}}]_{E-E_{Fh}} \quad (144)$$

in which,

$$\lambda_{84}(E,\eta_g) \equiv \frac{\lambda_{73}(E,\eta_g)}{\lambda_{74}(E,\eta_g)} and \lambda_{85}(E,\eta_g) \equiv \frac{\lambda_{75}(E,\eta_g)}{\lambda_{74}(E,\eta_g)}$$

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

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

$$m_{\perp}^{*}(E_F) = \frac{\hbar^2}{2}[-\{a_{11}(E)\}' + \frac{a_{511}\{T_{311}(E)\}'}{2\sqrt{T_{311}(E)}}]\Big|_{E-E_F} \qquad (145)$$

where,

$$\alpha_{11}(E) \equiv \frac{2m_t^+ m_t^-}{\alpha\hbar^2}\alpha_{211}(E), \alpha_{211}(E) \equiv [\frac{1}{2m_t^*} + \frac{\alpha E}{2m_t^*} + \frac{1+\alpha E}{2m_t^-}], \alpha_{511} \equiv \frac{2m_t^+ m_t^-}{\alpha\hbar^2}\omega_{11}(\omega_{11}) \equiv [\frac{\alpha^2}{16}[\frac{1}{m_t^+ m_t^-}]]$$

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

$$\omega_{311}(E) \equiv [\frac{\alpha E(1+\alpha E)}{m_t^+ m_t^-} + [\frac{1}{2m_t^*} - (\frac{\alpha E}{2m_t^+}) + \frac{(1+\alpha E)}{2m_t^-}$$

and

$$m_{\square}^{*}(E_F) = (\frac{m_t^+ m_l^-}{\alpha})[(\frac{\alpha}{2m_l^+} - \frac{\alpha}{2m_l^-}) + \frac{1}{2}\{\frac{2[\frac{1}{2m_l^*} + \frac{1+\alpha E}{2m_l^-} - \frac{\alpha E}{2m_l^+}](\frac{\alpha}{2m_l^-} - \frac{\alpha}{2m_l^-}) + \frac{\alpha(1+2\alpha E)}{m_l^- m_l^+}}{[[\frac{1}{2m_l^*} + \frac{1+\alpha E}{2m_l^-} - \frac{\alpha E}{2m_l^+}]^2 + \frac{\alpha E(1+\alpha E)}{m_l^- m_l^+}]}\}]_{E-E_F} \quad (146)$$

The volume in k- space as enclosed by (142) can be written through the integral as

$$V(E,\eta_g) = 2\pi\int_0^{\lambda_{86}(E,\eta_g)}[-[\lambda_{79}(E,\eta_g)k_z^2 + \lambda_{80}(E,\eta_g)] + \sqrt{\lambda_{81}(E,\eta_g)k_z^4 + \lambda_{82}(E,\eta_g)k_z^2 + \lambda_{83}(E,\eta_g)}]dk_z \quad (147)$$

$$where, \lambda_{86}(E,\eta_g) \equiv [\frac{\sqrt{[\lambda_{84}(E,\eta_g)]^2 + 4\lambda_{85}(E,\eta_g)} - \lambda_{84}(E,\eta_g)}{2}]^{1/2}, \lambda_{79}(E,\eta_g) \equiv \frac{\lambda_{71}(E,\eta_g)}{2\hbar^2 Z_0(E,\eta_g)}$$

$$\lambda_{81}(E,\eta_g) \equiv \frac{\lambda_{76}(E,\eta_g)}{4\hbar^4[Z_0(E,\eta_g)]^2}, \lambda_{76}(E,\eta_g) \equiv [\lambda_{71}(E,\eta_g)]^2, \lambda_{76}(E,\eta_g) \equiv [\lambda_{71}(E,\eta_g)]^2$$

$$\lambda_{77} \equiv [2\lambda_{71}(E,\eta_g)\lambda_{72}(E,\eta_g) - 4\lambda_{70}(E,\eta_g)\lambda_{73}(E,\eta_g) - 4\lambda_{70}(E,\eta_g)\lambda_{74}(E,\eta_g)]$$

$$\lambda_{77} \equiv [2\lambda_{71}(E,\eta_g)\lambda_{72}(E,\eta_g) - 4\lambda_{70}(E,\eta_g)\lambda_{73}(E,\eta_g) - 4\lambda_{70}(E,\eta_g)\lambda_{74}(E,\eta_g)]$$

$$\lambda_{83}(E,\eta_g) \equiv \frac{\lambda_{78}(E,\eta_g)}{9\hbar^4[Z_0(E,\eta_g)]^2} \text{ and } \lambda_{78}(E,\eta_g) \equiv [4\lambda_{70}(E,\eta_g)\lambda_{75}(E,\eta_g)]$$

Thus,

$$V(E,\eta_g) = [\lambda_{87}(E,\eta_g)]\int_0^{\lambda_{86}(E,\eta_g)}[\sqrt{k_z^4 + \lambda_{88}(E,\eta_g)k_z^2 + \lambda_{89}(E,\eta_g)} - \lambda_{90}(E,\eta_g)]dk_z \qquad (148)$$

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

$$and\ \lambda_{90}(E,\eta_g) \equiv 2\pi[\frac{\lambda_{79}(E,\eta_g)\{\lambda_{86}(E,\eta_g)\}^3}{3} + \lambda_{80}(E,\eta_g)\lambda_{89}(E,\eta_g)]$$

The (148) can be written as

$$V(E,\eta_g)=[\lambda_{87}(E,\eta_g)\lambda_{95}(E,\eta_g)-\lambda_{90}(E,\eta_g)] \tag{149}$$

in which,

$$\lambda_{95}(E,\eta_g)\equiv[\frac{\lambda_{91}(E,\eta_g)}{3}[-E_t[\lambda_{93}(E,\eta_g),\lambda_{94}(E,\eta_g)]]$$
$$[\{\lambda_{91}(E,\eta_g)\}^2+\{\lambda_{92}(E,\eta_g)\}^2+2\{\lambda_{92}(E,\eta_g)\}^2F_t[\lambda_{93}(E,\eta_g),\lambda_{94}(E,\eta_g)]]$$
$$+(\frac{\{\lambda_{86}(E,\eta_g)\}}{3})[\{\lambda_{86}(E,\eta_g)\}^2+\{\lambda_{91}(E,\eta_g)\}^2+2\{\lambda_{92}(E,\eta_g)\}^2]$$
$$[[\{\lambda_{91}(E,\eta_g)\}^2+\{\lambda_{86}(E,\eta_g)\}^2]^{1/2}[\{\lambda_{92}(E,\eta_g)\}^2+\{\lambda_{86}(E,\eta_g)\}^2]^{-1/2}],$$
$$\{\lambda_{91}(E,\eta_g)\}^2\equiv\frac{1}{2}[\sqrt{\{\lambda_{88}(E,\eta_g)\}^2-4\lambda_{89}(E,\eta_g)}+\lambda_{88}(E,\eta_g)], E_i[\lambda_{93}(E,\eta_g),\lambda_{94}(E,\eta_g)]$$

is the incomplete elliptic integral of the 2nd kind and is given by [105],

$$E_i[\lambda_{93}(E,\eta_g),\lambda_{94}(E,\eta_g)]\equiv\int_0^{\lambda_{93}(E,\eta_g)}[\{1-\{\lambda_{94}(E,\eta_g)\}^2\sin^2\xi\}^{1/2}]d\xi\,,$$

ξ is the variable of integration in this case,

$$\lambda_{93}(E,\eta_g)\equiv\tan^{-1}[\frac{\lambda_{86}(E,\eta_g)}{\lambda_{92}(E,\eta_g)}]\{\lambda_{92}(E,\eta_g)\}^2\equiv\frac{1}{2}[\lambda_{88}(E,\eta_g)-\sqrt{\{\lambda_{88}(E,\eta_g)\}^2-4\lambda_{89}(E,\eta_g)}],$$
$$\lambda_{94}(E,\eta_g)\equiv\frac{\sqrt{\{\lambda_{91}(E,\eta_g)\}^2-\{\lambda_{92}(E,\eta_g)\}^2}}{\lambda_{91}(E,\eta_g)}, F_i[\lambda_{93}(E,\eta_g),\lambda_{94}(E,\eta_g)]$$

is the incomplete elliptic integral of the 1st kind and is given by [105], $F_i[\lambda_{93}(E,\eta_g),\lambda_{94}(E,\eta_g)]\equiv\int_0^{\lambda_{93}(E,\eta_g)}[\{1-\{\lambda_{94}(E,\eta_g)\}^2\sin^2\xi\}^{-1/2}]d\xi\,.$

The DOS function in this case is given by

$$N_{HD}(E,\eta_g)=\frac{g_v}{4\pi^3}[\{\lambda_{87}(E,\eta_g)\}'\lambda_{95}(E,\eta_g)+\{\lambda_{95}(E,\eta_g)\}'\lambda_{87}(E,\eta_g)-\{\lambda_{90}(E,\eta_g)\}'] \tag{150}$$

Therefore the electron concentration can be expressed as

$$n_0=\frac{g_v}{4\pi^3}[\bar{I}_{125}(E_{F_h},\eta_g)+\sum_{r=1}^{s}L(r)[\bar{I}_{125}(E_{F_h},\eta_g)]] \tag{151}$$

where,

$$\bar{I}_{125}(E_{F_h},\eta_g)=[\{\lambda_{87}(E_{F_h},\eta_g)\}\lambda_{95}(E_{F_h},\eta_g)-\{\lambda_{90}(E_{F_h},\eta_g)\}]$$

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

$$E(1+\alpha E)+\alpha E(\frac{\hbar^2k_x^2}{2x_4}+\frac{\hbar^2k_y^2}{2x_5})+\alpha E\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})-(1+\alpha E)(\frac{\hbar^2k_x^2}{2x_1}+\frac{\hbar^2k_y^2}{2x_2})$$
$$-\alpha(\frac{\hbar^2k_x^2}{2x_1}+\frac{\hbar^2k_y^2}{2x_2})(\frac{\hbar^2k_x^2}{2x_4}+\frac{\hbar^2k_y^2}{2x_5})-\alpha(\frac{\hbar^2k_x^2}{2x_1}+\frac{\hbar^2k_y^2}{2x_2})\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-(1+\alpha E)\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2$$
$$-\alpha\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2(\frac{\hbar^2k_x^2}{2x_4}+\frac{\hbar^2k_y^2}{2x_5})-\alpha\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2=\frac{\hbar^2k_x^2}{2m_1}+\frac{\hbar^2k_y^2}{2m_2}+\frac{\hbar^2}{2m_3}(\frac{n_z\pi}{d_z})^2 \tag{152}$$

where, $x_4=m_t^+, x_5=\frac{m_t^++2m_l^+}{3}, x_6=\frac{3m_t^+m_l^+}{2m_l^++m_t^+}, x_1=m_t^-, x_2=\frac{m_t^-+2m_l^-}{3}, x_3=\frac{3m_t^-m_l^-}{2m_l^-+m_t^-}$

$m_1=m_t^*, m_2=\frac{m_t^*+2m_l^*}{3}$ and $m_3=\frac{3m_l^*m_t^*}{m_t^*+2m_l^*}$.

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

$$\gamma_2(E,\eta_g)+\alpha\gamma_3(E,\eta_g)(\frac{\hbar^2k_x^2}{2x_4}+\frac{\hbar^2k_y^2}{2x_5})+\alpha\gamma_3(E,\eta_g)\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-(1+\alpha\gamma_3(E,\eta_g))(\frac{\hbar^2k_x^2}{2x_1}+\frac{\hbar^2k_y^2}{2x_2})$$
$$-\alpha(\frac{\hbar^2k_x^2}{2x_1}+\frac{\hbar^2k_y^2}{2x_2})(\frac{\hbar^2k_x^2}{2x_4}+\frac{\hbar^2k_y^2}{2x_5})-\alpha(\frac{\hbar^2k_x^2}{2x_1}+\frac{\hbar^2k_y^2}{2x_2})\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-(1+\alpha\gamma_3(E,\eta_g))\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2$$
$$-\alpha\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2(\frac{\hbar^2k_x^2}{2x_4}+\frac{\hbar^2k_y^2}{2x_5})-\alpha\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2=\frac{\hbar^2k_x^2}{2m_1}+\frac{\hbar^2k_y^2}{2m_2}+\frac{\hbar^2}{2m_3}(\frac{n_z\pi}{d_z})^2 \tag{153}$$

Substituting, $k_x=r\cos\theta$ and $k_y=r\sin\theta$ (where r and θ are 2D polar coordinates in 2D wave vector space) in (153), we can write

$$r^4[\alpha\frac{1}{4}(\frac{\hbar^2\cos^2\theta}{x_1}+\frac{\hbar^2\sin^2\theta}{x_2})(\frac{\hbar^2\cos^2\theta}{x_4}+\frac{\hbar^2\sin^2\theta}{x_5})]+r^2\frac{1}{2}[(\frac{\hbar^2\cos^2\theta}{m_1}+\frac{\hbar^2\sin^2\theta}{m_2})$$
$$+\alpha\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2(\frac{\hbar^2\cos^2\theta}{x_4}+\frac{\hbar^2\sin^2\theta}{x_5})+\alpha(\frac{\hbar^2\cos^2\theta}{x_1}+\frac{\hbar^2\sin^2\theta}{x_2})\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2$$
$$+\hbar^2(1+\alpha\gamma_3(E,\eta_g))(\frac{\cos^2\theta}{x_1}+\frac{\sin^2\theta}{x_2})-\hbar^2\alpha\gamma_3(E,\eta_g)(\frac{\cos^2\theta}{x_4}+\frac{\sin^2\theta}{x_5})$$
$$-[\gamma_2(E,\eta_g)+\alpha\gamma_3(E,\eta_g)\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-(1+\alpha\gamma_3(E,\eta_g))\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2-\alpha(\frac{\hbar^4}{4x_3x_6}(\frac{n_z\pi}{d_z})^4)]=0 \tag{154}$$

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

$$A(E,n_z)=\bar{J}_1-\bar{J}_2 \tag{155}$$

where $\bar{J}_1\equiv 2\int_0^{\pi/2}\frac{c_1}{b_1}d\theta$ (156) in

and $\bar{J}_2\equiv 2\int_0^{\pi/2}\frac{ac_1^2}{b_1^3}d\theta$ (157)

which

$$a \equiv [\alpha(\frac{\hbar^4}{4})(\frac{\cos^2\theta}{x_1}+\frac{\sin^2\theta}{x_2})(\frac{\cos^2\theta}{x_4}+\frac{\sin^2\theta}{x_5})],$$

$$b_1 \equiv (\frac{\hbar^2}{2})[(\frac{\cos^2\theta}{m_1}+\frac{\sin^2\theta}{m_2})+\alpha(\frac{\hbar^2}{2x_3})(\frac{n_z\pi}{d_z})^2[(\frac{\cos^2\theta}{x_4}+\frac{\sin^2\theta}{x_5})$$

$$+\alpha(\frac{\hbar^2}{2x_6})(\frac{n_z\pi}{d_z})^2[(\frac{\cos^2\theta}{m_1}+\frac{\sin^2\theta}{m_2})$$

$$+(1+\alpha\gamma_3(E,\eta_g))(\frac{\cos^2\theta}{x_1}+\frac{\sin^2\theta}{x_2})-\alpha\gamma_3(E,\eta_g)(\frac{\cos^2\theta}{x_4}+\frac{\sin^2\theta}{x_5})]$$

$$and\ c_1 \equiv [\gamma_2(E,\eta_g)+\alpha\gamma_3(E,\eta_g)(\frac{\hbar^2}{2x_6})(\frac{n_z\pi}{d_z})^2-(1+\alpha\gamma_3(E,\eta_g))(\frac{\hbar^2}{2x_3})(\frac{n_z\pi}{d_z})^2-\alpha(\frac{\hbar^4}{4x_3x_6})(\frac{n_z\pi}{d_z})^4]$$

The (156) can be expressed as

$$\bar{J}_1 = 2\int_0^{\pi/2}\frac{t_{31}(E,n_z)d\theta}{A_{11}(E,n_z)\cos^2\theta+B_{11}(E,n_z)\sin^2\theta}$$

$$where,\ t_{31}(E,n_z)\equiv c_1, A_{11}(E,n_z)\equiv\frac{\hbar^2}{2m_1}t_{11}(E,n_z),$$

$$t_{11}(E,n_z)\equiv[1+m_1[\frac{1}{x_4}\frac{\alpha\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2+\frac{\alpha\hbar^2}{2x_1x_6}(\frac{n_z\pi}{d_z})^2+\frac{1+\alpha\gamma_2(E,\eta_g)}{x_1}-\frac{\alpha\gamma_3(E,\eta_g)}{x_4}]]$$

$$B_{11}(E,n_z)\equiv\frac{\hbar^2}{2m_2}t_{21}(E,n_z)$$

$$and\ t_{21}(E,n_z)\equiv[1+m_2[\frac{\alpha\hbar^2}{2x_3x_5}(\frac{n_z\pi}{d_z})^2+\frac{\alpha\hbar^2}{2x_2x_6}(\frac{n_z\pi}{d_z})^2+\frac{1+\alpha\gamma_3(E,\eta_g)}{x_2}-\frac{\alpha\gamma_3(E,\eta_g)}{x_5}]]$$

Performing the integration, we get

$$\bar{J}_1=\pi t_{31}(E,n_z)[A_{11}(E,n_z)B_{11}(E,n_z)]^{-1/2} \tag{158}$$

From (157)we can write

$$\bar{J}_2=\frac{\alpha t_{31}^2(E,n_z)\hbar^4}{2B_{11}^3(E,n_z)}I \tag{159}$$

$$where,\ I\equiv\int_0^{\infty}\frac{(a_1+a_2z^2)(a_3+a_4z^2)dz}{[(\bar{a})^2+z^2]^3},(\bar{a})^2=(\frac{A_{11}(E,n_z)}{B_{11}(E,n_z)}), \tag{160}$$

in which $a_1\equiv\frac{1}{x_1},a_2\equiv\frac{1}{x_2},z=\tan\theta,$ θ is a new variable, $a_3\equiv\frac{1}{x_4},a_4\equiv\frac{1}{x_5}$ and $(\bar{a})^2\equiv(\frac{A_1(E,n_z)}{B_1(E,n_z)})$.

The use of the Residue theorem leads to the evaluation of the integral in (160) as

$$I=\frac{\pi}{4\bar{a}}[a_1a_4+3a_2a_4] \tag{161}$$

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

$$A_{HD}(E,n_z)=\frac{\pi t_{31}(E,n_z)}{\sqrt{A_{11}(E,n_z)B_{11}(E,n_z)}}[1-\frac{1}{x_5}(\frac{1}{x_1}+\frac{3}{x_2})\frac{\alpha t_{31}(E,n_z)\hbar^4}{8B_{11}^2(E,n_z)}] \quad (162)$$

The EM for the HD QWs of IV-VI materials can thus be written as

$$m^*(E,n_z)=\frac{\hbar^2}{2}[\theta_{5HD}(E,n_z)]\Big|_{E=E_{F1HD}} \quad (163)$$

$$where,\ \theta_{5HD}(E,n_z)\equiv[1-\frac{1}{x_5}(\frac{1}{x_1}+\frac{3}{x_2})\frac{\alpha t_{31}(E,n_z)\hbar^4}{8[B_{11}(E,n_z)]^2}][A_{11}(E,n_z)B_{11}(E,n_z)]^{-1}$$

$$[\sqrt{A_{11}(E,n_z)\mathrm{B}_{11}(E,n_z)}\{t_{31}(E,n_z)\}'-t_{31}(E,n_z)\{\frac{1}{2}\{A_{11}(E,n_z)\}'[\frac{B_{11}(E,n_z)}{A_{11}(E,n_z)}]^{1/2}+\frac{1}{2}\{B_{11}(E,n_z)\}'[\frac{A_{11}(E,n_z)}{B_{11}(E,n_z)}]^{1/2}\}]$$

$$-\frac{1}{8}\frac{t_{31}(E,n_z)\alpha\hbar^4}{\sqrt{A_{11}(E,n_z)B_{11}(E,n_z)}}\frac{1}{x_5}(\frac{1}{x_1}+\frac{3}{x_2})[B_{11}(E,n_z)]^{-4}[\{B_{11}(E,n_z)\}^2\{t_{31}(E,n_z)\}'-2B_{11}(E,n_z)\{B_{11}(E,n_z)\}'t_{31}(E,n_z)]$$

Thus, the EM is a function of Fermi energy and the quantum number due to the band non-parabolicity.

The total DOS function can be written as

$$N_{2DT}(E)=(\frac{g_v}{2\pi})\sum_{n_z=1}^{n_{z_{\max}}}\theta_{5HD}(E,n_z)H(E-E_{n_{z7HD}}) \quad (164)$$

where the sub-band energy $(E_{n_{z7}})$ in this case can be written as

$$\gamma_2(E_{n_{z7HD}},\eta_g)+\alpha\gamma_3(E_{n_{z7HD}},\eta_g)\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-(1+\alpha\gamma_3(E_{n_{z7HD}},\eta_g))\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2$$

$$-\alpha\frac{\hbar^{2=0}}{2x_3}(\frac{n_z\pi}{d_z})^2\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-[\frac{\hbar^2}{2m_3}(\frac{n_z\pi}{d_z})^2] \quad (165)$$

The use (164) leads to the expression of 2D electron statistics as

$$n_{2D}=\frac{g_v}{2\pi}\sum_{n_z=1}^{n_{\max}}\left[T_{55HD}(E_{F1HD},n_z)+T_{56HD}(E_{F1HD},n_z)\right] \quad (166)$$

$$where T_{55HD}(E_{F1HD},n_z)\equiv\frac{A_{HD}(E_{F1HD},n_z)}{\pi} and T_{56HD}(E_{F1HD},n_z)\equiv\sum_{r=1}^{s}L(r)T_{55HD}(E_{F1HD},n_z)$$

In the absence of band-tails the EM in QWs of IV-VI materials can be written as

$$m^{*}(E,n_z)=\frac{\hbar^2}{2}[\theta_5(E,n_z)]\Big|_{E=E_{Fs}} \tag{167}$$

where,

$$\theta_5(E,n_z)\equiv[1-\frac{1}{x_5}(\frac{1}{x_1}+\frac{3}{x_2})\frac{\alpha t_{30}(E,n_z)\hbar^4}{8[B_{10}(E,n_z)]^2}][A_{10}(E,n_z)B_{10}(E,n_z)]^{-1}$$

$$[[\sqrt{A_{10}(E,n_z)B_{10}(E,n_z)}\{t_{30}(E,n_z)\}'-\{t_{30}(E,n_z)\}'\{\frac{1}{2}\{A_{10}(E,n_z)\}'[\frac{B_{10}(E,n_z)}{A_{10}(E,n_z)}]^{1/2}+\frac{1}{2}\{B_{10}(E,n_z)\}'[\frac{A_{10}(E,n_z)}{B_{10}(E,n_z)}]\}]$$

$$-\frac{1}{8}\frac{t_{30}(E,n_z)\alpha\hbar^4}{\sqrt{A_{10}(E,n_z)B_{10}(E,n_z)}}\frac{1}{x_5}(\frac{1}{x_1}+\frac{3}{x_2})[B_{10}(E,n_z)]^{-4}[\{B_{10}(E,n_z)\}^2\left\{t_{30}(E,n_z)\right\}'-2B_{10}(E,n_z)\{B_{10}(E,n_z)\}'t_{30}(E,n_z)]$$

$$t_{30}(E,n_z)=c_0,$$

$$c_0\equiv[E(1+\alpha E)+\alpha E(\frac{\hbar^2}{2x_6})(\frac{n_z\pi}{d_z})^2-(1+\alpha E)(\frac{\hbar^2}{2x_3})(\frac{n_z\pi}{d_z})^2-\alpha(\frac{\hbar^2}{4x_3x_6})(\frac{n_z\pi}{d_z})^4],$$

$$A_{10}(E,n_z)\equiv\frac{\hbar^2}{2m_1}t_{10}(E,n_z),t_{10}(E,n_z)\equiv[1+m_1[\frac{1}{x_4}\frac{\alpha\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2+\frac{\alpha\hbar^2}{2x_1x_6}(\frac{n_z\pi}{d_z})^2+\frac{1+\alpha E}{x_1}-\frac{\alpha E}{x_4}]]$$

$$B_{10}(E,n_z)\equiv\frac{\hbar^2}{2m_2}t_{20}(E,n_z)$$

and

$$t_{20}(E,n_z)\equiv[1+m_2[\frac{\alpha\hbar^2}{2x_3x_5}(\frac{n_z\pi}{d_z})^2+\frac{\alpha\hbar^2}{2x_2x_6}(\frac{n_z\pi}{d_z})^2+\frac{1+\alpha E}{x_2}-\frac{\alpha E}{x_5}]]$$

Thus, the EM is a function of Fermi energy and the quantum number due to the band non-parabolicity.

The total DOS function can be written as

$$N_{2DT}(E)=(\frac{g_v}{2\pi})\sum_{n_z=1}^{n_{z\max}}\theta_5(E,n_z)H(E-E_{n_{z7}}) \tag{168}$$

where the sub-band energy $(E_{n_{z7}})$ in this case can be written as

$$E_{n_{z7}}(1+\alpha E_{n_{z7}})+\alpha E_{n_{z7}}\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-(1+\alpha E_{n_{z7}})\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2$$

$$-\alpha\frac{\hbar^2}{2x_3}(\frac{n_z\pi}{d_z})^2\frac{\hbar^2}{2x_6}(\frac{n_z\pi}{d_z})^2-[\frac{\hbar^2}{2m_3}(\frac{n_z\pi}{d_z})^2]=0 \tag{169}$$

In the absence of band-tails, the expression of 2D electron statistics can be written as

$$n_{2D} = \frac{g_v}{2\pi}\sum_{n_z=1}^{n_{\max}} [T_{550}(E_{Fs}, n_z) + T_{560}(E_{Fs}, n_z)] \tag{170}$$

$$where, T_{550}(E_{Fs}, n_z) \equiv \frac{A_0(E_{Fs}, n_z)}{\pi}, A_0(E, n_z) = \frac{\pi t_{30}(E, n_z)}{\sqrt{A_{10}(E, n_z)}B_{10}(E, n_z)}[1 - \frac{1}{x_5}(\frac{1}{x_1} + \frac{3}{x_2})\frac{\alpha t_{30}(E, n_z)\hbar^4}{8B_{10}^2(E, n_z)}],$$

and

$$T_{560}(E_{Fs}, n_z) = \sum_{r=1}^{s} L(r) T_{550}(E_{Fs}, n_z)$$

For bulk specimens of IV-VI materials, the expression of electron concentration assumes the forms

$$n_0 = (\frac{g_v}{2\pi^2})[M_{A4}(E_{F_b}) + N_{A_4}(E_{F_b})] \tag{171}$$

where,

$$\omega_{A_1} = [\frac{\alpha^2}{16}[\frac{1}{m_t^- m_l^+} + \frac{1}{m_l^- m_t^+}] - \frac{\alpha^2}{4m_l^- m_t^+ m_l^- m_t^+}]$$

$$M_{A_4}(E_{F_b}) = [\alpha_5 J_{A_1}(E_{F_b}) - \alpha_3(E_{F_b})\bar{\tau}_{A_1}(E_{F_b}) - \frac{\alpha_4}{3}[\bar{\tau}_{A_1}(E_{F_b})]^3], \alpha_5 = [\frac{2m_t^+ m_t^-}{\alpha\hbar^2}\omega_{A_1}],$$

$$J_{A_1}(E_{F_b}) = \frac{A_4(E_{F_b})}{3} - [-(A_A^2(E_{F_b}) + B_A^2(E_{F_b}))E(\lambda, q) + 2B_A^2(E_{F_b})F(\lambda, q)] + \frac{\bar{\tau}_{A_1}(E_{F_b})}{3}$$

$$[(\bar{\tau}_{A_1}(E_{F_b}))^2 + A_A^2(E_{F_b}) + 2B_A^2(E_{F_b})][A_A^2(E_{F_b}) + \bar{\tau}_{A_1}^2(E_{F_b})]^{1/2}[B_A^2(E_{F_b}) + \bar{\tau}_{A_1}^2(E_{F_b})]^{-1/2}$$

$$\lambda = \tan^{-1}\frac{\bar{\tau}_A(E_{F_b})}{B_A(E_{F_b})},\ q = [\frac{\sqrt{A_A^2(E_{F_b}) - B_A^2(E_{F_b})}}{A_A(E_{F_b})}],\ A_A(E_{F_b}) = [\tau_{A_2}(E_{F_b}) + \sqrt{\tau_{A_2}^2(E_{F_b}) - 4\tau_{A_3}(E_{F_b})}]^{1/2}/\sqrt{2},$$

$$B_A(E_{F_b}) = [\tau_{A_2}(E_{F_b}) - \sqrt{\tau_{A_2}^2(E_{F_b}) - 4\tau_{A_3}(E_{F_b})}]^{1/2}/\sqrt{2},\ \tau_{A_2}(E_{F_b}) = \frac{\omega_{A_2}(E_{F_b})}{\omega_{A_1}^2},\ \tau_{A_3}(E_{F_b}) = \frac{\omega_{A_3}(E_{F_b})}{\omega_{A_1}^2},$$

$$\omega_{A_2}(E_{F_b}) = [\frac{\alpha}{2}[\frac{1}{2m_t^*} - \frac{\alpha.E_{F_b}}{2m_t^+} + \frac{1+\alpha.E_{F_b}}{2m_t^-}].[\frac{1}{m_t^- m_l^+} + \frac{1}{m_l^- m_t^+}] - \frac{\alpha}{m_t^+ m_t^-}[\frac{1}{m_l^*} + \frac{\alpha.E_{F_b}}{2m_l^+} + \frac{1+\alpha.E_{F_b}}{2m_l^-}]]$$

$$\omega_{A_3}(E_{F_b}) = [\frac{\alpha.E_{F_b} 1+\alpha.E_{F_b}}{m_t^+ m_t^-} + [\frac{1}{2m_t^*} - \frac{\alpha.E_{F_b}}{2m_t^+} + \frac{1+\alpha.E_{F_b}}{2m_t^-}]], \alpha_2(E_{F_b}) = [\frac{1}{2m_t^*} - \frac{\alpha E_{F_b}}{2m_t^+} + \frac{1+\alpha E_{F_b}}{2m_t^-}],$$

$$\alpha_3 = \frac{\alpha\hbar^2}{4}[\frac{1}{m_t^- m_l^+} + \frac{1}{m_l^- m_t^+}],$$

$$\tau_{A_1}(E_{F_b}) = [\frac{2m_l^+ m_l^-}{\alpha\hbar^2}]^{1/2}[-[\frac{1}{2m_l^*} + \frac{1+\alpha.E_{F_b}}{m_l^-} - \frac{\alpha.E_{F_b}}{2m_l^+}] + [[\frac{1}{2m_l^*} + \frac{1+\alpha.E_{F_b}}{m_l^-} - \frac{\alpha.E_{F_b}}{2m_l^+}]^2 + \frac{\alpha.E_{F_b}(1+\alpha.E_{F_b})}{m_l^- m_l^+}]^{1/2}]^{1/2},$$

is the in complete Elliptic integral of second kind, $F(\lambda, q)$ is the incomplete Elliptic integral of first kind,

$$N_{A_4}(E_{Fb}) = \sum_{r=1}^{s} L(r)[M_{A_4}(E_{Fb})]$$

$$I_{17}(E') = \frac{-I_{15}(E') + \sqrt{I_{15}^2(E') + 4I_{16}(E')}}{2}, \; I_{15}(E') = \frac{2m_l^+ m_t^-}{\alpha\hbar^2}[\frac{1}{m_l^*} + \frac{1}{m_l^-} + \alpha E'(\frac{1}{m_l^-} - \frac{1}{m_l^+})] \qquad (172)$$

$$and \;\; I_{16}(E') = \frac{4m_l^+ m_t^-}{\alpha\hbar^4} E'(1+\alpha E')$$

b) The dispersion relation of the conduction electrons in bulk specimens of IV-VI semiconductors in accordance with the model of Bangert and Kastner [111] is given by

$$\omega_1(E)k_s^2 + \omega_2(E)k_z^2 = 1 \qquad (173)$$

where,

$$\omega_1(E) = (2E)^{-1}[\frac{(\bar{R})^2}{E_{g_0}(1+\alpha_1 E)} + \frac{(\bar{S})^2}{\Delta_c'(1+\alpha_3 E)} + \frac{(\bar{Q})^2}{\Delta_c''(1+\alpha_3 E)}] \text{ and}$$

$$\omega_2(\mathrm{E}) = (2E)^{-1}[\frac{(\bar{\mathrm{A}})^2}{\mathrm{E_{g0}}(1+\alpha_1 \mathrm{E})} + \frac{(\bar{\mathrm{S}}+\bar{\mathrm{Q}})^2}{\Delta_c''(1+\alpha_3 \mathrm{E})}], (\bar{R})^2 = 2.3\times10^{-10}(eVm)^2,$$

$$(\bar{S})^2 = 4.6(\bar{R})^2, \alpha_1 = \frac{1}{\mathrm{E_{g0}}}, \alpha_2 = \frac{1}{\Delta_c'}, \alpha_3 = \frac{1}{\Delta_c''},$$

The electron energy spectrum in heavily doped IV-VI materials in this case can be expressed as

$$2I(4) = k_s^2[\{c_1(\alpha_1 E, E_g) - iD_1(\alpha_1, E, E_g)\}\frac{(\bar{R})^2}{E_{g_0}} + \{c_2(\alpha_2 E, E_g) - iD_2(\alpha_2, E, E_g)\}\frac{(\bar{S})^2}{\Delta_c'}$$

$$+\{c_3(\alpha_3 E, E_g) - iD_3(\alpha_3 E, E_g)\}\frac{(\bar{Q})^2}{\Delta_c''}] + k_z^2[\frac{2(\bar{A})^2}{E_{g_0}}\{c_1(\alpha_1 E, E_g) - iD_1(\alpha_1, E, E_g)\}$$

$$+\frac{(\bar{S}+\bar{Q})^2}{\Delta_c''}\{c_3(\alpha_3 E, E_g) - iD_3(\alpha_3 E, E_g)\}] \qquad (174)$$

where,

$$\alpha_1 = \frac{1}{E_g}, \alpha_2 = \frac{1}{\Delta_c'}, \alpha_3 = \frac{1}{\Delta_c''}, G_t = \frac{1+\alpha_i E}{\eta_g \alpha_i}$$

$$c_i(\alpha_i E, \eta_g) = [\frac{2}{\alpha_i \eta_g \sqrt{\pi}}]\exp(-u_i^2)\times[\sum_{p=1}^{\infty} \{\exp(\frac{-p^2}{4})(\sinh(pu_i))\}p^{-1}],$$

$i = 1,2,3,4,...$

and

$$D_i(\alpha_i, E, \eta_g) = [\frac{\sqrt{\pi}}{\alpha_i \eta_g}]\exp(-u_i^2)$$

Therefore (174) can be written as,

$$F_1(E,\eta_g)k_s^2 + F_2(E,\eta_g)k_z^2 = 1 \qquad (175)$$

where,

$$F_1(E,\eta_g) = [2\gamma_0(E,\eta_g)]^{-1}[\frac{(\bar{R})^2}{E_g}\{C_1(\alpha_1 E,E_g) - iD_1(\alpha_1,E,E_g)\} + \frac{(\bar{S})^2}{\Delta_c'}\{C_2(\alpha_2,E,E_g) - iD_2(\alpha_2,E,E_g)\}$$

$$+\frac{(\bar{Q})^2}{\Delta_c''}\{C_3(\alpha_3,E,E_g) - iD_3(\alpha_3,E,E_g)\}]$$

and

$$F_2(E,\eta_g) = [2\gamma_0(E,\eta_g)]^{-1}[\frac{2(\bar{A})^2}{E_g}\{C_1(\alpha_1,E,\eta_g) - iD_1(\alpha_1,E,\eta_g)\}$$

$$+\frac{(\bar{S}+\bar{Q})^2}{\Delta_c''}\{C_3(\alpha_3,E,E_g) - iD_3(\alpha_3,E,E_g)\}]]$$

Since $F_1(E,\eta_g)$ and $F_2(E,\eta_g)$ are complex, the energy spectrum is also complex in the presence of Gaussian band tails.

The EMs can be written as

$$m_{\perp}^{*}(E_{F_h},\eta_g) = (\frac{\hbar^2}{2}) \text{ Real part of } [\frac{F_1'(E_{F_h},\eta_g)}{F_2^2(E_{F_h},\eta_g)}] \qquad (176)$$

$$m_{11}^{*}(E_{F_h},\eta_g) = (\frac{\hbar^2}{2}) \text{ Real part of } [\frac{F_2'(E_{F_h},\eta_g)}{F_2^2(E_{F_h},\eta_g)}] \qquad (177)$$

It appears then that, the evolution of the masses needs an expression of the carrier concentration, which in turn is determined by the DOS function.

The DOS function in this case can be expressed as

$$N_{HD}(E,\eta_g) = \frac{g_v}{3\pi^2}F_3'(E,\eta_g), F_3(E,\eta_g) = [F_1(E,\eta_g)\sqrt{F_2(E,\eta_g)}]^{-1} \qquad (178)$$

The electron concentration is given by

$$n_0 = \frac{g_v}{3\pi^2}\text{Re}\,al\ \ part\ of\,[F_3(E_{F_h},\eta_g) + \sum_{r=1}^{s} L(r)[F_3(E_{F_h},\eta_g)]] \qquad (179)$$

The 2D dispersion relation in this case assumes the form

$$k_s^2 = F_6(E,\eta_g,n_z)$$

$$where,\ F_6(E,\eta_g,n_z) = [\frac{[1-F_2(E,\eta_g)(n_z\pi/d_z)]}{F_1(E,\eta_g)}] \qquad (180)$$

The EM in this case is given by

$$m^*(E_{F1HD},\eta_g,n_z) = \frac{\hbar^2}{2}\text{Re}\,al\ \ part\ of\,[F_6'(E_{F1HD},\eta_g,n_z)] \qquad (181)$$

The total DOS function can be written as

$$N_{2DT}(E) = \frac{g_v}{2\pi}\sum_{n_z=1}^{n_{z\max}} F_6'(E,\eta_g,n_z)H(E - E_{n_z 71HD}) \tag{182}$$

where $E_{n_z 71HD}$ is the quantized energy in this case and is given by

$$1 = F_2(E_{n_z 71HD},\eta_g)(\pi n_z / d_z)^2 \tag{183}$$

The surface electron concentration can be expressed as

$$n_0 = \frac{g_v}{2\pi}\mathrm{Re}al\ \ part\ of\,[\sum_{n_z=1}^{n_{z\max}}\ [F_6(E_{F1HD},\eta_g,n_z) + \sum_{r=1}^{s}\ L(r)[F_6(E_{F1HD},\eta_g,n_z)]]] \tag{184}$$

In the absence of band-tails the EMs can be written as

$$m_\perp^*(E_F) = (\frac{\hbar^2}{2})(\frac{F_{11}'(E_F)}{F_{11}^2(E_F)}) \tag{185}$$

$$m_\parallel^*(E_F) = (\frac{\hbar^2}{2})(\frac{F_{12}'(E_F)}{F_{12}^2(E_F)}) \tag{186}$$

$$where,\ F_{12}(E) = [\frac{(\bar{A})^2}{E_{go}(1+\alpha_1 E)} + \frac{(\bar{S}+\bar{Q})^2}{\Delta''_{go}(1+\alpha_3 E)}][2E]^{-1}$$

$$and\ \ F_{11}(E) = [\frac{(\bar{R})^2}{E_{go}(1+\alpha_1 E)} + \frac{(\bar{S})^2}{\Delta'_c(1+\alpha_2 E)} + \frac{(\bar{Q})^2}{\Delta''_{go}(1+\alpha_3 E)}][2E]^{-1}$$

It appears then that, the evolution of the masses needs an expression of the carrier concentration, which in turn is determined by the DOS function.

The DOS function in this case can be expressed as

$$N(E) = \frac{g_v}{3\pi^2}F_{13}'(E), \quad F_{13}(E) = [F_{11}(E)\sqrt{F_{12}(E)}]^{-1} \tag{187}$$

The electron concentration is given by

$$n_0 = \frac{g_v}{3\pi^2}[F_{13}(E_F) + \sum_{r=1}^{s}\ L(r)[F_{13}(E_F)]] \tag{188}$$

In the absence of band-tails, the 2D dispersion relation in this case assumes the form

$$k_s^2 = F_{16}(E,n_z)$$

$$where,\ F_{16}(E,n_z) = [\frac{[1 - F_{12}(E)(n_z\pi / d_z)^2]}{F_{11}(E,\eta_g)}] \tag{189}$$

The EM in this case is given by

$$m^*(E_{F_s},n_z) = \frac{\hbar^2}{2}[F_{16}'(E_{F_s},n_z)] \tag{190}$$

The total DOS function can be written as

$$N_{2DT}(E)=\frac{g_v}{2\pi}\sum_{n_z=1}^{n_{z_{\max}}} F_6'(E,\eta_g,n_z)H(E-E_{n_z71HD}) \qquad (191)$$

where E_{n_z711} is the quantized energy in this case and is given by

$$1=F_{12}(E_{n_z711},\eta_g)(\pi n_z/d_z)^2 \qquad (192)$$

The surface electron concentration can be expressed as

$$n_0=\frac{g_v}{2\pi}[\sum_{n_z=1}^{n_{z_{\max}}}[F_{16}(E_{F_s},n_z)+\sum_{r=1}^{s}L(r)[F_{16}(E_{F_s},n_z)]]] \qquad (193)$$

2.5The EM in Quantum Wells (QWs) of HD stressed Kane type materials

The electron energy spectrum in stressed Kane type semiconductors can be written [112] as

$$(\frac{k_x}{\bar{a}_0(E)})^2+(\frac{k_y}{\bar{b}_0(E)})^2+(\frac{k_z}{\bar{c}_0(\mathrm{E})})^2=1 \qquad (194)$$

$$where,\ [\bar{a}_0(E)]^2\equiv\frac{\bar{K}_0(E)}{\bar{A}_0(E)+\frac{1}{2}\bar{D}_0(E)},\ \bar{K}_0(E)\equiv[E-C_1\varepsilon-\frac{2C_2^2\varepsilon_{xy}^2}{3E_g'}](\frac{3E_g'}{2B_2^2})$$

C_1 is the conduction band deformation potential, ε is the trace of the strain tensor $\hat{\varepsilon}$ which can be written as $\hat{\varepsilon}=\begin{bmatrix}\varepsilon_{xx} & \varepsilon_{xy} & 0\\ \varepsilon_{xy} & \varepsilon_{yy} & 0\\ 0 & 0 & \varepsilon_{zz}\end{bmatrix}$, ,

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,

$$\bar{A}_0(E)\equiv[1-\frac{(\bar{a}_0+C_1)}{E_g'}+\frac{3\bar{b}_0\varepsilon_{xx}}{2E_g'}-\frac{\bar{b}_0\varepsilon}{2E_g'}],\ \bar{a}_0\equiv-\frac{1}{3}(\bar{b}_0+2\bar{m}),\ \bar{b}_0\equiv\frac{1}{3}(\bar{l}-\bar{m}),\ \bar{d}_0\equiv\frac{2\bar{n}}{\sqrt{3}},$$

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

$$[\bar{b}_0(E)]^2\equiv\frac{\bar{K}_0(E)}{\bar{A}_0(E)-\frac{1}{2}\bar{D}_0(E)},\ [\bar{c}_0(E)]^2\equiv\frac{\bar{K}_0(E)}{\bar{L}_0(E)}\ \text{and}\ \bar{L}_0(E)=[1-\frac{(\bar{a}_0+C_1)}{E_g'}+\frac{3\bar{b}_0\varepsilon_{zz}}{E_g'}-\frac{\bar{b}_0\varepsilon}{2E_g'}]$$

The use of (194) can be written as

$$(E-\alpha_1)k_x^2+(E-\alpha_2)K_Y^2+(E-\alpha_3)k_z^2=t_1E^3-t_2E^2+t_3E+t_4 \qquad (195a)$$

where,

$$\alpha_1 \equiv [E_g-C_1\varepsilon-(\bar{a}_0+C_1)\varepsilon+\frac{3}{2}\bar{b}_0\varepsilon_{xx}-\frac{\bar{b}_0}{2}\varepsilon+(\frac{\sqrt{3}}{2})\varepsilon_{xy}\bar{d}_0],$$

$$\alpha_2 \equiv [E_g-C_1\varepsilon-(\bar{a}_0+C_1)\varepsilon+\frac{3}{2}\bar{b}_0\varepsilon_{xx}-\frac{\bar{b}_0}{2}\varepsilon-(\frac{\sqrt{3}}{2})\varepsilon_{xy}\bar{d}_0],$$

$$\alpha_3 \equiv [E_g-C_1\varepsilon-(\bar{a}_0+C_1)\varepsilon+\frac{3}{2}\bar{b}_0\varepsilon_{zz}-\frac{\bar{b}_0}{2}\varepsilon], t_1 \equiv (\frac{3}{2B_2^2}), t_2 \equiv (\frac{1}{2B_2^2})[6(E_g-C_1\varepsilon)+3C_1\varepsilon]$$

$$t_3 \equiv (\frac{1}{2B_2^2})[3(E_g-C_1\varepsilon)^2+6C_1\varepsilon(E_g-C_1\varepsilon)-2C_2^2\varepsilon_{xy}^2]$$

and

$$t_4 \equiv (\frac{1}{2B_2^2})[3-C_1^{\varepsilon}(E_g-C_1\varepsilon)^2+2C_2^2\varepsilon_{xy}^2].$$

The (195a) can be written as

$$Ek^2-T_{17}k_x^2-T_{27}k_y^2-T_{37}k_z^2=[q_{67}E^3-R_{67}E^2+V_{67}E+\rho_{67}] \qquad (195b)$$

where, $T_{17}=\alpha_1$, $T_{27}=\alpha_2$, $T_{37}=\alpha_3$, $t_1=q_{67}$, $t_2=R_{67}$, $t_3=V_{67}$ and $t_4=\rho_{67}$

Under the condition of heavy doping, (195b) can be written as

$$I(4)k^2-T_{17}I(1)k_x^2-T_{27}I(1)k_y^2-T_{37}k_z^2I(1)=[q_{67}I(6)-R_{67}I(5)+V_{67}I(4)+\rho_{67}I(1)] \qquad (1.195c)$$

where,

$$I(6)=\int_{-\infty}^{E}(E-V)^3F(V)dV \qquad (196)$$

The (186) can be written as

$$I(6)=E^3I(1)-3E^2I(7)+3EI(8)-I(9) \qquad (197)$$

In which,

$$I(7)=\int_{-\infty}^{E}VF(V)dV \qquad (198)$$

$$I(8)=\int_{-\infty}^{E}V^2F(V)dV \qquad (199)$$

$$I(9)=\int_{-\infty}^{E}V^3F(V)dV \qquad (200)$$

Using (4), together with simple algebraic manipulations, one obtains

$$I(7)=\frac{-\eta_g}{2\sqrt{\pi}}\exp(\frac{-E^2}{\eta_g^2}) \qquad (201)$$

$$I(8)=\frac{\eta_g^2}{4}[1+Erf(\frac{E}{\eta_g})] \qquad (202)$$

and

$$I(9)=\frac{-\eta_g^3}{2\sqrt{\pi}}\exp(\frac{-E^2}{\eta_g^2})[1+\frac{E^2}{\eta_g^2}] \qquad (203)$$

Thus (197) can be written as

$$I(6)=[\frac{E}{2}[1+Erf(\frac{E}{\eta_g})][E^2+\frac{3}{2}\eta_g^2]+\frac{\eta_g}{2\sqrt{\pi}}\exp(\frac{-E^2}{\eta_g^2})[4E^2+\eta_g^2]] \tag{204}$$

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

$$P_{11}(E,\eta_g)k_x^2+Q_{11}(E,\eta_g)k_y^2+S_{11}(E,\eta_g)k_z^2=1 \tag{205}$$

$$where,\ P_{11}(E,\eta_g)\equiv[\frac{\gamma_0(E,\eta_g)-(T_{17}/2)[1+Erf(E/\eta_g)]}{\Delta_{14}(E,\eta_g)}],$$

$$\Delta_{14}(E,\eta_g)\equiv[q_{67}\{\frac{E}{2}[1+Erf(E/\eta_g)][E^2+\frac{3}{2}\eta_g^2]+\frac{\eta_g}{2\sqrt{\pi}}\exp(\frac{-E^2}{\eta_g^2})[4E^2+\eta_g^2]\}$$

$$-R_{67}\theta_0(E,\eta_g)+V_{67}\gamma_0(E,\eta_g)+\frac{\rho_{67}}{2}[1+Erf(E/\eta_g)]],$$

$$Q_{11}(E,\eta_g)\equiv[\frac{\gamma_0(E,\eta_g)-(T_{27}/2)[1+Erf(E/\eta_g)]}{\Delta_{14}(E,\eta_g)}]$$

and

$$S_{11}(E,\eta_g)\equiv[\frac{\gamma_0(E,\eta_g)-(T_{37}/2)[1+Erf(E/\eta_g)]}{\Delta_{14}(E,\eta_g)}]$$

Thus, the energy spectrum in this case is real since the dispersion relation of the corresponding materials in the absence of band tails as given by (194) has no poles in the finite complex plane. The EMs along x, y and z directions in this case can be written as

$$m_{xx}^*(E_{F_h},\eta_g)=\frac{\hbar^2}{2}[[\gamma_0(E_{F_h},\eta_g)-(T_{17}/2)[1+Erf(E_{F_h},\eta_g)]]^{-2}[\Delta_{14}(E_{F_h},\eta_g)\}'[\gamma_0(E_{F_h},\eta_g)-(T_{27}/2)[1+Erf(E_{F_h},\eta_g)]]]$$

$$-\Delta_{14}(E_{F_h},\eta_g)[\frac{1}{2}[1+Erf(\frac{E_{F_h}}{\eta_g})]-\{\frac{T_{17}}{\eta_g\sqrt{x}}\exp(\frac{E_{F_h}}{\eta_g})\}]] \tag{206}$$

$$m_{yy}^*(E_{F_h},\eta_g)=\frac{\hbar^2}{2}[[\gamma_0(E_{F_h},\eta_g)-(T_{27}/2)[1+Erf(E_{F_h},\eta_g)]]^{-2}[\Delta_{14}(E_{F_h},\eta_g)\}'[\gamma_0(E_{F_h},\eta_g)-(T_{27}/2)[1+Erf(E_{F_h},\eta_g)]]]$$

$$-\Delta_{14}(E_{F_h},\eta_g)[\frac{1}{2}[1+Erf(\frac{E_{F_h}}{\eta_g})]-\{\frac{T_{27}}{\eta_g\sqrt{x}}\exp(\frac{E_{F_h}}{\eta_g})\}]]] \tag{207}$$

and

$$m_{zz}^*(E_{F_h},\eta_g)=\frac{\hbar^2}{2}[[\gamma_0(E_{F_h},\eta_g)-(T_{37}/2)[1+Erf(E_{F_h},\eta_g)]]^{-2}[\Delta_{14}(E_{F_h},\eta_g)\}'[\gamma_0(E_{F_h},\eta_g)-(T_{37}/2)[1+Erf(E_{F_h},\eta_g)]]]$$

$$-\Delta_{14}(E_{F_h},\eta_g)[\frac{1}{2}[1+Erf(\frac{E_{F_h}}{\eta_g})]-\{\frac{T_{37}}{\eta_g\sqrt{x}}\exp(\frac{E_{F_h}}{\eta_g})\}]]] \tag{208}$$

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

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

$$m_{xx}^*(E_F)=\hbar^2\bar{a}_0(E_F)\{\bar{a}_0(E_F)\}' \tag{209}$$

$$m_{xx}^*(E_F)=\hbar^2\bar{b}_0(E_F)\{\bar{b}_0(E_F)\}' \tag{210}$$

$$m_{xx}^*(E_F)=\hbar^2\bar{c}_0(E_F)\{\bar{c}_0(E_F)\}' \tag{211}$$

The DOS function in this case can be written as

$$N_{HD}(E,\eta_g)=\frac{g_v}{3\pi^2}\Delta_{100}(E,\eta_g) \tag{212}$$

where,

$$\Delta_{100}(E,\eta_g)\{\Delta_{15}(E,\eta_g)\}^{-2}[\frac{3}{2}\{\Delta_{15}(E,\eta_g)\}\sqrt{\Delta_{14}(E,\eta_g)}\{\Delta_{14}(E,\eta_g)\}'-\{\Delta_{14}(E,\eta_g)\}^{3/2}\{\Delta_{15}(E,\eta_g)\}']$$

$$\Delta_{15}(E/\eta_g)\equiv[[\gamma_0(E/\eta_g)-(T_{17}/2)[1+Erf(E/\eta_g)]][\gamma_0(E/\eta_g)-(T_{27}/2)[1+Erf(E/\eta_g)]]$$

$$[\gamma_0(E,\eta_g)-(T_{37}/2)[1+Erf(E/\eta_g)]]]^{1/2}$$

Using (212), the electron concentration at can be written as

$$n_0=\frac{g_v}{3\pi^2}[\bar{I}_{126}(E_{F_h},\eta_g)+\sum_{r=1}^{s}L(r)[\bar{I}_{126}(E_{F_h},\eta_g)]] \tag{213}$$

where,

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

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

$$P_{11}(E,\eta_g)k_x^2+Q_{11}(E,\eta_g)k_y^2+S_{11}(E,\eta_g)(\frac{\pi n_z}{d_z})^2\equiv 1 \tag{214}$$

The EM can be expressed as

$$m^*(E_{F1HD},\eta_g,n_z)=\frac{\hbar^2}{2}A'_{56}(E_{F1HD},\eta_g,n_z) \tag{215}$$

$$where,\ A_{56}(E,\eta_g,n_z)=\frac{\pi[1-S_{11}(E,\eta_g)(\frac{\eta_z\pi}{d_z})^2]}{\sqrt{P_{11}(E,\eta_g)Q_{11}(E,\eta_g)}}$$

From (215), it appears that the EM is a function of Fermi energy, and size quantum number and the same mass exists in the band gap.

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

$$N_{2DT}(E)=\frac{g_v}{2\pi}\sum_{n_z=1}^{n_{z\max}}A'_{56}(E_{F1HD},\eta_g,n_z) \tag{216}$$

The sub band energies $(E_{n_{z8HD}})$ are given by

$$S_{11}(E_{n_{z8HD}},\eta_g)(\pi n_z/d_z)^2=1 \tag{217}$$

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

$$N_{2D}(E)=\frac{g_v}{2\pi}\sum_{n_z=1}^{n_{\max}}[T_{57HD}(E_{F1HD},\eta_g,\eta_z)+T_{58HD}(E_{F1HD},\eta_g,\eta_z)] \qquad (218)$$

$$where,\ T_{57HD}(E_{F1HD},\eta_g,\eta_z)\equiv A_{56HD}(E_{F1HD},\eta_g,\eta_z)$$

$$and T_{58HD}(E_{F1HD},\eta_g,\eta_z)\equiv\sum_{r=l}^{s}L(r)T_{57HD}(E_{F1HD},\eta_g,\eta_z)$$

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

$$\frac{k_x^2}{[\bar{a}_0(E)]^2}+\frac{k_y^2}{[\bar{b}_0(E)]^2}+\frac{1}{[\bar{c}_0(E)]^2}(n_z\pi/d_z)^2=1 \qquad (219)$$

The area of 2D wave vector space enclosed by (219) can be written as

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

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

From (219), the EM can be written as

$$m^*(E_{F_s},n_z)=\frac{\hbar^2}{2}[P^2(E_{F_s},n_z)\bar{a}_0(E_{F_s})\bar{b}_0(E_{F_s})]' \qquad (220)$$

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

$$N_{2DT}(E)=(\frac{g_v}{2\pi})\sum_{n_z=1}^{n_{z\max}}\theta_6(E,n_z)H(E-E_{n_{z11}}) \qquad (221)$$

in which,

$$\theta_6(E,n_z)=[2P(E,n_z)\{P(E,n_z)\}'\bar{a}_0(E)\bar{b}_0(E)+\{P(E,n_z)\}^2\{\bar{a}_0(E)\}'\bar{b}_0(E)+\{P(E,n_z)\}^2\{\bar{b}_0(E)\}'\bar{a}_0(E)]$$

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

$$\bar{c}_0(E_{n_{z11}})=n_z\pi/d_z \qquad (222)$$

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

$$n_{2D}=\frac{g_v}{2\pi}\sum_{n_z=1}^{n_{z\max}}[T_{61}(E_{Fs},n_z)+T_{62}(E_{Fs},n_z)] \qquad (223)$$

where,

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

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

$$D_0(E)=g_v(3\pi^2)^{-1}\bar{T}_0(E) \qquad (224)$$

where

$$\bar{T}_0(E)=[\bar{a}_0(E)\bar{b}_0(E)[\bar{c}_0(E)]'+\bar{a}_0(E)\left[\bar{b}_0(E)\right]'\bar{c}_0(E)+[\bar{a}_0(E)]'\bar{b}_0(E)\bar{c}_0(E)]$$

Combining (224) with the Fermi-Dirac occupation probability factor and using the generalized Sommerfeld lemma the electron concentration in this case can be expressed as

$$n_0 = g_v (3\pi^2)^{-1}[M_4(E_F) + N_4(E_F)] \tag{225}$$

where,

$$M_4(E_F) \equiv [\bar{a}_0(E_F)\bar{b}_0(E_F)\bar{c}_0(E_F)] \text{and } N_4(E_F) \equiv \sum_{r=1}^{s} L(r) M_4(E_F)$$

Thus, we can summarize the whole mathematical background in the following way.

Thus, we can summarize the whole mathematical background in the following way.

In this Paper, we have investigated the 3D and 2D EMs from HD bulk and QWs of non-linear optical materials on the basis of a newly formulated electron dispersion law considering the anisotropies of the effective electron masses, the spin orbit splitting constants and the influence of crystal field splitting within the framework of **k.p** formalism. The results for 3D and 2D EMs from HD bulk and QWs of III-V, ternary and quaternary compounds in accordance with the three and two band models of Kane form a special case of our generalized analysis. We have also studied the EM in accordance with the models of Stillman et al. and Palik et al. respectively since these models find use to describe the electron energy spectrum of the aforesaid materials. The 3D and 2D EMs has also been derived for HD bulk and QWs of II-VI, IV-VI, stressed materials, by using various appropriate band models respectively on the basis of the appropriate carrier energy spectra. The well-known expressions of the EMs in the absence of band tails for wide gap materials have been obtained as special cases of our generalized analysis under certain limiting conditions. This indirect test not only exhibits the mathematical compatibility of our formulation but also shows the fact that our simple analysis is a more generalized one, since one can obtain the corresponding results for relatively wide gap materials having parabolic energy bands under certain limiting conditions from our present derivation

3. RESULT AND DISCUSSIONS

Using the appropriate equations together with parameters as given elsewhere [113], we have plotted the real part of the energy spectrum (Re$[\theta_1(E,\eta_g)]$) as a function of election energy in Fig. 2.1(a) and the Fig. 2.1(b) exhibits the dependence of the imaginary part of the energy spectrum Im $[\theta_1(E,\eta_g)]$ on electron energy for HD n-Cd_3As_2(an example of tetragonal materials), respectively.

From Fig. 2.1(a), it appears that Re$[\theta_1(E,\eta_g)]$ has an increasing trend with energy E for positive values of E. Besides for negative values of E, the value of Re$[\theta_1(E,\eta_g)]$ is positive indicating its band-tailing nature. Beyond E=-1.0(eV), the value of Re$[\theta_1(E,\eta_g)]$ becomes negative and magnitude of the values are insignificant one. It is worth remarking that the band-tailing nature of Re$[\theta_1(E,\eta_g)]$ is clearly apparent from the Fig. 2.1(a).

From Fig. 2.1(b), we observe that Im $[\theta_1(E,\eta_g)]$ has the Gaussian nature of variation with energy E for both positive and negative values of E. The values of Im $[\theta_1(E,\eta_g)]$ are negative for all the values of E as considered in Fig. 2.1(b). It may be remarked that the graph of Fig. 2.1(b) clearly shows the tailing of Im $[\theta_1(E,\eta_g)]$ into conduction band (i.e., for positive values of E) and the tailing within the spin-splitting band (i.e., for negative values of E) respectively. The maximum contribution of Im $[\theta_1(E,\eta_g)]$ appears at E=-0.25 (eV) for η_g =0.8 (eV) which is beyond the band gap E_g =0.095 (eV). From Fig. 2.2(a), we observe that the Re$[\theta_2(E,\eta_g)]$ has an increasing trend with positive value of E. For negative value of E, the Re$[\theta_2(E,\eta_g)]$ becomes positive exhibiting clearly the band-tailing nature of it. Besides beyond E=-1.0 (eV), the value of Re$[\theta_2(E,\eta_g)]$ becomes negative. In addition, the band-tailing nature of Re$[\theta_2(E,\eta_g)]$ is clearly apparent from the Fig. 2.2(a).

From Fig. 2.2(b), we can write that the nature of variation of the Im $[\theta_2(E,\eta_g)]$ versus E is quite different from Im $[\theta_1(E,\eta_g)]$. Here, Im $[\theta_2(E,\eta_g)]$ has a positive alues with positive variations of E. Also, the positive values of Im $[\theta_2(E,\eta_g)]$ for negative E indicate the band-tailing nature. Beyond E=-0.5 (eV), Im $[\theta_2(E,\eta_g)]$ becomes negative and the magnitude of the negative values are significant. The nature of variation of Im $[\theta_2(E,\eta_g)]$ is not Gaussian type but can roughly be approximated to it. This occurs for δ=0.085 (eV) (i.e., positive value of δ). Because for δ=-0.21 (eV) for $CdGeAs_2$, the nature of variation of Im $[\theta_2(E,\eta_g)]$is Gaussian. The contribution of Re$[\theta_2(E,\eta_g)]$ is of significant value as compared to Im $[\theta_2(E,\eta_g)]$. The band-tailing is clearly shown in the variation of Im $[\theta_2(E,\eta_g)]$.

From Fig. 2.3(a), it appears that the nature of variation of the real part of the electron energy spectrum for $CdGeAs_2$(an example of non-linear optical materials) is more or les same as that for the tetragonal materials as given by Fig. 2.1(a). In this case, the band tailing nature of variation of Re$[\theta_1(E,\eta_g)]$for $CdGeAs_2$ is clearly shown in the graph. From Fig. 2.3(b), it appears that the nature of variation of the imaginary part of the electron energy spectrum for non-linear optical materials is more or less the same as that for the tetragonal material as given by Fig. 2.1(b). The Gaussian distribution of Im $[\theta_1(E,\eta_g)]$ with respect of E is apparent from the graph and the band tailing is clearly shown.

From Fig. 2.4(a), we can write that the band tailing effect is clearly shown in the graph. From Fig. 4(b), it appears that the variation of Im $[\theta_2(E,\eta_g)]$ with respect to E is a Gaussian type with negative From Fig. 2.5, we can write that the curve (a) is valid for $\delta \neq 0$ and $\Delta_{\parallel} \neq \Delta_{\perp}$ for the case of Cd_3As_2 and the curve (b) is valid for $\delta = 0$, $\Delta = (\Delta_{\parallel} + \Delta_{\perp})/2$ and $\Delta_{\parallel} = \Delta_{\perp}$ to obtain the corresponding three band model of Cd_3As_2. The curve (a) shows that the DOS increases with the increase in the positive values of E. The band tailing is clearly being observed from the graph. The variation of Im $[\theta_2(E,\eta_g)]$with respect to E are unlike that with respect of Im $[\theta_2(E,\eta_g)]$for Cd_3As_2 because of the negative value of δ (-0.21(eV) in $CdGeAs_2$.

The curve (b) also shows the same nature and finally the curve (b) merges with the curve (a). For negative value of E, the curves (a) and (b) exhibit tailing in the DOS together with the oscillations. It is worth remarking in this context that at the value of E corresponding to point MN, curve (a) shows that the DOS becomes negative indicating the formation of a **new forbidden zone in the material**. The value of E at those points lie between -1.45 (eV) at M and -1.65 (eV) at N which corresponds to the region away or near to the spin-orbit splitting band of the material. Besides, beyond -1.65 (eV), the DOS becomes positive.

The oscillatory nature of the DOS for negative values of E has been predicted by the present theory. **Also for $\psi_{11}(E,\eta_g) \geq \pi$, the cosine function becomes negative indicating the negative value of the DOS and hence the creation of a new forbidden zone**. The curve (b) is widely separated from the curve (a) for negative values of E. Also, it shows oscillation in this region with two points, P and Q where the DOS for curve (b) shows negative value. For this value of the DOS, the new forbidden zone appears for the curve (b). The value of E at P is -1.45 (eV) and at Q is -1.58 (eV). Thereafter, the DOS again becomes positive. **The oscillatory nature of the DOS for the Curve (b),is also predicted by the present formulation.** For the curve (b), the new forbidden zone (i.e., PQ) appears earlier than the same for the curve (a). The band tailing in the DOS for the curves (a) and (b) are clearly indicated in the graph for negative values of E. In the plot, the value of the DOS has been normalized by (1.0 x 10^{20}) factor.

From Fig. 2.6, it appears that both the curves (a) and (b) of the DOS increase with increase in E and finally the curve (b) converges with the curve (a). For negative value of E, the curve (a) exhibits oscillations with positive values of the DOS. Two oscillation peaks have been shown to appear over the region of study of energy, E. For the curve (a), the value of the DOS becomes negative as indicated by the region (X,Y), where the new forbidden zone has appeared. Besides, beyond the point Y, the DOS becomes positive with an oscillatory nature. The value of E at X is $\approx$-1.68 (eV) and at Y is $\approx$-1.8 (eV). The curve (a) is being widely separated from the curve (b) for the negative values of E. In addition, the appearance of oscillations with the new forbidden zone in the DOS has also been predicted by the theory. The curve (b) also shows oscillation in the DOS as indicated in the figure. Between the point (R, S), the curve (b) shows negative values of the DOS indicating the formation of a new forbidden zone for the three band Kane model representation of $CdGeAs_2$. The value of E at point R is E=-1.7(eV) and at point Sis E $\approx$-1.8(eV). Besides beyond point S, the DOS becomes positive with oscillatory nature. The curve (b) is widely separated from the curve (a) for negative values of E. The band tailing in the DOS for the curves (a) and (b) is clearly indicated in the graph.

In Fig. 2.7, we have plotted the energy spectra of n-InSb where the graph 3_R indicates the real part $T_{31}(E,\eta_g)$ for the perturbed three-band model of Kane in which the curve 3_{Im} exhibits the imaginary part $T_{32}(E,\eta_g)$ .The curve 3_{up} indicates the unperturbed three-band model of Kane. The curve (2) has been EESawn for the perturbed two-band model of Kane in which 2up indicates the corresponding unperturbed EES). In Fig. 2.7, I indicate the perturbed parabolic band model and I_{up} exhibits the energy spectrum for unperturbed parabolic energy bands (i.e. $E=\hbar^2k^2/2m_c$).

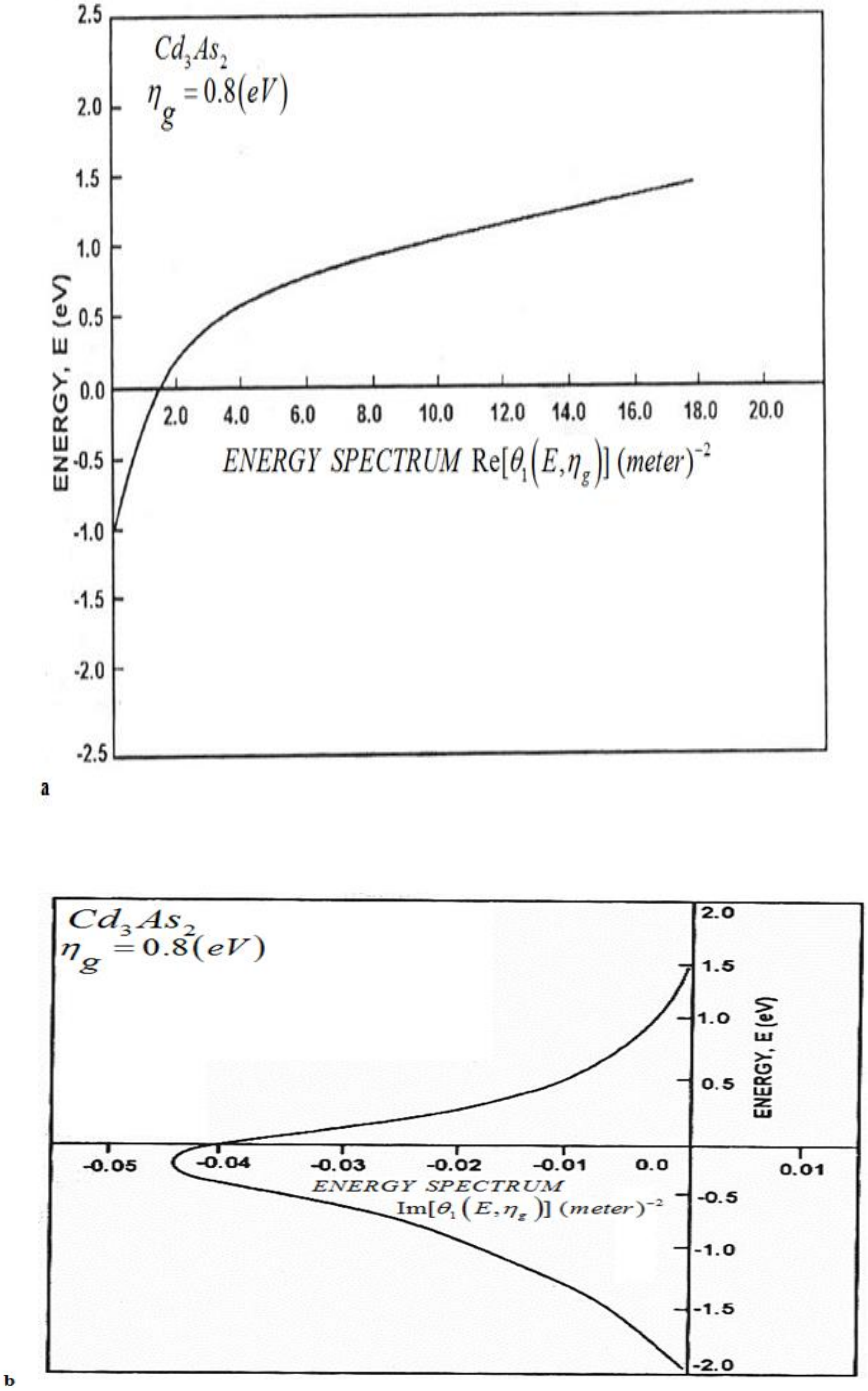

Fig. 2.1 (a) Plot of the electron energy spectrum of $\mathrm{Re}[\theta_1(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for Cd_3As_2. (b) Plot of the electron energy spectrum of $\mathrm{Im}[\theta_1(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for Cd_3As_2.

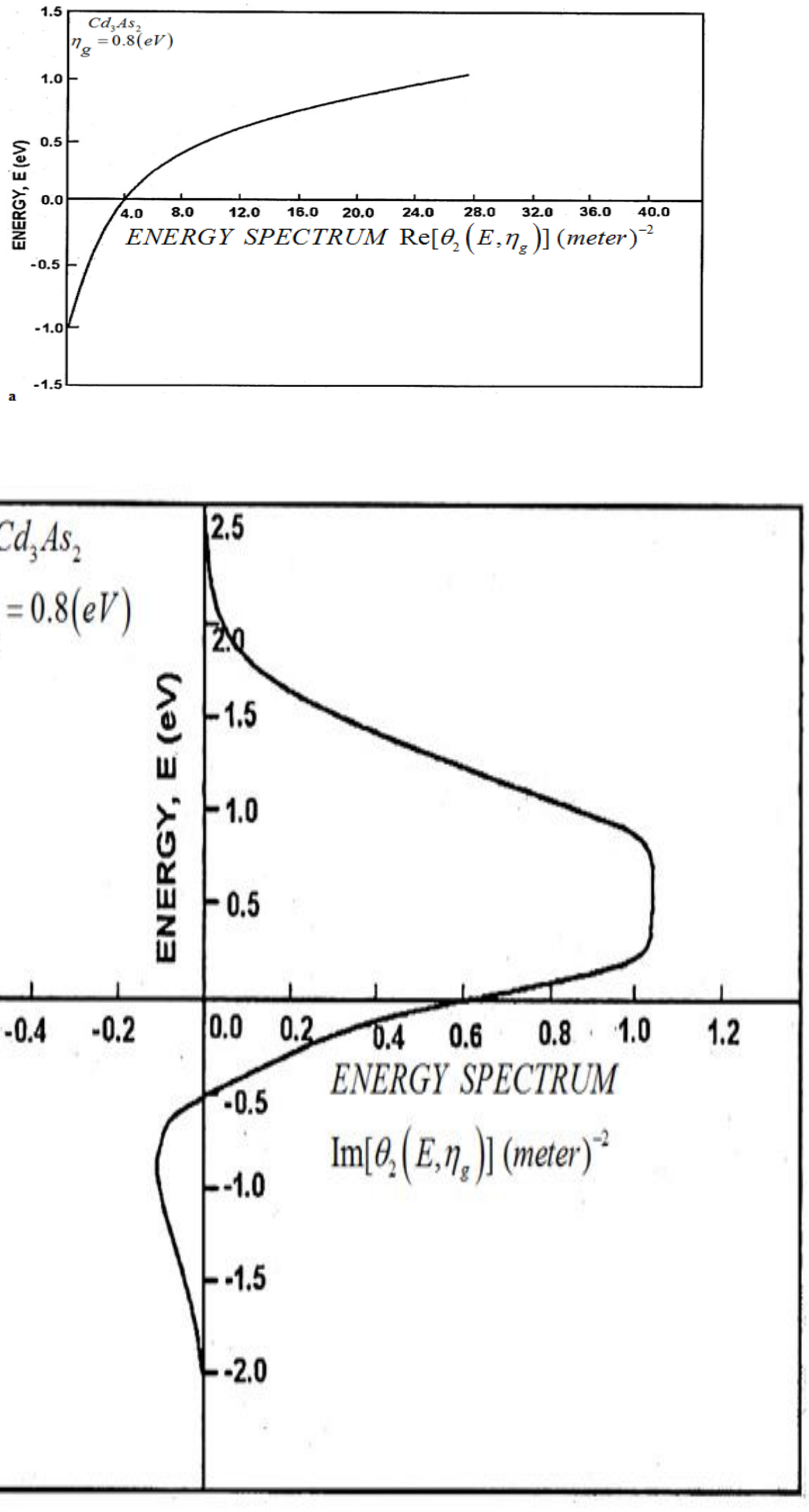

Fig.2.2(a) Plot of the electron energy spectrum of $\mathrm{Re}[\theta_2(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for Cd_3As_2. (b) Plot of the electron energy spectrum of $\mathrm{Im}[\theta_2(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for Cd_3As_2.

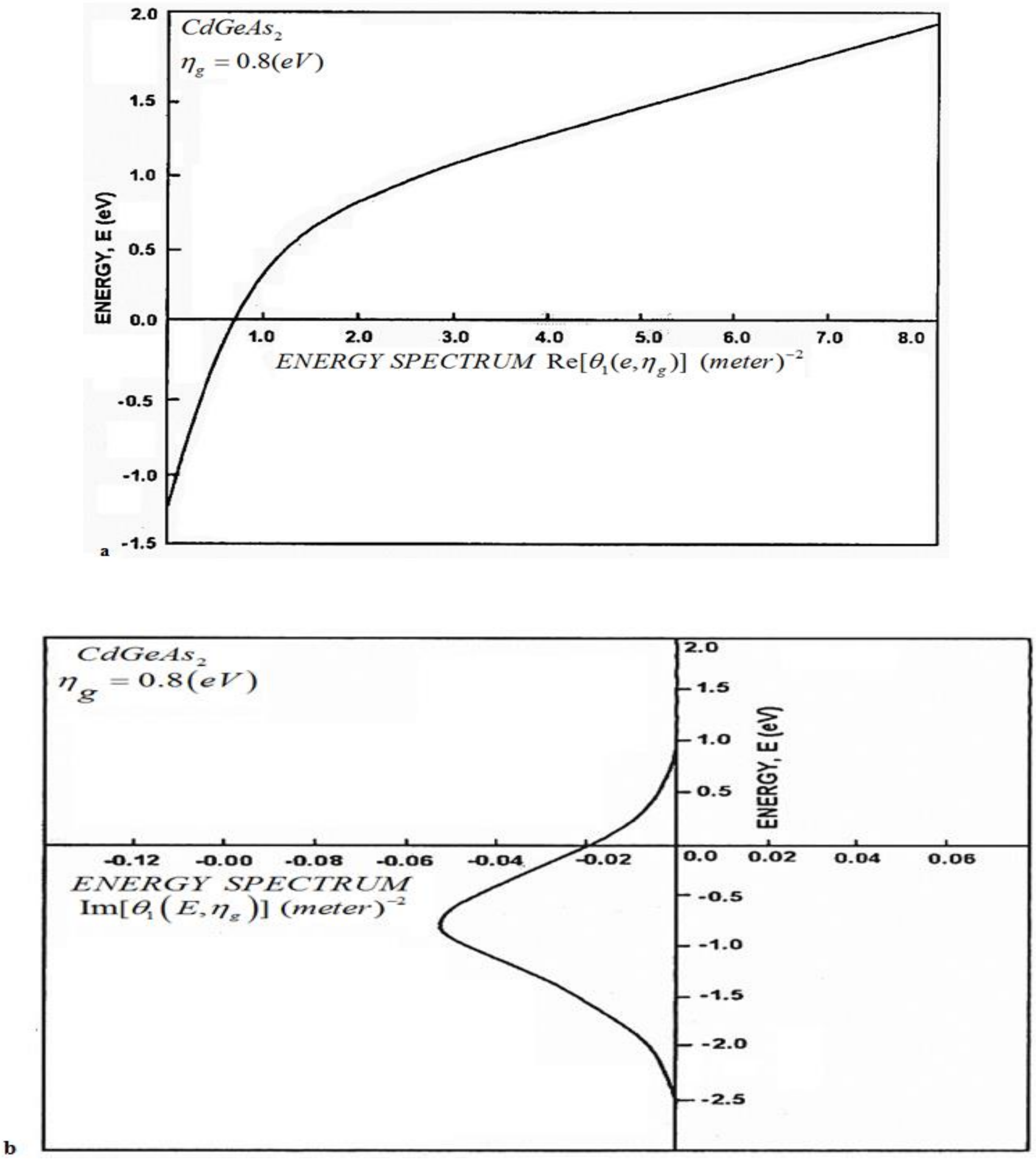

Fig. 2.3 (a) Plot of the electron energy spectrum of $\mathrm{Re}[\theta_1(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for CdGeAs$_2$. (b) Plot of the electron energy spectrum of $\mathrm{Im}[\theta_1(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for CdGeAs$_2$.

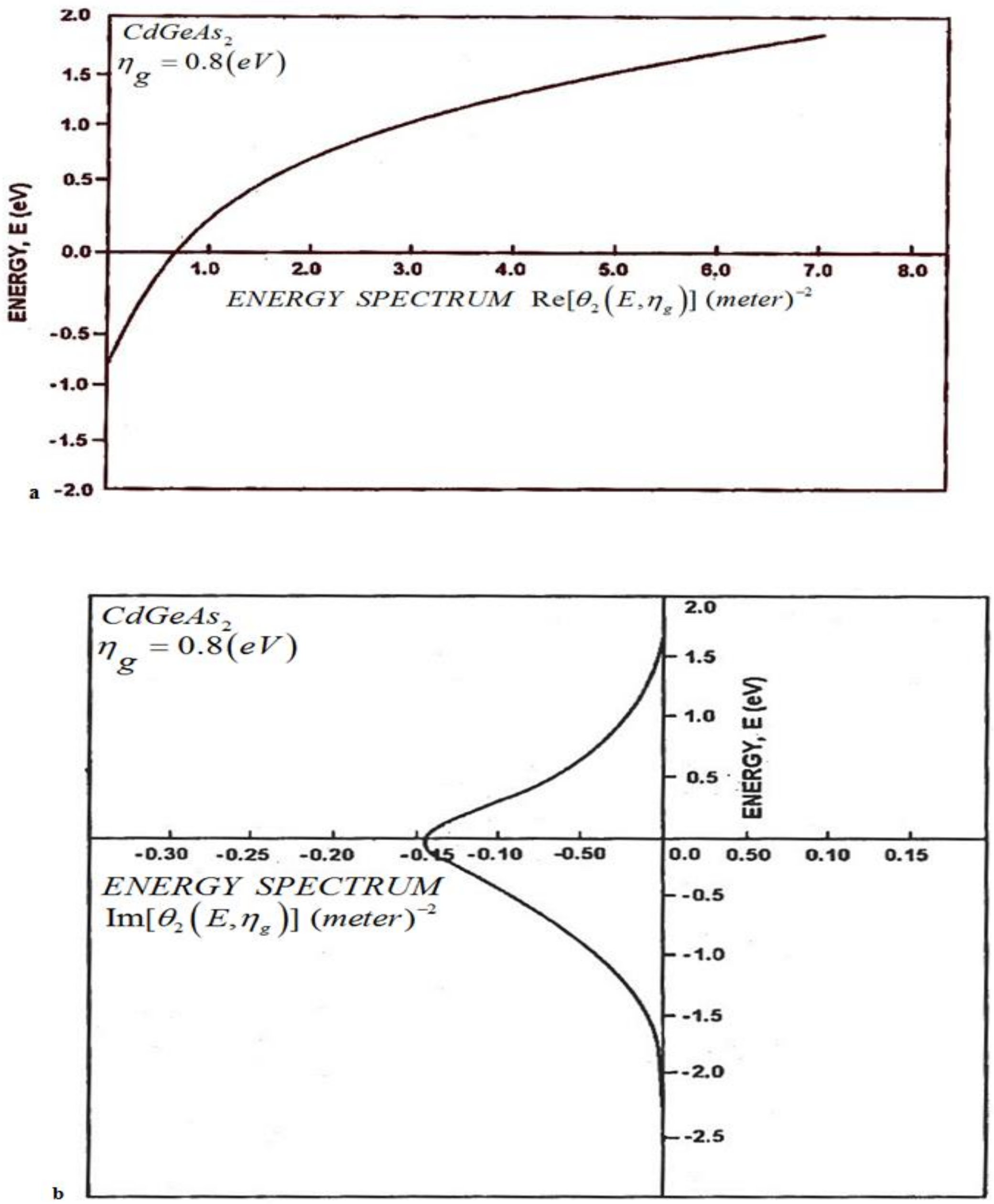

Fig. 2.4 (a) Plot of the electron energy spectrum of $\mathrm{Re}[\theta_2(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for CdGeAs$_2$. (b) Plot of the electron energy spectrum of $\mathrm{Im}[\theta_2(E,\eta_g)]$ (in m^{-2}) versus energy, E (eV) for CdGeAs$_2$.

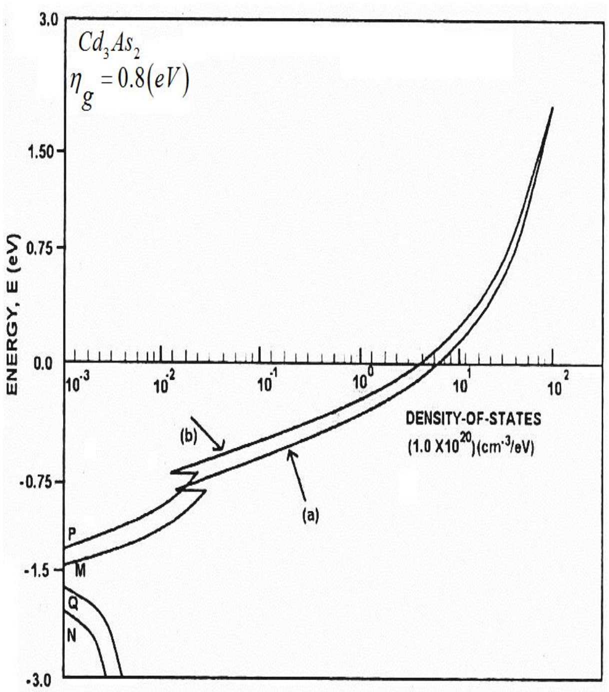

Fig. 2.5 The plots of the DOS, (cm^{-3}/eV) [normalized by 1.0 x 10^{20}] versus Energy, E (eV) for Cd_3As_2, (the curve (a)) and also for the HD three band Kane model of Cd_3As_2(curve (b)) respectively.

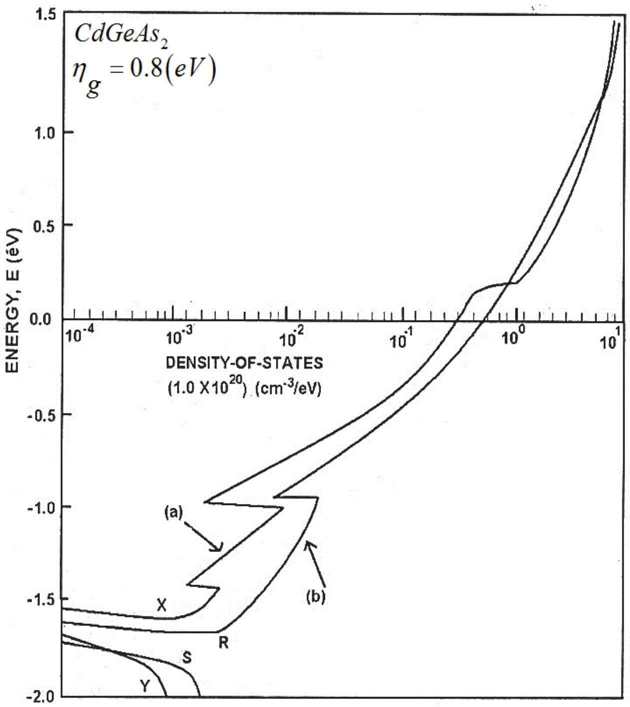

Fig. 2.6 The plots of the DOS, (cm^{-3}/eV) [normalized by 1.0 x 10^{20}] versus Energy, E (eV) for CdGeAs2, (the curve (a)) and also for the HD three band Kane model of $CdGeAs_2$(curve (b)) respectively.

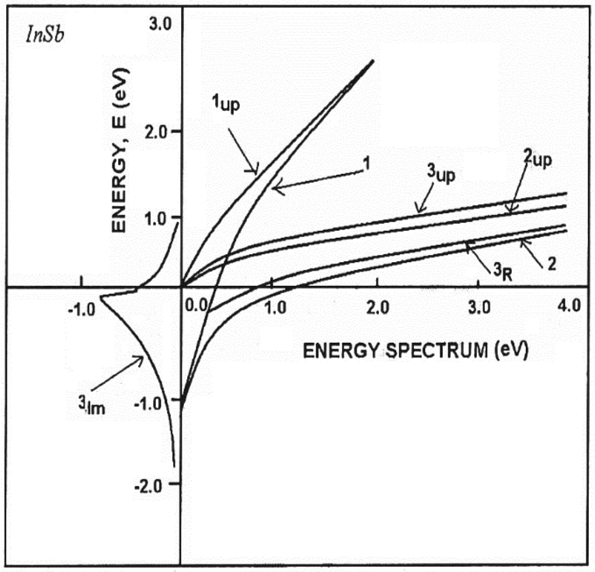

Fig. 2.7 The energy spectrum of InSb has been plotted with the following notations: (a) 3_R indicates the real part $T_{31}(E,\eta_g)$ for the perturbed three-band model of Kane; (b) 3_{Im} exhibits the imaginary part $T_{32}(E,\eta_g)$; (c) 3_{up} indicates the unperturbed three-band model of Kane; (d) (2) has been EESawn for the perturbed two-band model of Kane; (e) 2_{up} indicates the corresponding unperturbed EES; (f) I indicates the perturbed parabolic band model; (g)1_{up} exhibits the energy spectrum for unperturbed parabolic energy bands (i.e. $E=\hbar^2k^2/2m_c$).

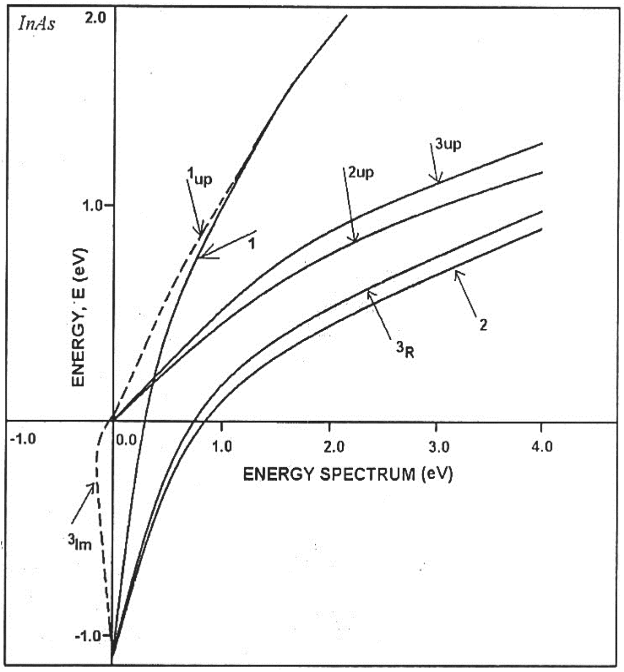

Fig. 2.8 The energy spectrum of InAs has been plotted for all the cases of Fig. 7

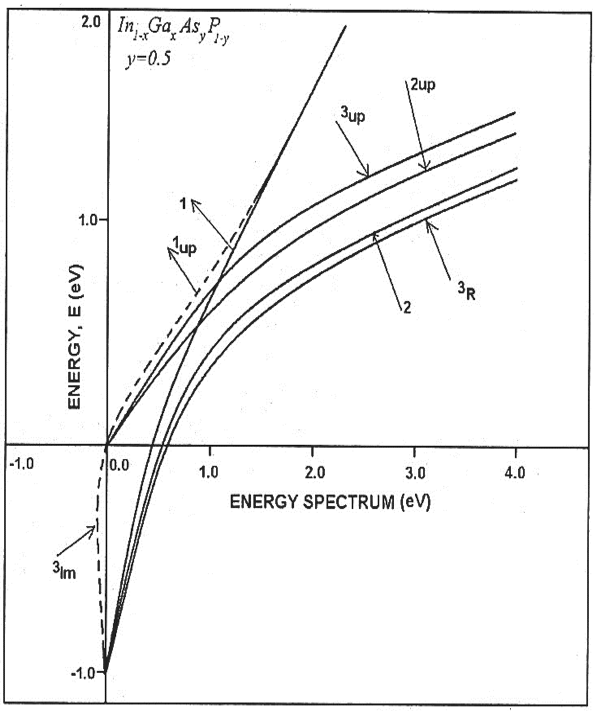

Fig. 2.9 The energy spectrum of $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InPhas been plotted for all the cases of Fig. 7

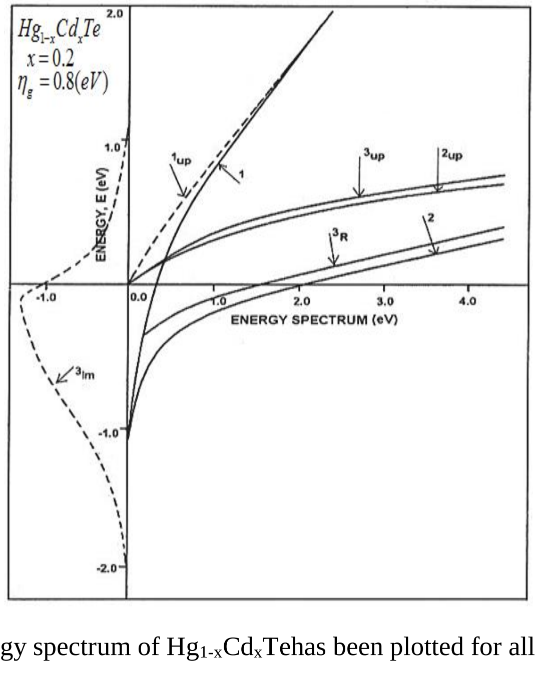

Fig. 2.10 The energy spectrum of $Hg_{1-x}Cd_xTe$has been plotted for all the cases of Fig. 7

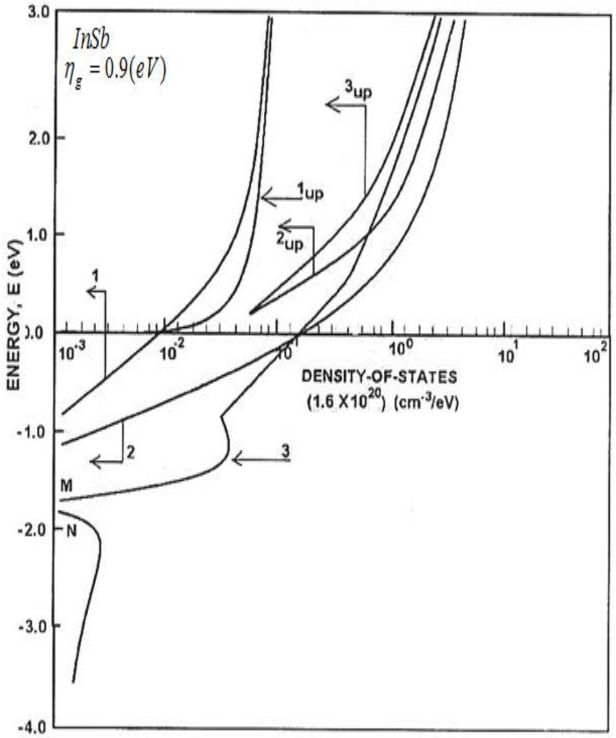

Fig. 2.11 The DOS functions have been plotted for all cases of Fig. 7 for n-InSb.

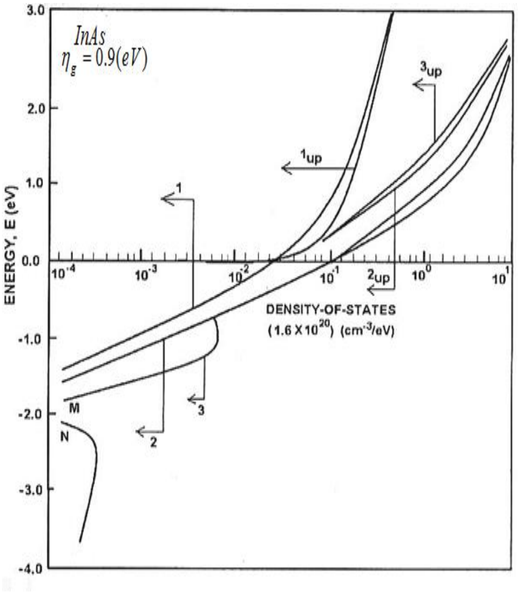

Fig. 2.12 The DOS functions have been plotted for all cases of Fig. 8 for n-InAs.

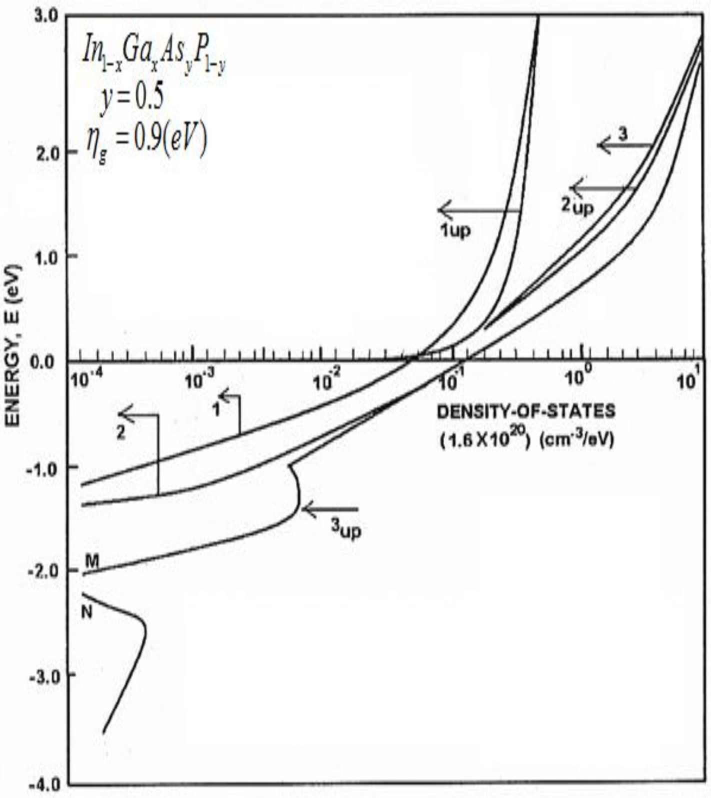

Fig. 2.13 The DOS functions have been plotted for all cases of Fig. 9 for $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP.

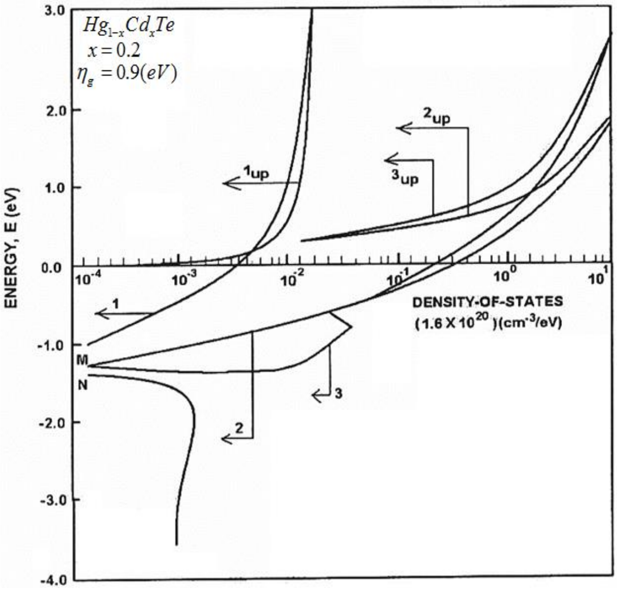

Fig. 2.14 The DOS functions have been plotted for all cases of Fig. 7 for $Hg_{1-x}Cd_xTe$.

Using the other material constants form the Table of the Appendixwe have plotted the EESs for n-InAs, $In_{1-x}Ga_xAs_yP_{1-y}$lattice matched to InP and $Hg_{1-x}Cd_xTe$ for all the cases of Fig. 2.7 in Figs. 8, 9, 10, respectively. In Figs. 11-14 we have plotted the DOS function for all cases of Fig. 7 for n-InSb, n-InAs, In_{1-x} $Ga_xAs_yP_{1-y}$ lattice matched to InP and $Hg_{1-x}Cd_xTe$, respectively. In this context, it may be noted that we have taken the first fifteen terms of the finite series in $T_{31}(E,\eta_g)$ for the purpose of numerical evaluations since we have observed that the contributions of the higher terms in the infinite series of $T_{31}(E,\eta_g)$ become negligible after it.

This statement is valid for all the cases in general. From Figs. 2.7-2.14, the following points can be noted:

1. When $E_g < \Delta$ (e.g. InSb and $Hg_{1-x}Cd_xTe$), the imaginary part of the energy spectrum (3_{Im}) is most prominent as compared to In_{1-x} $Ga_xAs_yP_{1-y}$ lattice matched to InP where $E_g < \Delta$. The imaginary part of energy spectrum enters in the conduction band where $E > 0$ (i.e. tails in the conduction band) as compared to the cases of n-InAs and In_{1-x} $Ga_xAs_yP_{1-y}$ lattice matched to InP where the tails are very small.
2. When the imaginary part (3_{Im}) is prominent (Figs. 2.1 and 2.3), the tails of the real part is shortened. The curves 3_{Im} exhibits tail of the conduction band and with this tail, the imaginary band enters into the region of conduction band ($E > 0$). For $Hg_{1-x}Cd_xTe$ and n-InSb, the 3_{Im}tails in to the split-off band.
3. When the EESs of the conduction electrons of the materials are defined by the perturbed two-band model of Kane, the imaginary part of the energy spectrum vanishes. The same is also true for perturbed parabolic band model. The unperturbed bands never exhibit tails in the energy spectrum.
4. The $\mathrm{N}_{HD}(E,\eta_g)$ as given by (1.43) shows oscillations with E for $E < 0$. The oscillatory part is not seen in Fig. 2.11 for $E > 0$. This is because, for $E < 0$, $\left|\mathrm{T}_{32}(E,\eta_g) \square \ \mathrm{T}_{31}(E,\eta_g)\right|$. So $\vartheta_{21}(E,\eta_g)$ is equal to zero leading to the non-oscillatory result Cos $\vartheta_{21}(E,\eta_g) \approx 1$ for $E > 0$. For $E < 0$, the value of $\vartheta_{21}(E,\eta_g)$ is significant and oscillations are found for $\mathrm{N}_{HD}(E,\eta_g)$ for $E > 0$, as evident from Fig. 2.11. For $\vartheta_{21}(E,\eta_g) \geq \pi$, Cos $\vartheta_{21}(E,\eta_g)$ becomes negative leading to the negative values of the DOS. The boundary points M and N in the graph mark the points where the DOS become negative. The electrons cannot exist for negative values of the DOS so this region is forbidden for electrons, which implies that, in the band-tails, there appears a new forbidden zone in addition to the normal band-gap of the semiconductor. It appears beyond the spin-orbit splitting band. No oscillations are found for the perturbed two band model of Kane and perturbed parabolic energy

bands respectively although there is tailing in the DOS. For $\eta_g \to 0,$ the oscillations and the appearance of new band gap in the tailed zone of the DOS are absent.

Form the above discussion, we observed that $\mathrm{T}_{31}(E,\eta_g)$ has a tail in the forbidden band and extended further. As this tail crosses the forbidden band (when $\mathrm{T}_{31}(E,\eta_g)$ $\mathrm{T}_{31}(E,\eta_g)$ does not vanish in the forbidden band for small E_g) and enters in to the split-off band where Δ exists and in the split-off band the tail vanishes, leaving behind some part of it to cross; then the remaining part of the split-off band interacts with the impurity atoms of the doped materials to produce a complex band. This interaction produces complex energy spectrum in the heavily doped materials whose unperturbed conduction electron are defined by the three-band model of Kane. Obviously for E_g □ $\Delta,$ the imaginary part of the complex energy spectrum will be most prominent and depth of the tail will be small. In the case when E_g □ $\Delta,$ the tails due to $\mathrm{T}_{31}(E,\eta_g)$ (i.e. the real part) lies almost within the forbidden region; only a very thin tail enters into the spin-split off band. This causes a prominent tail of $\mathrm{T}_{31}(E,\eta_g)$ and imaginary part is slightly present. For $E_g \approx \Delta$ (e.g, n-InAs shown in Fig. 2.8), the tail of $\mathrm{T}_{31}(E,\eta_g)$ is present considerably in the forbidden band, but $\mathrm{T}_{31}(E,\eta_g)$ does not vanishes to zero at the edge of the light-hole valance band where forbidden band ends; rather enters in to the split-off band. In the split-off band (when Δ is comparable to E_g), the tail covers the band considerably. So the tail due to $\mathrm{T}_{31}(E,\eta_g)$ and the imaginary energy spectrum due for to $\mathrm{T}_{32}(E,\eta_g)$ are present prominently.

So from Figs. 2.7-2.10, we observe that the complex energy spectrum is due to the interaction of the impurity atoms with the spin orbit splitting constant of the valance band for the three-band model of Kane where no real energy band as well as impurity band exist. More is the interaction (depends on the cross over region of Δ by the tail) causes more prominence of the imaginary part than the other case. Under undoped condition the band-tailing vanishes and there is no interaction with the splitting band. As a result, there exist no complex energy spectrum i.e. $\mathrm{T}_{32}(E,\eta_g)$ approaches to zero as $\eta_g \to 0.$

From the 2D EES in QWs of HD nonlinear optical and tetragonal materials (32), we observe that constant energy 2D wave vector surfaces are the series of concentric quantized circles in the complex energy plane which is the consequence of non-removable poles in the corresponding EES in the absence of band tails. The (174) represents the 2D EES of HD IV-VI materials in accordance with the model of Bangert and Kastner and same conclusion is also valid. From (43) we have the same inference for QWs of HD III-V materials whose unperturbed conduction electrons obey the three band model of Kane, which contains one non-removal pole in energy axis. The 3D electrons in HD III-V materials are also described by two band model of Kane, parabolic energy bands, model of Stillman et al and the model of Palik et al with the 2D EESs as given by (61), (78), (92) and (108) respectively. Since all the said EESs possess no poles in the finite energy planes, the constant energy of 2D wave vector surfaces are the series of

concentric quantized circles in the real plane instead of the complex one. The 2D EES (123) in HD II-VI materials reflects the fact that the constant energy 2D surface is series of concentric displaced quantized circles in the real plane. The 2D EES (153) of HD IV-VI materials represents constant energy 2D wave vector surface as the series of concentric quantized closed surfaces in accordance with Dimmock model. The 2D EES (214) in QWs of HD stressed Kane type materials reflects the fact that the constant energy 2D wave vector surfaces are the series of concentric ellipses in the real plane.

The influence of quantum confinement is immediately apparent from the said 2D equations since the EES depends strongly on the thickness of the quantum-confined materials in contrast with the corresponding bulk specimens. The energy decreases with increasing film thickness in an quantized way with different numerical magnitudes for QWs of HD materials. It appears that any electronic property exhibits spikes for particular values of film thicknesswhich, in turn, depends on the particular band structure of the specific material. Moreover, the electron energy in QWs of HD compounds can become several orders of magnitude larger than of bulk specimens of the same HD materials, which is also a direct signature of quantum confinement.

It may be noted that with the advent of MBE and other experimental techniques, it is possible to fabricate quantum-confined structures with an almost defect-free surface.If the direction normal to the film was taken differently from that as assumed in this work, the expressions for the EES forQWs of HDmaterials would be different analytically, since the basic EESs for many materials are anisotropic. In formulating the generalized electron energy spectrum for non-linear optical materials, we have considered the crystal-field splitting parameter, the anisotropies in the momentum-matrix elements, and the spin-orbit splitting parameters, respectively. In the absence of the crystal field splitting parameter together with the assumptions of isotropic effective electron mass and isotropic spin orbit splitting, our basic relation as given by (2) converts into the well-known three-band Kane model and is valid for III-V compounds, in general. It should be used as such for studying the electronic properties of n-InAs where the spin-orbit splitting parameter (Δ) is of the order of band gap (E_g). For many important materials $\Delta >> E_g$ and under this inequality, the three band model of Kane assumes the form $E(1+EE_g^{-1}) = \hbar^2 k^2 / 2m_c$ which is the well-known two-band Kane model. Also under the condition, $E_g \to \infty$, the above equation gets simplified to the well-known form of parabolic energy bands as $E = \hbar^2 k^2 / 2m_c$. It is important to note that under certain limiting conditions, all the results for all the models as derived here have transformed into the well-known expression of the EES for size quantized materials having parabolic bands. We have not considered other types of compounds or external physical variables for numerical computations in order to keep the presentation brief.

It may be noted that the complex band structures have already been studied for bulk materials and superlattices without heavy doping[114, 115] and bear no relationship with the complex energy spectrum as formulated in this Paper. The physical picture behind the formulation of complex energy spectrum in doped small gap materials, whose unperturbed conduction band is defined by the three band model of Kane, is the interaction of the impurity atoms in the tails with the spin-orbit splitting constant of the valence band as already noted. Besides, the complex spectra are not related to same evanescent modes (extinction modes) in the band tails and the conduction band. In this context, we wish to further note that many band tails models are proposed using the Gaussian distribution of the impurity potential variation. In this Paper we have used the Gaussian distribution function of the impurity potential and obtained an exact EES for heavily doped nonlinear optical and tetragonal compounds and other materials forming band tails. Our method is not at all related with the DOS technique as used in the aforementioned works. From the EES we can obtain the DOS but the DOS technique as used in the literature [114, 115] cannot provide the EES. 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 semiconductor devices, can be solved if and only if the EES is known. In this context it may be noted that although we have used the Gaussian model to explain the band tailing in heavily doped materials but it is not the only well-established one.

It may be noted that the presence of non-removable poles in the EES of the undoped material creates the complex energy spectrum of the corresponding heavily doped sample. All investigations of the transport properties of modern electronic devices made of heavily doped materials should be reformulated since the Boltzmann transport equation which controls all the transport properties should be solved at first for complex energy spectrum which is altogether a new field of research. Consequently, all the band structure dependent properties of all the electronic devices made of heavily doped materials will change leading to new physical ideas and new experimental findings under different physical conditions. We have not considered the many body effects in this simplified theoretical formalism due to the lack of availability in the literature of proper analytical techniques for including them in the generalized system as considered in this Paper. Our simplified approach will be useful for the purpose of comparison when methods of tackling the formidable problem after inclusion of the many body effects for the generalized systems appear. It is worth remarking in this context that the results of our simple theory, in the limit the band gap tends to infinity, get transformed to the well-known formulation for wide gap materials having parabolic energy bands. This indirect test not only exhibits the mathematical compatibility of our formulation but also shows the fact that our simple analysis is a more generalized one, since one can obtain the corresponding results for the relatively wide gap materials having parabolic energy bands under certain limiting conditions from our present derivation. The experimental results for the verification of the theoretical analyses of this Paper are still not available in the literature. It may be noted in this context that our theoretical formulation will be useful to analyze the experimental data when they appear. The inclusion of the said effect would certainly increase the accuracy of the results, although the qualitative features of the DOS discussed in this Paper would not change in the presence of the aforementioned effect. An important feature of the present work is that the influence of the energy band parameters on the EES and the DOS can be determined for various types of HD materials as considered in this Paper.

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