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A SIMPLE ANALYSIS OF THE THERMOELECTRIC POWER IN QUANTUM WIRES OF NON-PARABOLIC SEMICONDUCTORS IN THE PRESENCE OF CROSSED ELECTRIC AND MAGNETIC FIELDS

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In this paper a study is made of the thermoelectric power of electrons in quantum wires of nonparabolic semiconductors in the presence of crossed electric and magnetic fields on the basis of a newly derived electron dispersion law considering all types of anisotropies of the energy spectrum. It is found, taking n-CdGeAs$_2$ as an example, that the thermopower increases with increasing film thickness, magnetic field and electric field, respectively. The crystal field splitting enhances the thermopower with respect to all physical variables. In addition, the corresponding expressions for quantum wires of parabolic semiconductors have also been obtained from our generalized analysis under certain limiting conditions.

1. *Introduction*

With the advent of fine lithographical methods [1], molecular beam epitaxy [2], organo-metallic vapour-phase epitaxy [3] and other experimental techniques, low-dimensional structures [4,5] in the last few years attracted much attention not only for their potential in uncovering new phenomena in physical electronics but also for their interesting device applications [6]. In quantum well wires (QWW's) the electron gas is quantized in two transverse directions and charge carriers are free to move only in the single free direction. The potential use of these synthetic lD materials for high speed devices under different physical conditions makes the knowledge of their appropriate band structure desirable. It appears from the literature that the thermoelectric power of electrons (TPE) in QWW's in the presence of crossed electric and magnetic fields has yet to be investigated even for parabolic energy bands. With the advent of quantum Hall effect [7] there has been considerable interest in studying the TPE in quantized materials.

We have used the ternary chalcopyrite semiconductors having non-parabolic and non-standard energy band as an example of non-parabolic materials. We shall work out the problem for the more interesting case which occurs from the presence of various types of anisotropies of the energy spectrum. This will make our analysis a generalized one since we can obtain the TPE in QWW's of even parabolic semiconductors. Rowe and Shay [8] have demonstrated that the quasicubic model [9] can be used to explain the observed splitting and symmetry properties of the conduction and valence bands at the zone center of the ternary chalcopyrite semiconductors. The s-like conduction band is single degenerate and the p-like valence bands are triply degenerate. The latter splits into three subbands because of spin-orbit and crystal field interactions. The largest contribution to the crystal field splitting of the valence band occurs from the non-cubic potential [10]. The experimental data on the absorption constant [11], the effective masses [12], and the third order optical susceptibility [13] have produced strong evidence that the conduction band in the same semiconductor corresponds to a single ellipsoid of revolution at the zone center in $\vec{k}$ space. Incorporating the anisotropic crystal potential to the Hamiltonian, Kildal [11,14] proposed an E-$\vec{k}$ dispersion relation of the conduction electrons in the same semiconductor based on the assumptions of isotropic spin-orbit splitting parameters and isotropic interband momentum-matrix elements, respectively, though the anisotropies in the two aforementioned band parameters are significant physical features of the ternary chalcopyrite semiconductors [15].

In what follows, in Section 2.1. we shall derive the TPE in QWW of ternary chalcopyrite materials under cross-field configuration by using the generalized dispersion relation of the conduction electrons incorporating the above mentioned anisotropies as derived elsewhere [16]. In Section 2.2, we shall give the limiting cases of three-band Kane model, two-band model and that of parabolic energy bands in QWW's. We study the dependence of the TPE in QWW's of non-parabolic semiconductors in the presence of crossed electric and magnetic fields on electron concentration, electric and magnetic field strength and thickness. We take QWW's of n-CdGeAs$_2$ as an example.

2. *Theoretical background*

2.1. *Thermoelectrical power of electrons in quantum well wires*

The generalized dispersion relation of the conduction electrons, incorporating the aforementioned anisotropies of the energy bands in bulk specimens of ternary chalcopyrite semiconductors, can be expressed [16] as

$$U(E) = p_s^2/2M_\perp + p_z^2 V(E)/2M_\parallel \tag{1}$$

where $U(E) = [E(1+\alpha E)\{(E+E_g)(E+E_g+\Delta_\parallel) + \delta(E+E_g+\frac{2}{3}\Delta_\parallel) + \frac{2}{9}(\Delta_\parallel^2 - \Delta_\perp^2)\}]/\zeta(E)$, E is the electron energy as measured from the edge of the conduction band in the vertically upward direction in the absence of any quantization, $\alpha = 1/E_g$, E_g is the band gap, $\zeta(E) = [(E+E_g)(E+E_g+\frac{2}{3}\Delta_\parallel + \delta(E+E_g+\frac{2}{3}\Delta_\parallel) + \frac{1}{9}(\Delta_\parallel^2 - \Delta_\perp^2)]$, $\Delta_\parallel$ and $\Delta_\perp$ are the spin-orbit splitting parameters parallel and perpendicular to the direction of the c-axis, respectively, δ is the crystal field splitting parameter, $\vec{p}_s = \hbar\vec{k}_s$, $\hbar = h/2\pi$, h is the Plancks constant, $k_s^2 = k_x^2 + k_y^2$, $M_{\parallel,\perp} = m_{\parallel,\perp}^*[(E_g+\frac{2}{3}\Delta_{\parallel,\perp})[(E_g+\Delta_{\parallel,\perp})]^{-1}]$, $m_\parallel^*$ and $m_\perp^*$ are the band edge effective electron masses along and perpendicular to the direction of the c-axis, $\vec{p}_z = \hbar\vec{k}_z$ and $V(E) = [(E+E_g)(E+E_g+\frac{2}{3}\Delta_\parallel)]/\zeta(E)$.

Thus, extending the method as given in the literature [17], the modified electron energy spectrum in QWW of the same materials in the presence of crossed electric field E_0 along x-axis and magnetic field B along z-axis can be written as

$$f + (q^2/2)\sin^{-1}(\psi) = eB\pi\hbar l \tag{2}$$

where the symbols are defined in Appendix A.1. The use of (2) leads to the expression for electron concentration n_0 as,

$$F + \frac{1}{2}Q^2\sin^{-1}(\Phi) = eB\pi\hbar l \tag{3}$$

where the symbols are defined in Appendix A.2.

The TPE in the present case can be expressed as

$$D = s_0/en_0 \tag{4a}$$

where s_0 is the entropy in the present case. Then using (3) and (4a) we get

$$D = (\pi^2 k^2 T/3en_0)(q_1/q_2) \tag{4b}$$

where the symbols are defined in Appendix A.3.

2.2. *Special cases*

1. Under the conditions $\delta = 0$, $\Delta_{\parallel} = \Delta_{\perp} = \Delta$ (the isotropic spin-orbit splitting parameter) and $m^*_{\perp} = m^*_{\parallel} = m^*$ (the isotropic effective electron mass at the edge of the conduction band), (1) assumes the form

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E), \qquad \gamma(E) = \frac{E(E+E_g)(E+E_g+\Delta)(E_g+\frac{2}{3}\Delta)}{E_g(E+E_g+\frac{2}{3}\Delta)(E_g+\Delta)} \tag{5}$$

which is the three-band Kane model [18] for III-V semiconductors, and ternary and quaternary alloys. It is used in this form for the study of electronic properties of n-InAs where $\Delta \simeq E_g$. Thus with the above mentioned substitutions, the electron statistics and the TPE can, respectively, be expressed as

$$F_1 + \frac{1}{2}Q_1^2 \sin^{-1}(\Phi_1) = eB\pi\hbar l \tag{6}$$

and

$$D = (\beta_1/\beta_2)(\pi^2 k_B^2 T/3en_0) \tag{7}$$

where the notations are defined in Appendix A.4.

2. Under the conditions $\Delta \gg E_g$ (e.g. in n-InSb, n-HgTe) or $\Delta \ll E_g$ (e.g. n-InP, n-GaAs), (5) assumes the form

$$E(1+\alpha E) = \hbar^2 k^2/2m^*, \qquad \alpha = 1/E_g \tag{8}$$

which is the two-band Kane model [19]. Therefore in this case, the basic forms of (6) and (7) will not change where $\gamma(E) = E(1+\alpha E)$ and $\psi_0(E) = (1+2\alpha E)$. Finally under the condition $\alpha \to 0$, as for wide band gap materials, the forms (6) and (7) remain same where $\gamma(E) = E$ and $\psi_0(E) = 1$.

3. *Results and discussion*

Using the appropriate equations together with the parameters [14] $m^*_{\parallel} = 0.030m_0$, $m^*_{\perp} = 0.039m_0$, $\Delta_{\parallel} = 0.34$ eV, $\Delta_{\perp} = 0.36$ eV, $\delta = -0.21$ eV, $E_g = 0.57$ eV, $E_0 = 10^3$ V/m, $B = 3.5$ T, $d_1 = 40$ nm and $d_2 = 60$ nm, we have calculated the normalised TPE as a function of electron concentration. The results are shown as curve a in Fig. 1. For the purpose of comparison, curve b in Fig. 1 shows the same dependence, but taking the crystal field parameter as zero. In addition, in Fig. 1, curve c corresponds to the degenerate three-band Kane model of n-CdGeAs$_2$ (taking $\Delta = 0.35$ eV and $m^* = 0.34m_0$ for the purpose of numerical computations). We have also plotted the TPE according to with two-band Kane model and that of parabolic energy bands, using the same parameters as in the calculations of results shown in Fig. 1. We have presented the TPE as functions of film thickness (taking square QWW), magnetic field and electric field as shown in Figs. 2, 3 and 4, respectively. The various simplified limiting cases have further been considered for the purpose of assessing the influence of energy band models on the TPE in QWW's of nonparabolic materials.

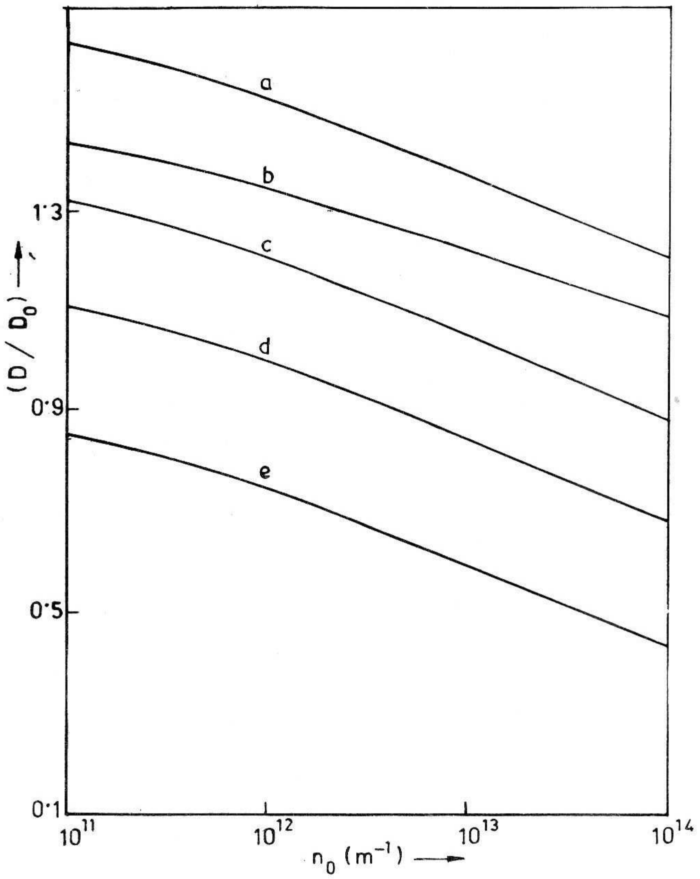

Fig. 1. Plot of the normalized TPE as a function of the electron concentrations per unit length under cross field configuration in QWW of n-CdGeAs$_2$*: curve a, our proposed dispersion relation; curve b,* $\delta = 0$, *curve c, the three-band Kane model, curve d, the two-band Kane model, curve e, the parabolic energy bands.*

It appears from Fig. 1 that the TPE decreases with increasing electron concentration at a rate lower than in the case $\delta = 0$. Moreover, for relatively low values of the electron concentration, the effect of crystal field splitting decreases wheras the same parameter affects significantly the TPE for relatively large values of the carrier degeneracy. The TPE increases with increasing thickness, magnetic field and electric field is shown in Figs. 2, 3 and 4, respectively. The TPE exhibits largest value with respect to all the variables in accordance with our proposed generalized

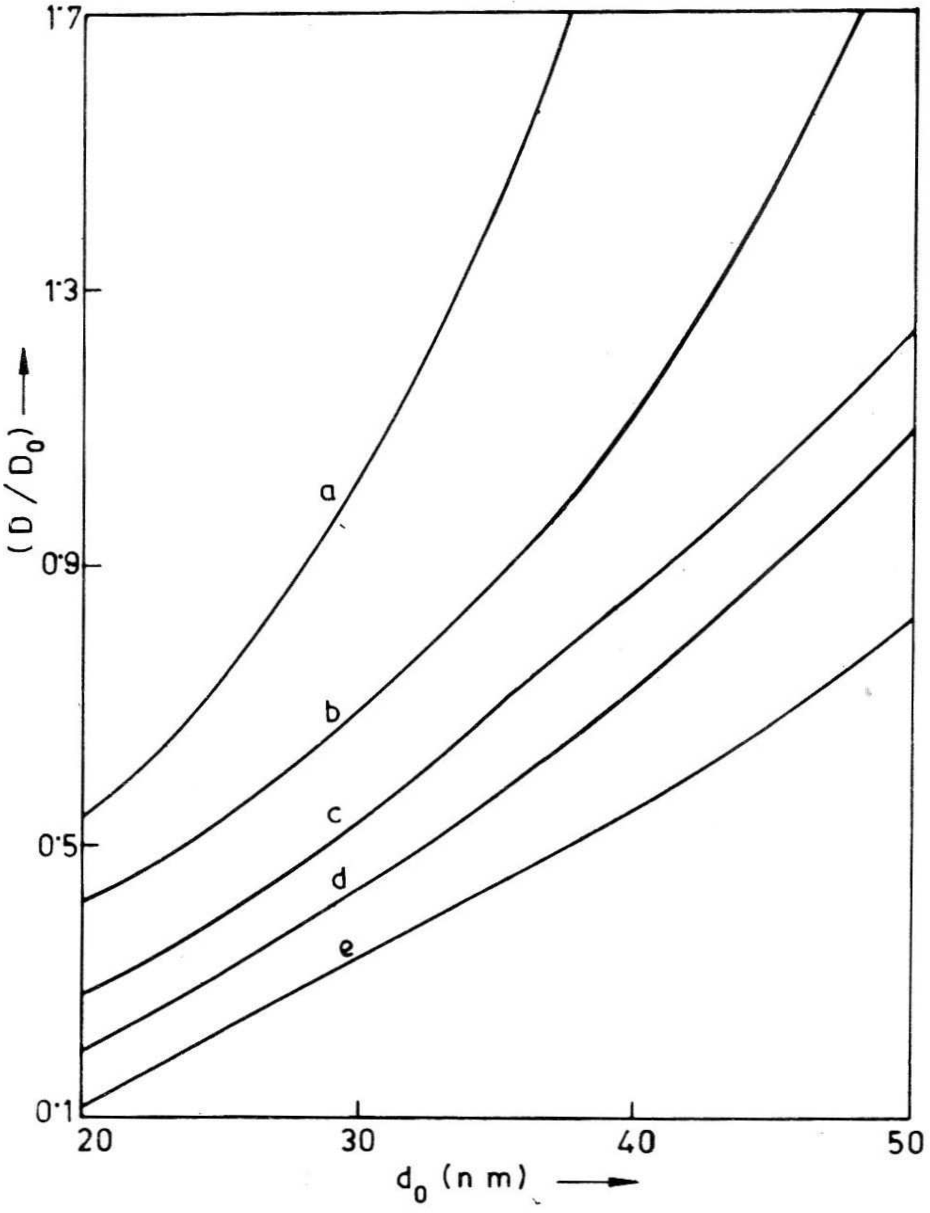

Fig. 2. Plot of the normalized TPE as function of the film thickness (assuming square QWW) under cross field configuration in QWW of n-CdGeAs$_2$: curve a, our proposed dispersion relation; curve b, $\delta = 0$; curve c, the three-band Kane model; curve d, the two-band Kane model; curve e, the parabolic energy bands. ($n_0 = 10^{16}\,\mathrm{m}^{-1}$, $E_0 = 10^3\,\mathrm{V/m}$ and $B = 3$ T).

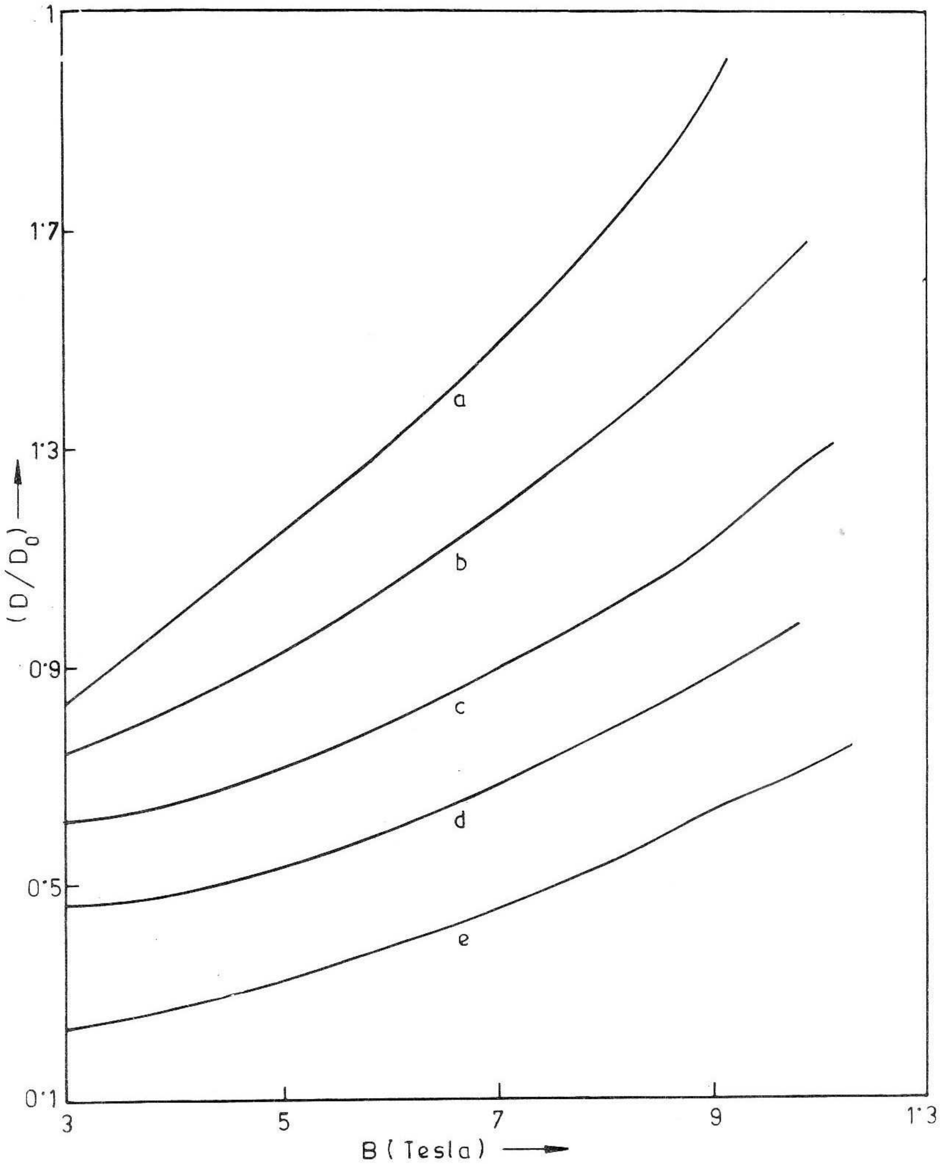

Fig. 3. Plot of the normalized TPE as function of the magnetic field under cross-field configuration in QWW in n-CdGeAs$_2$: curve a, our proposed dispersion relation; curve b, $\delta = 0$; curve c, the three-band Kane model; curve d, the two-band Kane model; curve e, the parabolic energy bands. ($n_0 = 10^{11}$ m^{-1}, $d_1 = 40$ nm, $d_2 = 50$ nm, $E_0 = 10^3$ V/m).

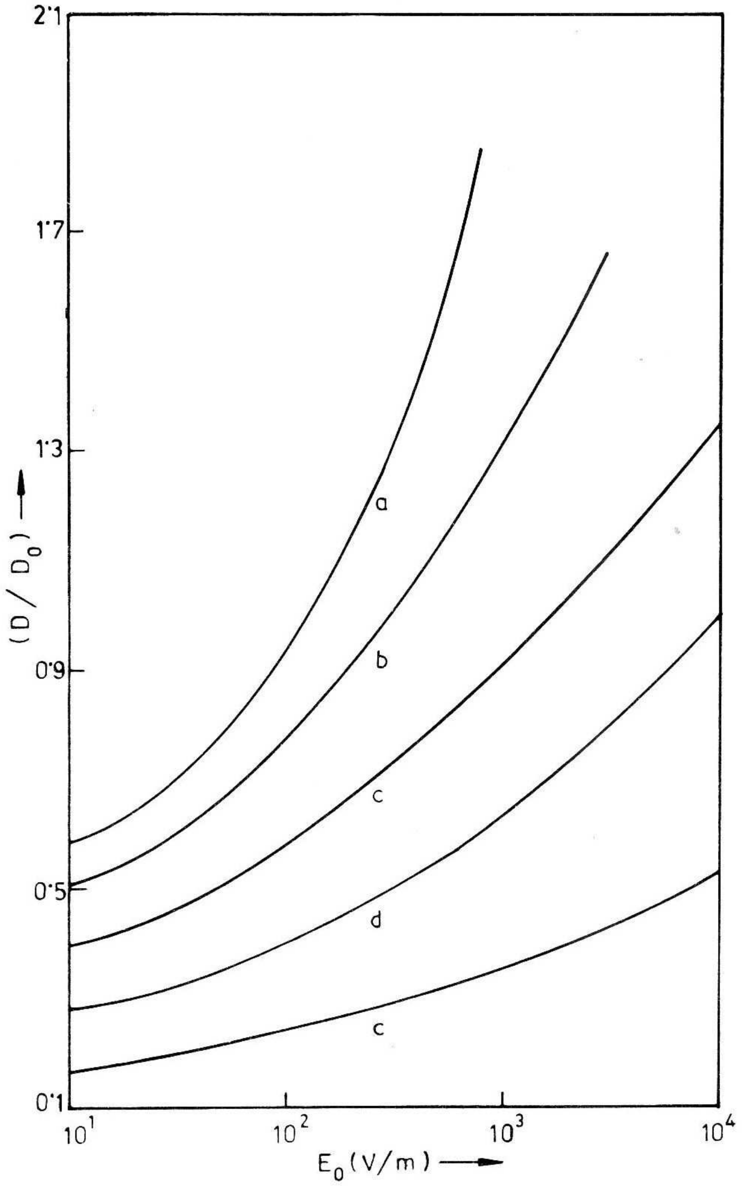

Fig. 4. Plot of the normalized TPE as function of the electric field under cross field configuration in QWW of n-CdGeAs$_2$: curve a, our proposed dispersion relation; curve b, $\delta = 0$; curve c, the three-band Kane model; curve d, the two-band Kane model; curve e, the parabolic energy bands. ($n_0 = 10^{-10}\,\mathrm{m}^{-1}$, $d_1 = 40$ nm, $d_2 = 50$ nm, $B = 3$ T).

dispersion law and the smallest for the parabolic energy bands. The variations of the TPE with n_0, B, d_0 and E_0 are completely band structure dependent for all models of QWW of degenerate ternary chalcopyrite semiconductors. Since the experimental data of the thermoelectric power are not available in the literature to the best of our knowledge, we can not compare our theoretical analysis with the experiment. We wish to note that the theoretical results, as given here, would be useful in analysing the experimental results when they appear. The experimental values of D will provide an experimental check on the TPE and also serve as a technique for probing the band structure in degenerate materials.

We wish to note the basic form of (2) remains unaltered for our proposed dispersion relation, three-band Kane model, two-band Kane model and that of parabolic energy bands in QWW of semiconductors in crossed fields. Thus (2) covers various semiconductors under different physical conditions. The functions F, Q and Φ are band structure dependent quantities. The above statement is also true in the presence of magnetic field only. This peculiarity of transcendental nature of our present problem, which is valid even for parabolic energy bands, is not at all true in bulk materials. From the expressions of TPE and electron concentration as given by Eqs. (4b) and (3) we can get the corresponding expressions for QWW's of even parabolic semiconductors in the absence of electric field. It is worth remarking that the quantization of energy of transverse plane of the direction of application of the magnetic field, valid for the 3D electron gases in a cross-field configuration, is not at all valid for QWW under the same physical condition. Besides, the subband energies can be calculated from Eq. (2).

It may be stated that the analysis of our present work be useful in determining theoretically the diffusion constant both in the presence and in the absence of electrical field, even for parabolic semiconductors since the TPE is inversely proportional to the diffusivity-to-mobility ratio. Finally it may be remarked that the basic purpose of our present paper is not only to investigate the TPE in QWW of non-parabolic semiconductors under cross-field configuration, but also to formulate the appropriate generalized electron energy spectrum since the study of the transport phenomena and the formulation of the electronic properties of semiconductors are based on the dispersion relations in such materials.

Appendix

A.1. $f = \Big[(b - eBd_1)\, 2^{-1} \left[q^2 - (b + eBd_1)^2\right]^{1/2} - 2^{-1} (b + eBd_1) \left[q^2 - (b - eBd_1)^2\right]^{1/2}\Big]$, $b = (eB)^{-1} \left[2M_\perp \varrho(E) eE_0 + \pi\hbar elBd_2^{-1}\right]$, $q^2 = \left[2M_\perp U(E) - M_\perp p_z^2 a^{-1}(E) - \pi^2\hbar^2 t^2 \left(4d_2^2\right)^{-1} + b^2\right]$, $\psi = \Big[\bar{\zeta}_+ \left(1 - \bar{\zeta}_-^2\right)^{1/2} - \bar{\zeta}_- \left(1 - \bar{\zeta}_+^2\right)^{1/2}\Big]$, $\bar{\zeta}_\pm = (b \pm eBd_1)/2$, $2d_1$ and $2d_2$ are the widths along x and y directions, respectively, $t = 1, 2, 3, \ldots$, $l = 1, 2, 3, \ldots$, $\varrho(E) =$

$= \ U(E)\left[(1+2\alpha E)\{E(1+\alpha E)\}^{-1} - J(E)\{I(E)\}^{-1} + (E+E_g+\Delta_{\|})^{-1} - \left(E+E_G+\frac{2}{3}\Delta_{\|}\right)^{-1}\right]$, $J(E) = I(E)\left[C(E)\{1+A(E)\}^{-1} - H(E)\{1+G(E)\}^{-1}\right]$, $I(E) = [1+A(E)][1+G(E)]^{-1}$, $A(E) = [(E+E_g+\Delta_{\|})(E+E_g)]^{-1}[\frac{1}{9}(\Delta_{\|}^2-\Delta_{\perp}^2)+\delta(E+E_g+\frac{1}{3}\Delta_{\|})]$, $G(E) = [(E+E_g)(E+E_g+\frac{2}{3}\Delta_{\|})]^{-1}[\delta(E+E_g+\frac{1}{3}\Delta_{\|})+\frac{1}{9}(\Delta_{\|}^2-\Delta_{\perp}^2)]$, $C(E) = A(E)[\delta\{\frac{2}{9}(\Delta_{\|}^2-\Delta_{\perp}^2)+\delta(E+E_g+\frac{2}{3}\Delta_{\|})\}^{-1} - (2E+2E_g+\Delta_{\|})\{(E+E_g)(E+E_g+\Delta_{\|})\}^{-1}]$ and $H(E) = G(E)[\{\delta(E+E_g+\frac{1}{3}\Delta_{\|})+\frac{1}{9}(\Delta_{\|}^2-\Delta_{\perp}^2)\}^{-1}\delta - (2E+2E_g+\frac{2}{3}\Delta_{\|})\{(E+E_g)(E+E_g+\frac{2}{3}\Delta_{\|})\}^{-1}]$.

A.2. $F = [[C-eBd_1]2^{-1}[X^2-(C-eBd_1)^2]^{1/2} - 2^{-1}(C+eBd_1)[X^2-(C-eBd_1)^{1/2}]$, $C = (eB)^{-1}[2M_{\perp}eE_0\varrho(E_F)+\pi\hbar leBd_2^{-1}]$, $X^2 = [2M_{\perp}U(E_F)+C^2-M_{\perp}\hbar^2n_0^2\pi^2a^{-1}(E_F)-\pi^2\hbar^2t^2(4d_2^2)^{-1}]$, $\Phi = [\lambda_+(1-\lambda_-^2)^{1/2}-\lambda_-(1-\lambda_+^2)^{1/2}]$ and $\lambda_{\pm} = (C \pm eBd_1)/2$.

A.3. $q_1 = A_1 - QA_2 + Q^2[2\sqrt{1-\Phi^2}]^{-1}$, $A_1 = (a_1/2)[Q^2-(C+eBd_1)^2]^{1/2} + (1/4)(C-eBd_1)[Q^2-(C+eBd_1)^2]^{1/2}[2Qa_2-2a_1(C+eBd_1)] - (a_1/2)[Q^2-(C-eBd_1)^2]^{1/2} - \frac{1}{4}(C+eBd_1)[Q^2-(C-eBd_1)^2]^{1/2}[2Qa_2-2a_1(C-eBd_1)]$, $a_1 = (eB)^{-1}[2M_{\perp}eE_0\varrho'(E_F)]$, $'$ denotes the differentiation w.r.t. E_F, $a_2 = (2Q)^{-1}[2M_{\perp}U(E_F)+M_{\perp}\hbar^2n_0^2\pi^2a^{-2}(E_F)a'(E_F)+(eB)^{-1}(4CM_{\perp}\cdot\varrho'(E_F)eE_0)]$, $a_2 = A_2$, $A_3 = [-s_+(1-\Gamma_-^2)^{1/2}+(\Gamma_+\Gamma_-)s_-(1-\Gamma_-^2)^{1/2}+s_-(1-\Gamma_+)^{1/2}-(\Gamma_+\Gamma_-)s_+(1-\Gamma_+^2)^{1/2}]$, $s_{\pm} = [a_1Q^{-1}-Q^{-2}A_2(C \pm eBd_1)]$, $\Gamma_{\pm} = (C \pm eBd_1)/2$, $q_2 = [A_4 - QA_5(\sin^{-1}\Phi)+Q^2A_6\{2\cdot\sqrt{1-\Phi^2}\}^{-1}]$; $A_4 = [[Q^2-4\Gamma_+^2]^{1/2}(-\Gamma_{,-}QA_5)+\frac{1}{2}\Gamma_+(Q^2-4\Gamma_-^2)^{-1/2}(2QA_5)]$, $A_5 = n_0M_{\perp}\hbar^2Q^{-1}$, $A_6 = [\lambda_+\sqrt{1-\Gamma_-^2}-\lambda_-(\Gamma_+\Gamma_-)(1-\Gamma_-^2)^{-1/2}+\lambda_+(\Gamma_+\Gamma_-)\cdot(1-\Gamma_+^2)^{-1/2}-\lambda_-(1-\Gamma_+^2)^{1/2}]$, $\lambda_{\pm} = (A_5/Q)(2\Gamma_{\pm})$.

A.4. $F_1 = \frac{1}{2}[\Theta_+(Q_1^2-\Theta_+^2)^{1/2}-\Theta_-(Q_1^2-\Theta_-^2)^{1/2}]$, $\Theta_{\pm} = [[\hbar t\pi(2d_2)^{-1}+m^*E_0\psi_0(E_F)B^{-1}\pm eBd_1]]$, $\psi_0(E_F) = \{\gamma(E_F)\{(1+\alpha E_F)E_F\}^{-1}[1+2\alpha E_F+E_F(1+\alpha E_F)\{(E_F+E_g+\Delta)^{-1}-(E_F+E_g+\frac{2}{3}\Delta)^{-1}\}]\}$, $Q_1^2 = [2m^*\gamma(E_F)-(\hbar^2\pi^2n_0^2)+m^*2E_0^2\psi_0^2(E_F)B^{-2}+m^*E_0\psi_0(E_F)\pi t\hbar(Bd_2)^{-1}]$, $\Phi_1 = [\zeta_{1,+}(1-\zeta_{1,-})^{1/2}-\zeta_{1,-}(1-\zeta_{1,+}^2)^{1/2}]$, $\zeta_{1,\pm} = \Theta_{\pm}/Q_1$, $\beta_1 = [\frac{1}{2}m^*E_0\psi_0(E_F)B^{-1}(Q_1^2-\Theta_+^2)^{1/2}+\frac{1}{2}\Theta_-^2E_0m^*\psi'(E_F)B^{-1}(Q_1^2-\Theta_-^2)^{-1/2}-\frac{1}{2}Q_1a_2\Theta_-(Q_1^2-\Theta_-^2)^{-1/2}+$

$+ \frac{1}{2}(Q_1^2 - \Theta_+^2)^{-1/2} Q a_1 \Theta_+ - \frac{1}{2} m^* E_0 \psi'(E_F) B^{-1} (Q_1^2 - \Theta_+^2)^{-1/2} \cdot (Q_+^2) -$ $- \frac{1}{2} m^* E_0 \psi'(E_F) B^{-1} (Q_1^2 - \Theta_-^2)^{1/2} + Q_1 a_1 (\sin^{-1} \Phi_1) + (Q_1^2 s_1/2 \cdot \sqrt{1 - \Phi^2})]$, $a_1 = (2Q)^{-1}[2m^* \gamma'(E_F) + 2(m^*)^2 E_0^2 B^{-2} \psi_0(E_F) \psi_0'(E_F) + m^* E_0 \psi'(E_F) \cdot$ $\cdot\, t\pi\hbar (B d_2)^{-1}]$, $s_1 = [p_{1,+}(1 - \zeta_{1,-}^2)^{1/2} - \zeta_{1,+}\zeta_{1,-}(p_{1,-})(1 - \zeta_{1,-}^2)^{-1/2} -$ $- p_{1,-}(1 - \zeta_{1,+}^2)^{1/2} + \zeta_{1,+}\zeta_{1,-} p_{1,+}(1 - \zeta_{1,+}^2)^{1/2}]$, $p_{1,\pm} = (m^* E_0 \psi'(E_F) \cdot$ $\cdot\, (B Q_1)^{-1} - a_1 Q_1^{-2} \Theta_\pm)$, $\beta_2 = [\frac{1}{2}\Theta_+ Q_1 a_2 (Q_1^2 - \Theta_+^2)^{-1/2} + \frac{1}{2} Q_1 a_2 \Theta_- (Q_1^2 -$ $- \Theta_-^2)^{-1/2} + Q a_2 \sin^{-1}(\Phi_1) + Q^2 s_2 \{2\sqrt{1 - \Phi^2}\}^{-1}]$, $a_2 = \hbar^2 \pi^2 n_0 / Q_1$, $s_2 = [p_{2,+}\sqrt{1 - \zeta_{1,-}^2} - \zeta_{1,+}\zeta_{1,-} p_{2,-}(1 - \zeta_{1,-}^2)^{-1/2} - p_{2,-}(1 - \zeta_{1,+}^2)^{1/2} +$ $+ \zeta_{1,+}\zeta_{1,-} p_{2,+}(1 - \zeta_{1,+}^2)^{-1/2}]$ and $p_{2,\pm} = a_2 \Theta_\pm / Q_1^2$.

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JEDNOSTAVNA ANALIZA TERMOELEKTRIČNE SNAGE U KVANTNIM ŽICAMA NEPARABOLIČNIH POLUVODIČA U PREKRIŽENOM ELEKTRIČNOM I MAGNETSKOM POLJU

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Razmatrana je termoelektrična snaga elektrona u tzv. kvantnim žicama neparaboličnih poluvodiča u prekriženom električnom i magnetskom polju koristeći nedavno dobiven zakon disperzije za energiju elektrona koji uzima u obzir sve tipove anizotropije u energetskom spektru. Uzevši n-CdGeAs$_2$ kao primjer, nađeno je da termoelektrična snaga opada porastom debljine filma, te jakošću električnog i magnetskog polja. Isto tako, kristalno polje jača termoelektričnu snagu u odnosu na sve fizikalne parametre.