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THE THERMOELECTRIC POWER IN QUANTUM DOTS OF SEMIMETALS UNDER STRONG MAGNETIC FIELD

KAMAKHYA PRASAD GHATAK

Department of Electronics and Telecommunication Engineering, Faculty of Engineering and Technology, University of Jadavpur, Calcutta 700032, India

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We study the thermoelectric power of the carriers in quantum dots of semimetals under strong magnetic field, taking Bi as an example. The numerical results are presented for the McClure and Choi, the hybrid, the Cohen, the Lax and the ellipsoidal parabolic energy band models of Bi. It is observed that the thermopower increases with decreasing electron concentration, increasing magnetic field and increasing film thickness, respectively. The oscillations of the TPM in Bi, in accordance with McClure and Choi model, show up much more significantly as compared to other models. In addition, the corresponding well known expression for the thermoelectric power in the presence of a classically strong magnetic field in bulk specimens of parabolic semiconductors has been obtained as a special case of our generalized expressions.

1. *Introduction*

The remarkable developments of fine lithographical methods, molecular beam epitaxy, organo-metallic vapour phase epitaxy and other experimental techniques have generated significant possibilities of fabrication of new artificial materials known as quantum wells formed between two plannar heterojunctions[1)]. The heterojunctions based on various materials are currently being studied because of the enhancement of carrier mobility[2)]. The properties make such structures suitable for the applications in quantum well lasers[3)], heterojunction FET's[4)], high-speed digital network[5)], optical modulators[6)] and other devices. As the dimension of the quantum confinement increases from 1D to 3D, the degree of the free-carrier motion decreases drastically and the density-of-states function changes from the step function to the Dirac's delta function (i.e. from a stepped cummulative one to a complete discrete one)[7,8)]. Though considerable work has already been done, still the interest for further research of the different other aspects of such systems is becoming increasingly important. In the present communication we shall study the thermoelectric power in quantum dots of semimetals, under strong magnetic field (TPM).

It is well-known that the analysis of the thermoelectric power gives information about the band structure, the density-of-state function and the effective electron mass[9)]. The remarkable feature of the TPM is that it is independent of scattering mechanisms, and in the case of spherical energy surface the shape of the conduction band can be determined from its experimental investigations[9)]. The TPM can be connected to the Einstein relation of the diffusivity-mobility ratio[10)] and the carrier contribution to elastic constants in degenerate materials having arbitrary dispersion laws[11)]. The aforementioned physical properties are considered to be the two most widely used parameters of electron transport in electron devices. The discovery of quantum Hall effect[12)] has brought interest to the study of the TPM in fully quantized systems. In recent years, the different modifications of the TPM have extensively been investigated[13,14)]. Nevertheless, it appears from the literature that the TPM in quantum dots of semimetals has yet not been investigated. It is well known that the E-$\vec{k}$ dispersion relation of the carriers in semimetals differ considerably from simpler spherical surfaces of the degenerate electron gas. We shall take Bi as an example of semimetals. Several models have been developed to describe the energy spectrum of the carriers in Bi. Earlier works demonstrated[15)] that the carrier properties of Bi could be described by ellipsoidal parabolic model or one band model. Shoenberg indicated that the Haas-Van Alphen and cyclotron resonance experiments supported the one band model[16)] though the later work showed that Bi could be described by the band model since the magnetic field dependence of many physical parameters of Bi supports the above model[17)]. Magneto-optical results[18)] and ultrasonic quantum oscillation data[19)] favour the Lax ellipsoidal non-parabolic model[20)] where as Kao[21)], Dinger and Lawson[22)] and Koch and Jensen[23)] indicated that the Cohen model[24)] is in better agreement with the experimental results. In a work on magnetic surface resonance, Takaoka et al.[25)] concluded that neither the Lax model nor the Cohen model is adequate and they proposed the hybrid model. In 1977, McClure and Choi[26)] proposed a new model of Bi which is more accurate and general than those currently in use. They showed that it can fit the data for a large number of magneto-oscillatory and resonance experiments.

In what follows, we shall formulate the TPM for QDs of Bi in accordance with the McClure and Choi, the hybrid, the Cohen, the Lax and the ellipsoidal parabolic energy band model on the basis of the newly formulated carrier energy spectra for the QDs of each model. We shall study the doping, magnetic field and thickness dependence of the TPM in QDs of Bi.

2. *Theoretical background*

(a) McClure and Choi Model:

The E-$\vec{k}$ dispersion law of the carriers in bismuth in accordance with the McClure-Choi model can be expressed[27)] as

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

where E is the carrier energy as measured from the band-edge in the absence of any quantization, m_1, m_2 and m_3 are the effective carrier masses at the band edge along x, y and z-directions, respectively, and m_2^1 is the effective mass tensor component at the top of the valence band (for electrons) or at the top of the conduction band (for holes).

Therefore, the modified electron energy spectrum in the presence of a strong magnetic field B_y along y-direction, in QDs of Bi, whose electron dispersion law is given by Eq. (1), can be written as

$$(L_{\prime +})(d_1^2 - L_+^2)^{1/2} - (L_{\prime -})(d_1^2 - L_-^2)^{1/2} + d_1^2\left[\sin^{-1}\frac{L_+}{d_1} - \sin^{-1}\frac{L_-}{d_1}\right] = 2a_1\hbar n_z\,, \tag{2}$$

where

$$L_\pm = b_1/(2a_1) \pm a_1 d_z\,, \qquad d_1^2 = c_1 + b_1^2/(2a_1)^2,$$

$$a_1^2 = \left[\frac{1}{2m_3} - \frac{\alpha\hbar^2}{4m_1m_3}\left(\frac{\pi n_y}{2d_y}\right)^2\right]^{-1} e^2B_y^2\left[\frac{1}{2m_1} - \frac{\alpha\hbar^2}{4m_1m_2}\left(\frac{\pi n_y}{2d_y}\right)^2\right],$$

$$b_1 = \left[\frac{1}{2m_3} - \frac{\alpha\hbar^2}{4m_2m_3}\left(\frac{\pi n_y}{2d_y}\right)^2\right]^{-1}\left[\frac{\hbar n_x \pi e B_y}{d_x}\left(\frac{1}{2m_1} - \frac{\alpha\hbar^2}{4m_1m_2}\left(\frac{\pi n_y}{2d_y}\right)^2\right)\right],$$

$$c_1 = \left[\frac{1}{2m_3} - \frac{\alpha\hbar^2}{4m_1m_3}\left(\frac{\pi n_y}{2d_y}\right)^2\right]^{-1} \times\left[E + \alpha E^2 - \hbar^2\left(\frac{\pi n_x}{2d_x}\right)^2\right]\left[\frac{1}{2m_1} - \frac{\alpha\hbar^2}{4m_1m_2}\left(\frac{\pi n_y}{2d_y}\right)^2\right] - \hbar^2\left(\frac{\pi n_y}{2d_y}\right)^2\left[\frac{1}{2m_2} + \frac{\alpha E}{2m_2}\left(1-\frac{m_2}{m_2^1}\right) + \frac{\alpha\hbar^2}{4m_2m_2^1}\left(\frac{\pi n_y}{2d_y}\right)^2\right].$$

n_x, n_y and n_z are the size quantum numbers along x, y and z directions, respectively, and $2d_x$, $2d_y$ and $2d_z$ are the widths of QDs of Bi along the x, y and z-directions, respectively. Thus we note that the magnetic field which is parallel to y-axis does not give rise to magnetic quantization. In the absence of magnetic field, $B_y \to 0$ and Eq. (2) gets simplified as

$$E(1+\alpha E)=\frac{\hbar^2}{2m_1}\left(\frac{\pi n_x}{2d_x}\right)^2+\frac{\hbar^2}{2m_2}\left(\frac{\pi n_y}{2d_y}\right)^2+\frac{\hbar^2}{2m_3}\left(\frac{\pi n_z}{2d_z}\right)^2+\frac{\hbar^2}{2m_2}\left(\frac{\pi n_y}{2d_y}\right)^2\alpha E\left(1-\frac{m_2}{m_2^1}\right)$$

$$+\frac{\alpha\hbar^4}{4m_2m_2^1}\left(\frac{\pi n_y}{2d_y}\right)^4-\frac{\alpha\hbar^4}{4m_1m_2}x\left(\frac{\pi^2 n_x n_y}{4d_x d_y}\right)^2-\frac{\alpha\hbar^4}{4m_2m_3}\left\{\left(\frac{\pi n_y}{2d_y}\right)^2\cdot\left(\frac{\pi n_z}{2d_z}\right)^2\right\}. \quad (3)$$

The use of Eq. (2) leads to the expression of the density-of-states function as

$$N(E) = \left[(g_s g_v)\left(8d_x d_y d_z\right)^{-1}\right]\sum_{n_x,n_y,n_z}\delta'(E-E'), \quad (4)$$

where δ' is the Dirac's delta function, g_s is the spin degeneracy, g_v is the valley degeneracy and E' is the root of Eq. (2). The TPM under present condition can be expressed[9] as

$$G = S_0/(en_0), \quad (5)$$

where S_0 is the entropy per unit volume in the present case, e the electron charge and n_0 the electron concentration per unit volume. Using Eqs. (4) and (5) we get

$$G = (eT)^{-1}\left[\frac{\sum_{n_x,n_y,n_z} E' F_{-2}(\eta)}{\sum_{n_x,n_y,n_z} F_{-2}(\eta)} - E_F\right], \quad (6)$$

where T is the temperature, $\eta = (k_B T)^{-1}(E_F - E')$, E_F is the Fermi energy in the present case and $F_j(\eta)$ is the one parameter Fermi-Dirac integral as defined by Blakemore[28].

Thus, to evaluate G as a function of electron concentration, we need an expression for the electron statistics which can, in turn, be written as

$$n_0 = \left[(g_s g_v)\left(8d_x d_y d_z\right)^{-1}\right]\sum_{n_x,n_y,n_z} F_{-2}(\eta)). \quad (7)$$

(b) Hybrid model:

The electron dispersion law in accordance with the hybrid model can be written[25] as

$$E(1+\alpha E) = \frac{p_x^2}{2m_1} + \frac{p_z^2}{2m_3} + \frac{p_y^2}{2m_2}\left[\beta(E)\right] + \frac{8p_y^4}{4E_g M_2}, \quad (8)$$

where $\beta(E) = 1 + \delta_0 + aE(1-\gamma)$, $\delta = M_2/m_2$, $\gamma = M_2/M_1^1$, M_2 is the effective mass tensor component along the bisectrix axis due to the influence of the remote bands at the bottom of the conduction band (for electrons) or at the top of the valence bands (for holes) and M_2^1 is the effective mass tensor component along the bisectrix axis due to the influence of the remote bands at the top of the valence bands (for electrons) or at the bottom of the conduction bands (for holes). Thus the basic forms of Eqs. (6) and (7) will be unaltered where

$$a_1^2 = (m_3/m_1)e^2 B_y^2\,,$$

$$b_1 = 2m_3 \frac{\hbar e B_y}{m_1} \frac{\pi n_x}{2d_x}\,,$$

and

$$c_1 = 2m_3 \left[E(1+\alpha E) - \frac{\hbar^2}{2m_1} \left(\frac{\pi n_x}{2d_x}\right)^2 \right.$$

$$\left. - \frac{\hbar^2}{2M_2} \left(\frac{\pi n_y}{2d_y}\right)^2 \left[1 + \delta_0 + \alpha E(1-\gamma)\right] - \frac{\alpha\gamma\hbar^4}{4M_2^2} \left(\frac{\pi n_y}{2d_y}\right)^4 \right].$$

(c) Cohen model:

The energy dispersion law in accordance with the Cohen model[24] can be expressed as

$$E(1+\alpha E) = \frac{p_x^2}{2m_1} + \frac{p_z^2}{2m_3} - \frac{\alpha E p_y^2}{2m_2^1} + \frac{\alpha p_y^2}{4m_2 m_2^1} + \frac{p_y^2}{2m_2}(1+\alpha E). \qquad (9)$$

In this case basic forms of Eqs. (6) and (7) will not change, where

$$a_1^2 = (m_3/m_1)e^2 B_y^2\,, \qquad b_1 = 2m_3\big(\hbar e B_y \pi n_x m_1^{-1} d_x^{-1}\big)/2\,,$$

and

$$c_1 = 2m_3 \left[E(1+\alpha E) - \frac{\hbar^2}{2m_1} \left(\frac{\pi n_x}{2d_x}\right)^2 \right.$$

$$\left. + \frac{\alpha E \hbar^2}{2m_2^1} \left(\frac{\pi n_y}{2d_y}\right)^2 - \frac{(1+\alpha E)}{2m_2} \left(\frac{\hbar \pi n_y}{2d_y}\right)^2 - \frac{\alpha \hbar^4}{4m_2 m_2^1} \left(\frac{n_y \pi}{2d_y}\right)^4 \right].$$

(d) Lax ellipsoidal model:

The E-$\vec{k}$ relation in Bi in accordance with the Lax non-parabolic ellipsoidal model[20] can be written as

$$E(1+\alpha E) = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{p_z^2}{2m_3}\,. \qquad (10)$$

The basic forms of Eqs. (6) and (7) will be unaltered for the Lax model where

$$a_1^2 = (m_3/m_1)\, e^2 B_y^2\,, \qquad b_1 = (m_3/m_1)\, eB_y n_x \pi\hbar/d_x\,,$$

and

$$c_1 = 2m_3 \left[E(1+\alpha E) - \frac{\hbar^2}{2m_1}\left(\frac{n_x\pi}{2d_x}\right)^2 - \frac{\hbar^2}{2m_2}\left(\frac{n_y\pi}{2d_y}\right)^2 \right].$$

(e) The ellipsoidal parabolic model:

The carrier dispersion law for the model is given by

$$E = \frac{p_x^2}{2m_1} + \frac{p_y^2}{2m_2} + \frac{p_z^2}{2m_3}\,. \tag{11}$$

We wish to note that under the condition $\alpha \to 0$, the McClure and Choi, the Cohen and the Lax model as given by Eqs. (1), (9) (10), respectively, reduce to Eq. (11). Also under the limiting conditions $\alpha \to 0$ and $\delta_0 \gg 1$, the hybrid model as given by Eq. (8) gets simplified to Eq. (11). For the parabolic model, the forms of Eqs. (6) and (7) will not change in forms where

$$a_1^2 = (m_3/m_1)\, e^2 B_y^2\,, \qquad b_1 = (m_3/m_1)\, eB_y n_x \pi\hbar/d_x\,,$$

and

$$c_1 = 2m_3 \left[E - \frac{\hbar^2}{2m_1}\left(\frac{n_x\pi}{2d_x}\right)^2 - \frac{\hbar^2}{2m_2}\left(\frac{n_y\pi}{2d_y}\right)^2 \right].$$

For bulk specimens, the quantum numbers, n_x, n_y and n_z would vary from zero to infinity and, hence, the summation over n_x, n_y and n_z is replaced by the integrals over n_x, n_y and n_z to express the TPM and n_0 in isotropic parabolic ellipsoidal energy bands as[9)]

$$G = \frac{k_B}{e}\left[\left(\frac{5}{2} F_{3/2}(\eta_0)/F_{1/2}(\eta_0) \right) - \eta_0 \right], \tag{12}$$

and

$$n_0 = N_c F_{1/2}(\eta_0) g_v\,, \tag{13}$$

where $\eta_0 = E_{F0}/k_B T$, E_{F0} is the Fermi energy in bulk specimens of Bi as measured from the edge of the conduction band in the vertically upward directions in the absence of any quantization, $N_c = 2(2\pi m_d k_B T/h^2)^{3/2}$ and $m_d = (m_1 m_2 m_3)^{1/3}$. Under the condition of non-degeneracy $\exp(-\eta_0) \ll 1$ and we get

$$G = \frac{k_B}{e}\left[\frac{5}{2} - \eta_0 \right], \tag{14}$$

and

$$n_0 = g_p N_0 \exp(\eta_0)\,. \tag{15}$$

Thus, we can summarize the whole mathematical background in the following way. We have formulated the expressions for the TPM and n_0 in quantum dots of Bi in accordance with the McClure and Choi, the hybrid, the Cohen, the Lax and the ellipsoidal parabolic models by using the basic fundamental expression of

TPM as given by Eq. (5) for all models after formulating the appropriate electron energy spectra in QDs of Bi under strong magnetic field. We have shown that under certain limiting conditions all four models reduce to the ellipsoidal energy bands as given by Eq. (11), and Eqs. (6) and (7) represent the generalized expressions of TPM and n_0 where E' is the only band structure dependent quantity. Replacing the summations over n_x, n_y and n_z by integrations over n_x, n_y and n_z we have obtained the well known expressions of TPM and n_0 for bulk specimens of parabolic semiconductors as given by Eqs. (12) and (13)[9]. Thus we can write that from the simple theoretical expressions of TPM and n_0 in QDs of bismuth in accordance with various band models, we have obtained the well known results of TPM and n_0 in bulk specimens of both degenerate and nondegenerate parabolic semiconductors, respectively. The above sentence is the indirect theoretical test of our mathematical formulations.

3. Results and discussion

Using Eqs. (6) and (7) and taking the parameters[29,30] $g_p = 3$, $g_s = 2$, $m_1 = m_0/172$, $M_2 = 1.28m_0$, $m_2 = m_0/0.8$, $m_3 = m_0/88.5$, $E_g = 0.153$ eV, $B_y = 1$ T, $T = 4.2$ K and $d_x = d_y = d_z = 25$ nm, we have plotted in Fig. 1 the normalized

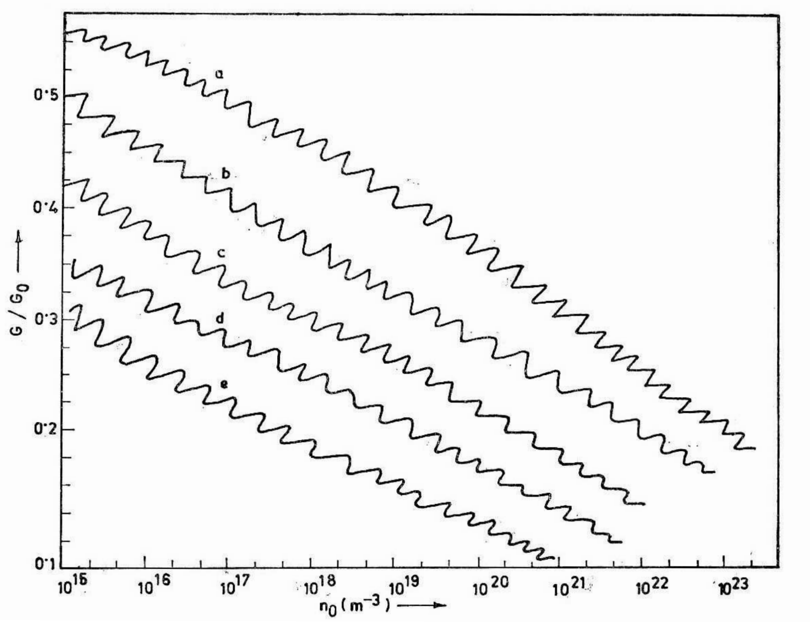

Fig. 1. Plot of normalized TPM versus n_0 in QDs of Bi *in accordance with: curve a – McClure and Choi model, curve b – hybrid model, curve c – Cohen model, curve d – Lax model and curve e – the parabolic ellipsoidal model.*

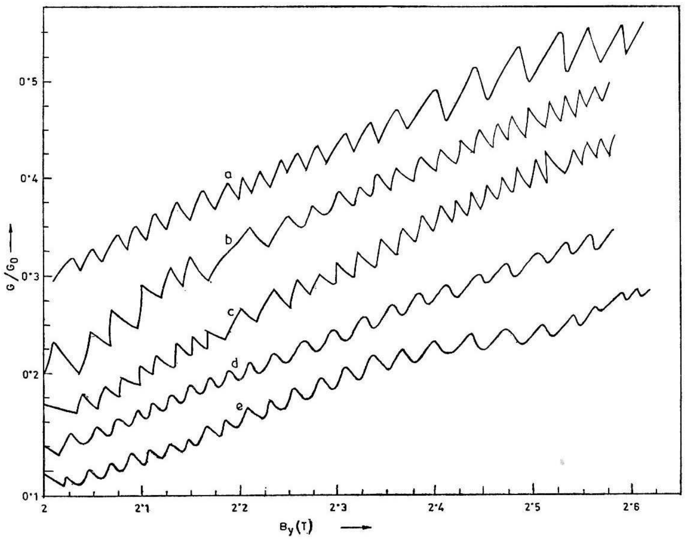

Fig. 2. Plot of normalized TPM in QDs of Bi *versus* B_y *in accordance with: curve a – McClure and Choi model curve b – hybrid model, curve c – Cohen model, curve d – Lax model and curve e – the parabolic ellipsoidal model.* ($n_0 = 10^{23}$ m^{-3} *and* $d_x = d_y = d_z = 25$ nm).

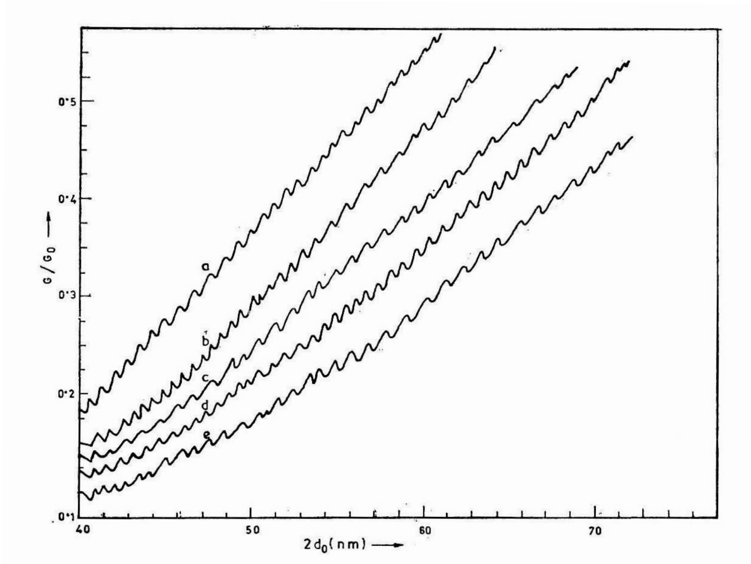

Fig. 3. Plot of normalized TPM of Bi *versus film thickness in accordance with: curve a – McClure and Choi model curve b – hybrid model, curve c – Cohen model, curve d – Lax model and curve e – the parabolic ellipsoidal model.* ($B_y = 1$ T, $n_0 = 10^{23}$ m^{-3}).

TPM versus n_0 in cubic QDs of Bi in accordance with various band models. Plots for the normalized TPM versus B_y and $2d_0$ are shown in Figs. 2 and 3, respectively, in accordance with the mentioned band models of Bi.

It appears from Fig. 1 that the TPM in QDs of Bi decreases with increasing electron concentration and the McClure and Choi model enhances the TPM in the whole range of concentrations considered. It appears from Fig. 2 that the TPM increases with increasing magnetic field. With varying magnetic field, a change is reflected in the TPM through the redistribution of the electrons among the size-quantized levels. It may be noted that the 3D quantization leads to the discrete energy levels, somewhat like atomic energy levels, which produces very sharp changes. This follows from the inherent nature of the 3D quantization of the carrier gas dealth with here. Under such quantization, there remain no free electron states inbetween any two allowed set of size-quantized levels unlike that found for 3D carrier gases in semiconductors under 2D quantization of k space. Consequently, the crossing of the Fermi level by the size-quantized levels under 3D quantization would have much greater impact on the redistribution of the electrons among the allowed states, as compared to the results for 2D quantization. It appears from Fig. 3 that the TPM increases with increasing film thickness. Though the TPM varies nonlinearly in all band models of Bi, as evident from all figures, the rates of variations are totally band structure dependent. It appears from all figures that the oscillations of the TPM in Bi is greatest for the McClure and Choi model and least for the ellipsoidal parabolic energy bands.

The Eqs. (6) and (7) are generalized expressions of TPM and electron concentration in QDs of Bi under strong magnetic field. Only E' is the band-structure dependent quantity. This is only possible for 3D quantization of $\vec{k}$ space. We wish to note that we have formulated the TPM in accordance with all types of band models of Bi for the purpose of relative comparison as evident from all figures which are self explanatory. Though the experimental verification of the basic content of the present work is not available in the literature to the best of our knowledge, the importance of the TPM in semiconductor physics is already well known. Besides, our analysis is also valid for holes with the proper change in band parameters. The carrier energy spectra in Bi could be described by the McClure and Choi, the hybrid, the Cohen, the Lax and the ellipsoidal parabolic models as often used by various authors to describe the different physical properties of semimetals. We have formulated the expressions of TPM for all the models. We have shown that under certain limiting conditions the four models reduce to the ellipsoidal parabolic energy bands and expressions of n_0 and TPM under the same conditions reduce to the well known expressions as given by Eqs. (15) and (14), respectively. The Cohen model is used to describe the carrier dispersion law of lead chalcogenide materials[31)]. The Lax model under the condition of isotropic effective electron mass at the band edge reduces to the two-band Kane model which is often used in studying the physical features of III-V semiconductors, excluding n-InAs[31)]. Furthermore under the condition $E_g \to \infty$, together with the above mentioned equality, the two-band Kane model reduces to the well known form of isotropic parabolic energy bands which is often used for investigating the electronic properties of wide band gap materials. Thus the analysis of the present paper is valid not only for Bi but also for all types of lead chalcogenides, III-V semiconductors excluding n-InAs, and wide-gap materials. It may be noted that the basic purpose of the present work is not solely to investigate the TPM in QDs of Bi in accordance with various band models, but also to formulate the density-of-states function by deriving new carrier energy spectrum since the various transport phenomena and the derivation of the expressions of many important physical properties are based on the appropriate density-of-states function in such materials. Finally, it may be remarked that the nature of variations of TPM as shown here would be similar for most of other non-parabolic semiconductors, since narrow-gap materials having Kane-type energy bands obey the two-band Kane model, whereas the present analysis is based on the generalized Kane's theory[31)].

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TERMOELEKTRIČNA SILA U KVANTNIM TOČKAMA POLUMETALA U PRISUSTVU JAKOG MAGNETSKOG POLJA

KAMAKHYA PRASAD GHATAK

Department of Electronics and Telecommunication Engineering, Faculty of Engineering and Technology, University of Jadavpur, Calcutta 700032, India

UDC 538.915

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Razmatrana je termoelektrična sila u kvantnim točkama u prisustvu jakog magnetskog polja. Kao primjer uzet je Bi. Prikazani su numerički rezultati za nekoliko modela energetskih vrpci Bi. Opaženo je da termonapon raste s padom koncentracije nosilaca naboja, porastom magnetskog polja te povećanjem debljine filma.