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# ON THE EFFECTIVE MASS IN SMALL-GAP MATERIALS UNDER MAGNETIC QUANTIZATION

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An attempt is made to study the effective mass in small-gap materials under strong magnetic quantization taking Bi and $p$-CdSb as examples. It is found that for Bi the effective electron mass at the Fermi level depends on Fermi energy, and the magnetic quantum number due to the influence of band non-parabolicity, resulting in different effective masses corresponding to different magnetic sub-bands. The same mass increase with increasing electron concentration and oscillates of the orientation of the quantizing magnetic field, respectively. The effective hole mass in $p$-CdSb depends on the magnetic quantum number which in the characteristic feature of the Yamada model. Besides, the effective quantum number dependent Fermi level masses differ widely with each other for relatively small values of hole concentration and for all values of the quantizing magnetic field, respectively

## 1. Introduction

The effective mass of the carriers in semiconductors, which is strongly connected with the carrier mobility, is known to be one of the most important device parameters[1]. In semiconductors with parabolic $E - \vec{k}$ dispersion relations ($E$ is the total energy as measured from the band edge and $\vec{k}$ is the wave-vector of the carriers, respectively) the effective mass is independent of energy whereas for non-parabolic energy band the same mass increases with increasing carrier energy in a monotonous manner. Among the various definitions of the effective mass[2], it is the momentum effective mass that should be regarded as the basic quantity[3] since it is this mass which appears in the description of transport phenomena and all other properties of the electron gas in a band with arbitrary band non-parabolicity. Momentum effective mass enters in various transport coefficients and plays the most dominant role in explaining the experimental results of different types of scattering mechanisms[4-5]. The carrier degeneracy in semiconductors influences the effective mass when it is energy dependent. Under degenerate conditions, only the carriers at the Fermi surface of degenerate semiconductors participate in conduction process and hence, the effective momentum mass of the carriers (hereafter referred to as EMM) corresponding to the Fermi energy would be of interest in carrier transport under such conditions. The Fermi energy is again determined by the dispersion relation and the carrier concentration and, therefore, these two parameters would determine the dependence of EMM in degenerate semiconductors on the degree of degeneracy.

In recent years various $E - \vec{k}$ relations of the carriers for different semiconductors have been proposed[6-10], which have created interest for studying the EMM in such semiconductors under various physical conditions[5-14]. Besides, it is well-known that the quantizing magnetic field drastically changes the energy spectrum by reshaping the band structure[15]. Incidentally, it appears from the literature that the EMM in Bi and $p$-CdSb has yet to be investigated for the more interesting case which occurs from the presence of a quantizing magnetic field. We wish to note that Bi has been the subject of a large number of experimental and theoretical researches. Several models have been developed to describe the energy-band-structure of Bi[16-18]. Earlier works demonstrated that the electronic properties of Bi could be described by one-band model[19]. Sohenberg indicated that de Haas-Van Alphen and cyclotron resonance experiments supported the one-band model[19]. Later work showed that Bi could be described by two-band model[20] since the magnetic field dependences of many physical phenomena of Bi supports the above model. Magneto-optical results[21], longitudinal magneto-striction[22] and ultrasonic quantum oscillations data[23] favour the Lax ellipsoidal non-parabolic model[24], but Kao[25], Dinger and Lawson[26 and Koch and Jensen[27] indicated that Cohen's model[28] is in better agreement with the experimental results. In a work on magnetic surface resonance, Takaoka et al.[29] concluded that neither the Lax model nor the Cohen model is adequate and proposed a hybrid model. McClure and Choi[17] presented a new energy-band model of Bi, which gives very good fits to a large number of magneto oscillatory and resonance experiments. Chen et al.[8] proposed a new model in the presence of a quantizing magnetic field along $z$-axis. Recently, Cankurtaran et al.[30] obtained the generalized magneto-dispersion relation of the conduction electrons in Bi in the presence of an arbitrarily oriented quantizing magnetic field. It may also be noted from the literature that EMM of $p$-type semiconductors has relatively been less investigated specially under magnetic quantization. In this paper we shall also study the EMM in $p$-CdSb in the presence of a quantizing magnetic field by considering the generalized dispersion relation of the holes as derived by Yamada[31] including all types of anisotropies in the energy spectrum.

In what follows, in Section 1 of theoretical background we shall derive the magneto EMM in Bi by using the model of Cankurtaran et al.[30]. We shall study the doping, magnetic field and orientational dependences of EMM at the Fermi level in Bi. In Section 2, we shall formulate the EMM in $p$-CdSb by deriving the appropriate dispersion relation. We shall investigate the doping and magnetic field dependences of EMM at the Fermi level in $p$·CdSb.

## 2. *Theoretical background*

### 2.1. *Formulation of EMM in Bi under magnetic quantization*

The magneto dispersion relation of the carriers in Bi can be expressed[30] as

$$E(1 + \alpha E) = A_1 k_H^4 + A_2 k_H^2 + A_3 \tag{1}$$

where $\alpha \equiv 1/E_g$, $E_g$ is bandgap, $E$ is the total energy in the presence of magnetic quantization as measured from the band edge in the absence of any quantization, $k_H$ is the direction of application of the quantizing magnetic field $H$ which makes an angle $\Theta$ with the $x$-axis while lying in the $xy$ plane and the other notations are defined in the above reference. The EMM at the Fermi level $E_F$ along the direction of magnetic quantization is given by

$$m^* = \left[\hbar k_H \Big/ \frac{1}{\hbar}\frac{\partial k_H}{\partial E}\right]\Bigg|_{E=E_F} \tag{2}$$

since in non-parabolic bands the EMM has to be obtained by dividing the momentum by velocity. Thus using Eqs. (2) and (1), the EMM at the Fermi level in Bi can be expressed as

$$m_{\pm}^* (n, E_F, \Theta) = \hbar^2 \left(\alpha E_F + \frac{1}{2}\right) [A_4 + 4A_1 E_F (1 + \alpha E_F)]^{-1/2} \tag{3}$$

where

$$A_4 \equiv \{A_2^2 - 4A_1 A_3].$$

From Eq. (3) it appears that the EMM at the Fermi level in Bi is a function of magnetic quantum number, quantizing magnetic field and the angle of orientation of the same field, respectively. The evaluation of EMM as a function of carrier concentration requires an expression of carrier statistics which, in turn, is determined by the density-of-states function. Using Eq. (1) the density-of-states function per ellipsoid can be written, incorporating spin and broadening of Landau levels, as

$$N(E) = (e\,H/4\pi^2\,\hbar\,\sqrt{2})\sum_{n=0}^{n_{max}}[[a_1 + \{a_1^2 + b_1^2\}^{1/2}]^{-1/2}$$

$$[a_1' + \{a_1\,a_1' + b_1\,b_1'\}\{a^2 + b^2\}^{-1/2}]] \tag{4}$$

where

$$a_1 \equiv [2A_1]^{-1}\,[\sqrt{t_1} - A_2],$$

$$t_1 \equiv [x + \sqrt{a^2 + y^2}],$$

$$x \equiv [A_4 + 4A_1\{E + a\,E^2 - a\,\Gamma^2\}],$$

$\Gamma$ is the broadening of Landau levels and is given by $\Gamma = \pi\,k_B\,T_D$ in which $k_B$ is Boltzmann constant and $T_D$ is Dingle temperature,

$$y \equiv 4A_1\,\Gamma(1 + 2a\,E),$$

$$b \equiv [2A_1]^{-1}\,[\sqrt{t_2}],$$

$$t_2 \equiv [[-x + \sqrt{x^2 + y^2}]^{1/2}]/2$$

and $'$ denotes differentiation with respect to energy.

Combining Eq. (4) with the Fermi-Dirac occupation probability factor the carrier concentration per ellipsoid can be expressed as

$$n_0 = \frac{e\,H}{2\pi^2\,\hbar}\sum_{n=0}^{n_{max}}[U + V] \tag{5}$$

where

$$U \equiv [\{a + \{a^2 + b^2\}^{1/2}\}]^{1/2}/2,$$

$$V \equiv \sum_{r=1}^{s} 2\,(k_B\,T)^{2r}\cdot(1 - 2^{1-2r})\,\zeta(2r)\,\frac{\mathrm{d}E_F^{2r}}{\mathrm{d}^{2r}}\,[U],$$

$T$ is the temperature, $r$ is the set of the real positive integers, $\zeta(2r)$ is the zeta function of order $2r$[32].

Under the condition $a \to 0$, Eq. (1) takes the form

$$E = \left(n' + \frac{1}{2}\right)\hbar\,\omega_c + \frac{\hbar^2\,k_H^2}{2m_H}, \qquad n' = n + S\,r \tag{6}$$

which is the well-known expression of the magneto-dispersion relation of ellipsoidal parabolic energy bands[15]. Thus using the above substitution, Eqs. (3) to (5) get simplified as

$$m^* = m_H \tag{7}$$

$$N(E) = (eH\sqrt{m_H}/h^2) \sum_{n=0}^{n_{max}} Y(E)/X(E) \tag{8}$$

$$n_0 = (2eH\sqrt{m_H}/h^2) \sum_{n=0}^{n_{max}} [Y(E_F) + Z(E_F)] \tag{9}$$

where

$$Y(E) \equiv [\Delta_0(E) + \sqrt{\Delta_0^2(E) + \Gamma^2}]^{1/2},$$

$$\Delta_0(E) \equiv \left[E - \left(n' + \frac{1}{2}\right)\hbar\omega_0\right],$$

$$X(E) \equiv [\Gamma^2 + \Delta_0^2(E)]^{1/2}$$

and

$$Z(E_F) \equiv \sum_{r=1}^{s} 2(k_B T)^{2r} \cdot (1 - 2^{1-2r})\,\zeta(2r)\,\frac{\mathrm{d}^{2r}}{\mathrm{d}E_F^{2r}}[Y(E_F)].$$

It may be noted in the absence of splitting equation (8) assumes the form[33a)]

$$N(E) = \frac{eH\sqrt{m_H}}{h^2} \sum_{n=0}^{n_{max}} [E_z + \sqrt{E_z^2 + \Gamma^2}]\,[E_z^2 + \Gamma^2]^{-1/2} \tag{10}$$

where

$$E_z \equiv \left[E - \left(n + \frac{1}{2}\right)\hbar\omega_c\right].$$

Under the condition $\Gamma \to 0$, the carrier concentration assumes the well-known form[33b)]

$$n_0 = \frac{N_c\Theta_0}{2} \sum_{n=0}^{n_{max}} F_{-1/2}(\eta') \tag{11}$$

where

$$N_c \equiv 2(2\pi m_H k_B T/h^2)^{3/2}, \qquad \Theta_0 \equiv \hbar\omega_c/k_B T,$$

$$\eta' \equiv (k_B T)^{-1}\left[E_F - \left(n' + \frac{1}{2}\right)\hbar\omega_c\right] .$$

and $F_j(\eta')$ is the one parameter Fermi-Dirac integral of order $j$ as defined by Blakemore[34)].

### 2.2. *Formulation of the magneto EMM in p-CdSb*

The energies of the two valence bands in *p*-type CdSb in the absence of any quantization can be expressed[31] as

$$E_{1,2} = \frac{1}{2}(a_1 + b_1)k_x^2 + \frac{1}{2}(a_2 + b_2)k_y^2 + \frac{1}{2}(a_3 + b_3)k_z^2 +$$

$$+ \frac{1}{2}(A + B)k_x \pm \left[\left\{\frac{1}{2}(a_1 - b_1)k_x^2 + \frac{1}{2}(a_2 - b_2)k_y^2 + \frac{1}{2}(A - B)k_x\right\}^2 +\right.$$

$$\left. + G^2 k_y^2 + \Delta^2\right]^{1/2} \tag{12}$$

where the notations are the same as in the above reference.

Thus in the presence of a quantizing magnetic field $H$ along $k_y$ direction, the modified $E - \vec{k}_y$ dispersion relations are given by

$$k_y^2 = \bar{a}E_{1,2} + \beta(E, n) \pm [\gamma(E_{1,2})^2 + \Theta(n)(E_{1,2}) + \Omega(n)]^{1/2} \tag{13}$$

where

$$\bar{a} \equiv d(d^2 - f^2)^{-1}, \quad d \equiv \frac{1}{2}(A + B), \quad f \equiv \frac{1}{2}(a_2 - b_2),$$

$$\beta(E, n) \equiv [G^2 + 2f Q(n) - 2d P(n)][2(d^2 - f^2)]^{-1},$$

$$Q(n) \equiv \left[2eH\hbar^{-1}\left(n + \frac{1}{2}\right)\sqrt{\bar{G}\bar{e}}\right]\left[1 + \frac{b^2}{4\bar{e}}\right]^{-1},$$

$$\bar{e} \equiv \frac{1}{2}(a_1 - b_1), \quad \bar{G} \equiv \frac{1}{2}(a_3 - b_3), \quad b^2 \equiv \frac{1}{4}(A - B)^2,$$

$$P(n) = 2eH\hbar^{-1}\left(n + \frac{1}{2}\right)\sqrt{ac}\left(1 + \frac{d^2}{4a}\right)^{-1},$$

$$a \equiv \frac{1}{2}(a_1 + b_1), \quad c \equiv \frac{1}{2}(a_3 + b_3), \quad \gamma \equiv f^2(d^2 - f^2)^{-2},$$

$$\Theta(n) \equiv [(d^2 - f^2)^{-2}\{dG^2 + 2fd\,Q(n) - 2P(n)\,d^2\}]$$

and

$$\Omega(n) \equiv [2(d^2 - f^2)]^{-2}[G^4 + 4G^2 f\,Q(n) - 4G^2 d\,P(n) -$$

$$- afd\,P(n)\,Q(n) + 4d^2 Q^2(n) + 4d^2\Delta^2 + 4f^2 P^2(n) + 4\Delta^2 f^2]$$

Therefore, the effective mass at the Fermi level $E_F$ corresponding to the $n$-th magnetic subband can be written as

$$m^*_{n,\pm}(E_F) = \frac{\hbar^2}{2}\left[\bar{a} \pm \frac{\{\gamma E_F + \frac{1}{2}Q(n)\}}{\sqrt{\gamma E_F^2 + Q(n)E_F + \Omega(n)}}\right]. \qquad (14)$$

It appears then that the evaluation of the effective Fermi level mass requires expression of the hole-statistics which in turn can be expressed, as

$$p_0 = \frac{eHg_v}{2\pi^2\hbar^2}\sum_{n=0}^{n_{max}}[\tau_1(E_F) + \tau_2(E_F)] \qquad (15)$$

where $g_v$ is the valley degeneracy,

$$\tau_1(E_F) \equiv [E_F\bar{a} + \beta(n) \pm \sqrt{\gamma E_F^2 + Q(n)E_F + \Omega(n)}]^{1/2}$$

and

$$\tau_2(E_F) \equiv \sum_{r=1}^{s} 2(k_B T)^{2r}(1 - 2^{1-2r})\,\zeta(2r)\frac{\mathrm{d}^{2r}}{\mathrm{d}E_F^{2r}}[\tau_1(E_F)].$$

## *3. Results and discussion*

Using Eqs. (3) and (5) together with the parameters[34–36] $H = 3\,\mathrm{T}$, $m_1 = m_0/172$, $m_2 = m_0/0.8 \approx m_2'$, $m_3 = m_0/88.5$, $E_g = 0.0153\,\mathrm{eV}$, $T_D = 2\mathrm{K}$, $T = 4.2\,\mathrm{K}$, $g_v = 3$ and $\Theta = 60°$, the normalized EMM of a few subbands in Bi are plotted as functions of the electron concentrations in Fig. 1. Plots of normalized EMM for a few subbands as functions of $H$ and $\Theta$ are given in Figs. 2 and 3, respectively. Again using Eqs. (14) and (15) and taking the parameters[31] $a_1 = -3.23 \times 10^{-19}\,\mathrm{eV \cdot m^2}$, $a_2 = -1.63 \times 10^{-19}\,\mathrm{eV \cdot m^2}$, $a_3 = -9.19 \times 10^{-19}\,\mathrm{eV \cdot m^2}$, $b_1 = -6.07 \times 10^{-19}\,\mathrm{eV \cdot m^2}$, $b_2 = -2.44 \times 10^{-19}\,\mathrm{eV \cdot m^2}$, $b_3 = -1.05 \times 10^{-6}\,\mathrm{eV \cdot m}$, $A = 2.97 \times 10^{-10}\,\mathrm{eV \cdot m}$, $B = -3.47 \times 10^{-10}\,\mathrm{eV \cdot m}$, $|G| = 1.30 \times 10^{-10}\,\mathrm{eV \cdot m}$, $\Delta = 0.070\,\mathrm{eV}$, $H = 3\,\mathrm{T}$ and $T = 4.2$, K we have plotted $m^*_{n\pm}(E_F)/m_0$ versus $p_0$ for the first two magnetic subbands as shown in Fig. 4. In Fig. 5, using the same procedure, we have also plotted the normalized magneto EMM versus $H$ for first two magnetic subbands corresponding to $p_0 = 10^{22}\,\mathrm{m^{-3}}$. From these figures and the above discussion the following features follow:

1. The EMM's increase with increasing electron concentration in a monotonic manner as expected for degenerate semiconductors and differ widely with $n_0$ for relatively small values for carrier degeneracy, whereas they converge to a single value for relatively larger values of $n_0$ in the whole range of concentrations considered.
2. The EMM's exhibit oscillatory dependence with magnetic field. It appears from the Figs. 1 to 3 that, the EMM's in Bi under arbitrary magnetic quantization depend on the electron concentration, the magnetic quantum number

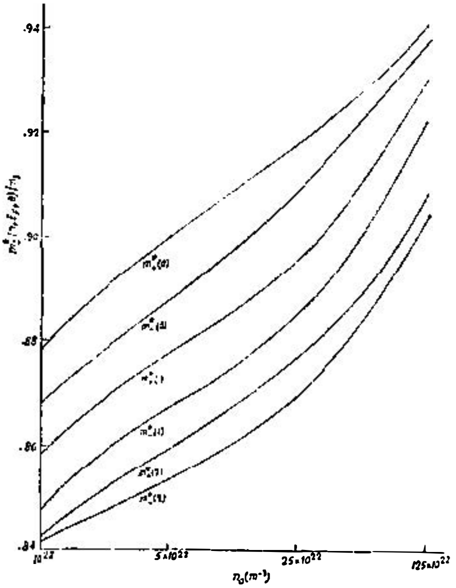

Fig. 1. Plot of the normalized EMM in Bi as a function of electron concentration under magnetic quantization for few magnetic subbands.

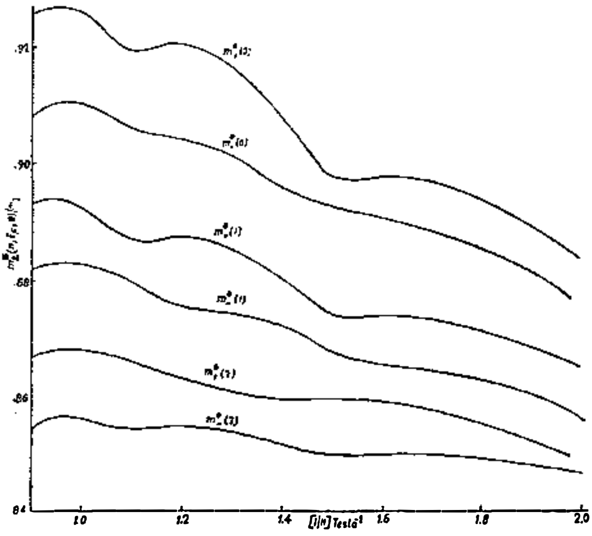

Fig. 2. Plot of the normalized EMM in Bi as a function of magnetic field for few magnetic subbands.

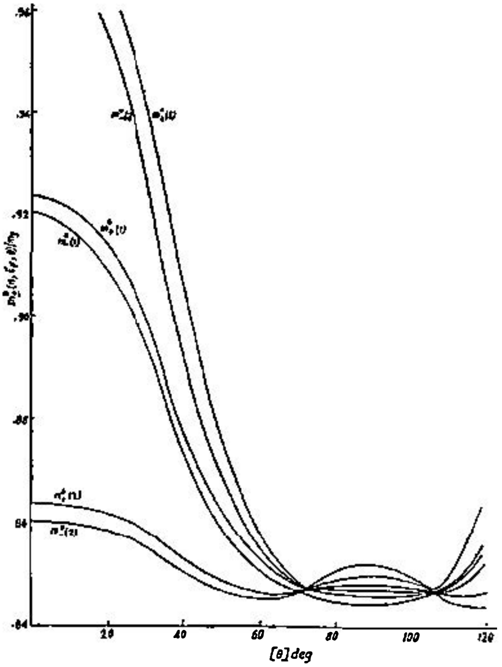

Fig. 3. Plot of the normalized EMM in Bi as a function of the orientation of the magnetic field for few magnetic subbands.

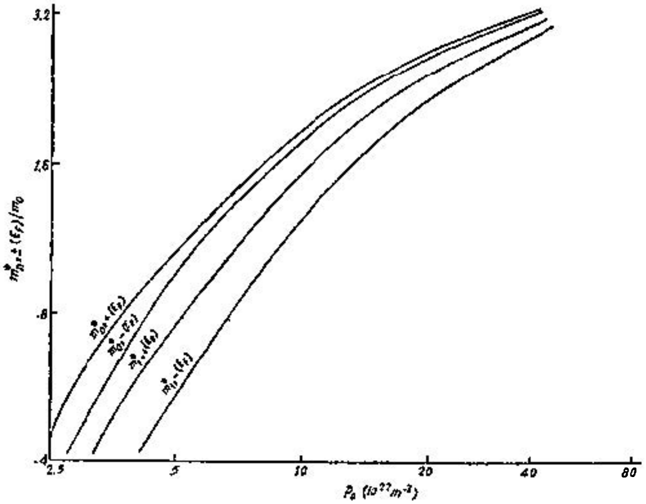

Fig. 4. Plot of the doping dependence of the normalized effective hole mass at the Fermi level in *p*-CdSb for the first two magnetic subbands at 4.2 K.

and the angle of orientation of the quantizing magnetic field, respectively, resulting in different effective masses at the Fermi level corresponding to different magnetic subbands. The dependence of EMM on $n_0$ and $n$ is solely due to band non-parabolicity while the reason behind the variation of effective mass with $\Theta$ lies in the anisotropies band edge effective masses. The EMM's show the oscillatory dependence both with $H$ and $\Theta$ in different manners. The SdH oscillations which occur in degenerate semiconductors would further be influenced by the index dependent EMM and the contribution of the oscillatory effective mass on the oscillatory mobility would be important.

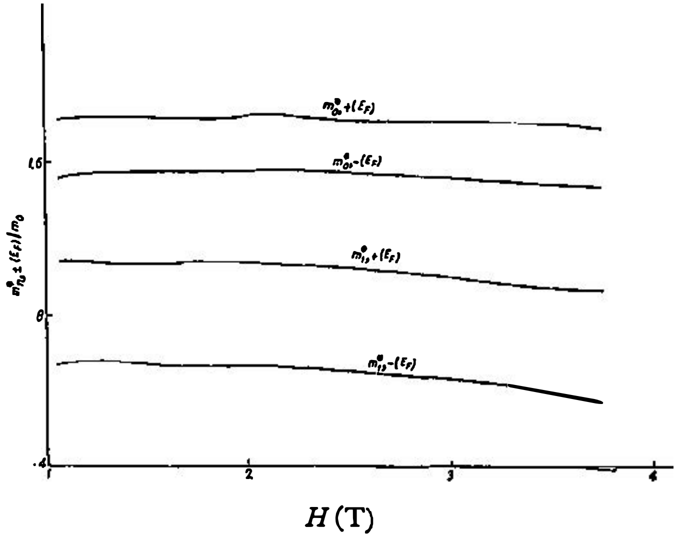

Fig. 5. Plot of the magnetic field dependence of the normalized effective hole mass at the Fermi level in $p$-CdSb for the first two magnetic subbands at 4.2 K.

3. The quantum number dependent behaviour of the effective hole mass in $p$-CdSb is a characteristic feature of the Yamada model and the same masses corresponding to different $n$ differ widely with each other for relatively small values of $p_0$ and,
4. the effective masses corresponding to different $n$ also differ widely in $p$-CdSb with each other for all values of $H$ in the whole range of magnetic field considered.

To the best of our knowledge, the experimental data concerning our results are not available, though the importance of understanding the EMM is already well-known in the field of semiconductor science. Finally we wish to note that although in a more rigorous treatment the many-body effects and the completely arbitrary orientation of the quantizing magnetic field should be considered along with a self-consistent procedure, our simplified analysis exhibits the basic qualitative features of the quantum number dependent EMM in Bi and $p$-CdSb under magnetic quantization, respectively.

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# O EFEKTIVNOJ MASI U MATERIJALIMA S MALIM ENERGETSKIM PROCIJEPOM PRI MAGNETSKOJ KVANTIZACIJI

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Razmatran je problem efektivne mase u materijalima s malim energetskim procijepom pri jakoj magnetskoj kvantizaciji. Kao primjer uzeti su Bi i *p*-CdSb. Za Bi je nađeno da efektivna masa na Fermi plohi ovisi o Fermijevoj energiji i magnetskom kvantnom broju kao posljedica neparaboličnosti energetske vrpce. Posljedica je različita efektivna masa za razne magnetske podvrpce. Kod *p*-CdSb efektivna masa šupljina također ovisi o magnetskom kvantnom broju.