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LETTER TO THE EDITOR

Magnetic field dependence of electron density in bismuth†

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Abstract. Using time-independent perturbation theory, the energy eigenvalue equation for a free-electron gas in bismuth with the McClure–Choi modified non-ellipsoidal non-parabolic (MNENP) model in the presence of a uniform DC magnetic field has been solved. We investigate the effect of the magnetic field on the electron density at very low temperatures and compare numerical results for this new band model with those for the Cohen NENP, Lax ENP, and EP models. Results show that quantum oscillations of the electron density for the MNENP model appear much more salient and considerable than those for other models. It seems that this MNENP model could be better for describing some physical phenomena of the magnetic field effect in bismuth for the very low-temperature limit.

Bismuth has been the subject of a large number of experimental and theoretical works. It is a semimetal with highly anisotropic Fermi surfaces. Some early works demonstrated that the Fermi surface for electrons in bismuth can be satisfactorily described by the ellipsoidal parabolic (EP) model (Shoenberg 1957). From theoretical calculations (Cohen 1961, Wu and Tsai 1974) and experimental results (Koch and Jensen 1969, Dinger and Lawson 1970, 1971, 1973), it was pointed out that the energy band in the bismuth structure follows the Cohen non-ellipsoidal non-parabolic (NENP) model. However, the magneto-optical results (Maltz and Dresselhaus 1970, Vecchi *et al* 1976) and the longitudinal magnetostriction (Michenaud *et al* 1981, 1982) supported the Lax ellipsoidal non-parabolic (ENP) model (Lax 1958). McClure and Choi (1977) presented a new energy band model for bismuth electrons which is more general than those currently in use. They showed that it can fit the data for a large number of magneto-oscillatory and resonance experiments. This new energy band model is called the McClure–Choi modified non-ellipsoidal non-parabolic (MNENP) model. It is the purpose of this report to calculate the magnetic energy levels in bismuth and study the effect of the DC magnetic field on the electron density for this new band model. We also make a comparison between these models.

From the report of McClure and Choi (1977), the new energy band model can be represented in the form of the relation between the energy E and momentum $\boldsymbol{p} = (p_x, p_y, p_z)$ of an electron gas as

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$$E\left(1+\frac{E}{E_g}\right)=\frac{p_x^2}{2m_1}+\frac{p_y^2}{2m_2}\left[1+\frac{E}{E_g}\left(1-\frac{m_2}{m_2'}\right)\right]+\frac{p_z^2}{2m_3}+\frac{p_y^4}{4m_2m_2'E_g}$$
$$-\frac{p_x^2p_y^2}{4m_1m_2E_g}-\frac{p_y^2p_z^2}{4m_2m_3E_g} \qquad (1)$$

where E_g is the energy gap between the L point valence and conduction bands. From experimental results (Antcliffe and Bate 1967, Dinger and Lawson 1970, 1971, 1973),

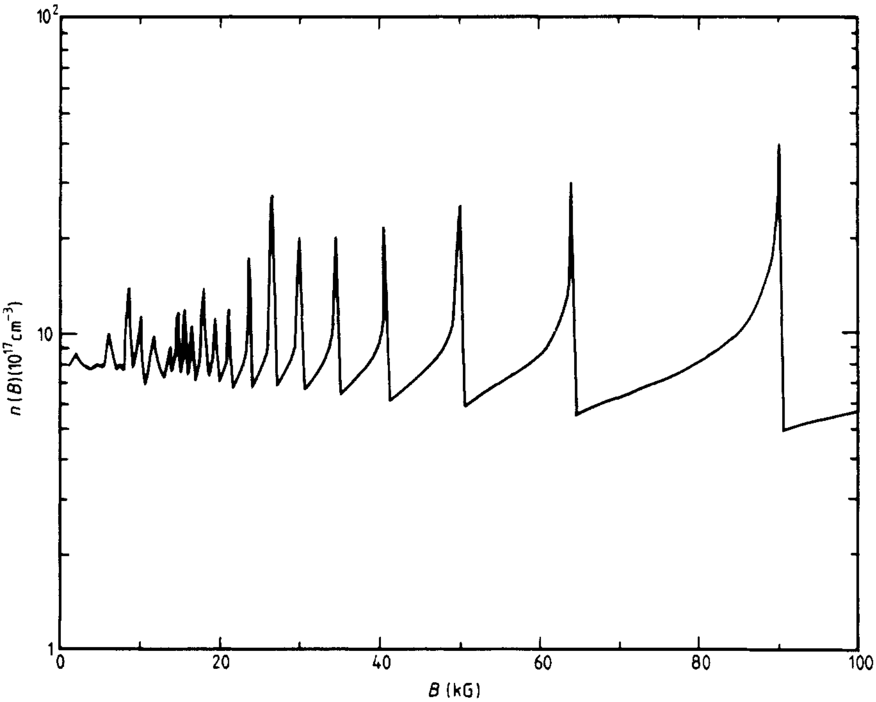

Figure 1. Electron density $n(B)$ as a function of DC magnetic field B in bismuth for the McClure–Choi MNENP model.

it has been indicated that the difference between m_2 and m_2' is quite small, i.e. $m_2 \simeq m_2'$. Thus the term in the square brackets of equation (1) can be considered as constant. For the sake of convenience, some parameters are defined by $\alpha_1 = m/m_1$, $\alpha_2 = (m/m_2)[1+(E/E_g)(1-m_2/m_2')] \simeq m/m_2$, $\alpha_3 = m/m_3$, $\alpha_4 = m/2m_2m_2'E_g$, $\alpha_5 = m/2m_1m_2E_g$, and $\alpha_6 = m/2m_2m_3E_g$, where m is the mass of the free electron. The difference between the MNENP and NENP models is that there are two extra terms of $-p_x^2p_y^2/4m_1m_2E_g$ and $-p_y^2p_z^2/4m_2m_3E_g$ in equation (1) for the MNENP model. Thus the energy eigenvalue equation in a DC magnetic field $\boldsymbol{B}$ directed along the z direction can be written as

$$H_0(1+H_0/E_g)\Psi_{kns} = (1/2m)\{\alpha_1p_x^2+\alpha_2(p_y-eBx/c)^2+\alpha_3p_z^2+\alpha_4$$
$$\times(p_y-eBx/c)^4-(\alpha_5/2)[p_x^2(p_y-eBx/c)^2+(p_y-eBx/c)^2p_x^2]$$
$$-\alpha_6p_z^2(p_y-eBx/c)^2\}\Psi_{kns}$$
$$=E_{kns}(1+E_{kns}/E_g)\Psi_{kns} \qquad (2)$$

where E_{kns} is the true energy of the system defined by $H_0\Psi_{kns} = E_{kns}\Psi_{kns}$. Using time-independent perturbation theory and considering

$$H' = \alpha_4(p_y - eBx/c)^4 - (\alpha_5/2)[p_x^2(p_y - eBx/c)^2 + (p_y - eBx/c)^2 p_x^2] - \alpha_6 p_z^2(p_y - eBx/c)^2 \tag{3}$$

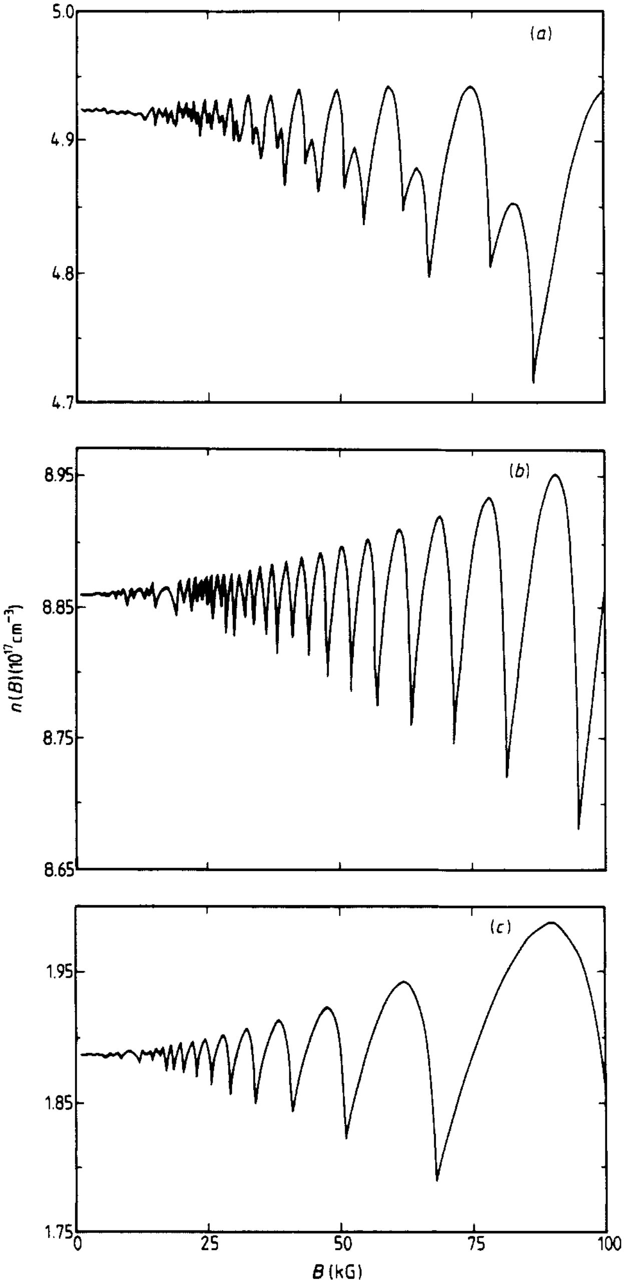

Figure 2. Electron density $n(B)$ as a function of DC magnetic field B in bismuth for: (a) the Cohen NENP model: (b) the Lax ENP model; and (c) the EP model.

as perturbation terms, the eigenfunctions and eigenvalues up to first order for equation (2) are given by

$$\Psi_{kns}(\boldsymbol{r}) = \begin{pmatrix} \dfrac{1+s}{2} \\ \dfrac{1-s}{2} \end{pmatrix} \exp(\mathrm{i}k_y y + \mathrm{i}k_z z)\Big\{\Phi_n(x-x_0) + \left(\frac{\hbar\omega_c}{32E_g}\right)[n(n-1)$$
$$\times (n-2)(n-3)]^{1/2}\Phi_{n-4}(x-x_0) + \left(\frac{\hbar\omega_c}{16E_g}\right)\left[(2n-1) - \frac{(\hbar k_z)^2/m^*}{\hbar\omega_c}\right]$$
$$\times [n(n-1)]^{1/2}\Phi_{n-2}(x-x_0) - \left(\frac{\hbar\omega_c}{16E_g}\right)\left((2n+3) - \frac{(\hbar k_z)^2/m^*}{\hbar\omega_c}\right)$$
$$\times [(n+1)(n+2)]^{1/2}\Phi_{n+2}(x-x_0) - \left(\frac{\hbar\omega_c}{32E_g}\right)[(n+1)(n+2)$$
$$\times (n+3)(n+4)]^{1/2}\Phi_{n+4}(x-x_0)\Big\} \qquad (4)$$

and

$$E_{kns} = -\tfrac{1}{2}E_g\Bigg(1 - \Bigg\{1 + \left(\frac{4}{E_g}\right)\Bigg[(n+\tfrac{1}{2})\hbar\omega_c + \tfrac{1}{2}s\hbar\omega_s$$
$$+ \frac{(\hbar k_z)^2}{2m^*}\left(1 - \frac{(n+\frac{1}{2})\hbar\omega_c}{2E_g}\right) + (n^2+n+1)\frac{(\hbar\omega_c)^2}{4E_g}\Bigg]\Bigg\}^{1/2}\Bigg) \qquad (5)$$

where $s = \pm 1$, $\omega_c = (|e|B/mc)(\alpha_1\alpha_2)^{1/2}$, $x_0 = ck_y\hbar/eB$, $m^* = m/\alpha_3$, and $\Phi_n(x)$ is the harmonic oscillator wavefunction. ω_s is defined by $\omega_s = |e|B/m_s c$, where m_s is the spin effective mass that has a relation with the spin-splitting factor g such that $m_s/m = 2/g$. For bismuth, the spin effective mass is equal to the cyclotron mass (Giura *et al* 1969), i.e., $m_s = m/(\alpha_1\alpha_2)^{1/2}$. Consequently $\omega_s = \omega_c$ for the pure bismuth.

For the calculation of the electron density in the conduction band, it is assumed that the interesting temperature is near absolute zero. Then one can obtain

$$n(B) = (\omega_c/\sqrt{2}\pi^2\hbar^2)(m^3/\alpha_1\alpha_2\alpha_3)^{1/2}$$
$$\times \sum_{s=\pm1}\sum_{n=0}^{N}\left[\frac{E_F(1+E_F/E_g) - (n+s/2+\frac{1}{2})\hbar\omega_c - (n^2+n+1)(\hbar\omega_c)^2/4E_g}{1-(n+\frac{1}{2})\hbar\omega_c/2E_g}\right]^{1/2} \qquad (6)$$

where $N = \min(N_1, N_2)$, and N_1 and N_2 should satisfy the conditions

$$(N_1^2 + N_1 + 1)(\hbar\omega_c)^2/4E_g + (N_1 + \tfrac{1}{2}s + \tfrac{1}{2})\hbar\omega_c < E_F(1 + E_F/E_g) \qquad (7)$$

and

$$(N_2 + \tfrac{1}{2})\hbar\omega_c < 2E_g \qquad (8)$$

where E_F is the Fermi energy at $B = 0$.

As a numerical example for bismuth, the relevant parameters are (Fal'kovskiĭ 1968) $\alpha_1 = 172$, $\alpha_2 = 0.8$, $\alpha_3 = 88.5$, $E_g = 0.0153$ eV, and $E_F = 0.0276$ eV. In figure 1, the electron density for the McClure–Choi MNENP model is shown as a function of the DC magnetic field. It can be seen that the electron density for the MNENP model oscillates saliently and considerably with the magnetic field, and the amplitude and period of quantum oscillations increase with the field. In figure 2, the electron density as a function of magnetic field for the NENP, ENP, and EP models is shown on a larger scale for the values of $n(B)$. It can be seen that in these three band models, some quantum oscillations with the magnetic field also appear, although their amplitudes are much smaller than those for the MNENP model. However, the number of quantum oscillations for the NENP and ENP models is much larger than that for the EP model.

From our numerical results presented here, it shows that the mean value of the electron density for the MNENP model is almost the same as that for the ENP model (Édel'man 1975), but not the same as that for the NENP model. Moreover, the quantum oscillations of the electron density for the MNENP model appear much more saliently than those for other models. From equation (6) it can be seen that there exists a singular point for each period when the quantum number n satisfies

$$(x + \tfrac{1}{2})\hbar\omega_c = 2E_g \tag{9}$$

with $n = [x]$, where $[x]$ denotes the greatest integer $\leqslant x$. From this relation, $n(B)$ will increase rapidly and then abruptly decrease with the magnetic field for each period when n is very close to x. These quantum oscillations of the electron density with the magnetic field have a sharp cusp-like peak for each period as the same type of de Haas–van Alphen oscillations (Liu and Toxen 1965). Consequently, the MNENP model could be better for describing some physical phenomena of the magnetic-field effect in bismuth for the very low-temperature limit.

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