PHYSICAL REVIEW B **79**, 081102(R) (2009)

Origin of the peaks in the Nernst coefficient of bismuth in strong magnetic fields

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(Received 20 December 2008; published 17 February 2009)

We explain the origin of most of the peaks in the Nernst coefficient that were recently observed at magnetic fields directed along the trigonal axis and the bisectrix direction in bismuth. Additional experiments are discussed that enable one to verify our explanation.

DOI: 10.1103/PhysRevB.79.081102 PACS number(s): 71.70.Di, 71.18.+y, 72.15.Jf

In a recent paper[1] oscillations of the Nernst coefficient in bismuth were observed for the magnetic fields directed along the trigonal and bisectrix axes of the crystal. Moreover, several unusual peaks of this coefficient were discovered for very high magnetic fields H ($14 \leq H \leq 33$ T) parallel to the trigonal axis.[2] These peaks were concomitant with quasiplateaus in the Hall coefficient, and the authors of Ref. 2 suggested that these results are a signature of an exotic quantum fluid reminiscent of the fluid associated with the fractional quantum Hall effect. Interestingly, in the same interval of the high magnetic fields several jumps of the magnetization were observed, which were ascribed to field-induced instabilities of the ground state of interacting electrons in bismuth.[3]

In this paper we show that positions of the peaks in the Nernst signal for H along the bisectrix axis and for $H < 12$ T applied along the trigonal axis can be explained using a simple model of the electron energy spectrum of bismuth in magnetic fields. In particular, the most of the peaks are due to the hole Fermi surface of bismuth, while some peaks result from its electron part. On the basis of our calculation we also predict additional peaks that have not yet been observed. However, the unusual peaks observed in the Nernst signal at high magnetic fields cannot be explained in this way directly. Nevertheless, we show that at least some of these peaks can be reproduced if one assumes that a small deviation in the magnetic-field direction from the trigonal axis occurred in the experiments. We also theoretically analyze dependences of the peaks on this tilt angle of the magnetic field. These angular dependences will enable one to distinguish between the peaks that appear even in the one-electron approximation and the peaks that are really due to collective effects.

The electron-band structure of bismuth is well known; see, e.g., Refs. 4 and 5 and the references cited therein. The Fermi surface of bismuth consists of one hole ellipsoid located at the T point of its Brillouin zone and of three closed electron surfaces of nearly ellipsoidal shape centered at the points L. The spectrum of the holes in bismuth is well approximated by the simple parabolic model.[4] On the other hand, the electron spectrum near point L is accurately described by the model of McClure,[6] and the parameters of this model are well known.[5,7] However, in the framework of the McClure model the spectrum of the electrons *in a magnetic field* H can be found analytically only if H is directed along the longest axis of the electron ellipsoid, i.e., if $\mathbf{H}$ practically coincides with the bisectrix axis.[7] To find the Landau levels of the electrons for an arbitrary direction of H, two empirical expressions for these levels were proposed many years ago.[8,9] These expressions permitted one to describe a number of experimental data.[8–11] Below we shall use the expression suggested in Ref. 8 to analyze the oscillations of the Nernst coefficient.

The electron ellipsoid at point L is elongated along the bisectrix axis. If one describes this ellipsoid by the so-called model of Lax[12] in which only linear terms in quasimomentum p are taken into account in the electron Hamiltonian, the electron spectrum in the magnetic field H can be found analytically at any direction of H. But the Lax model cannot accurately describe the electron ellipsoid along its elongation, and that is why McClure[6] took into account also quadratic terms in p for this direction in his Hamiltonian. It is these terms that do not permit one to find the spectrum analytically at the arbitrary directed magnetic fields within the McClure model.

To allow for the deviation in the real electron spectrum from the Lax model, Smith *et al.*[8] suggested a simple generalization of the formula that describes the Landau levels in the model of Lax. According to Ref. 8, in the presence of the magnetic field H the nth Landau level E_n for an electron with the quasimomentum p_H along $\mathbf{H}$ can be found from the equation

$$E\left(1+\frac{E}{E_G}\right)=\left(n+\frac{1}{2}\right)\hbar\omega_c+\frac{p_H^2}{2m_H}\pm\frac{1}{2}g\beta_0 H, \qquad (1)$$

where signs $\pm$ correspond to the electron spins that are antiparallel and parallel to $\mathbf{H}$, respectively; the energy E is measured from the edge of the conduction band; ω_c is the cyclotron frequency

$$\omega_c=\frac{eH}{m_c c},$$

E_G is the gap between the conduction and valence bands at point L; g is the effective electron g factor at this point; β_0 is the Bohr magneton; and the longitudinal and the cyclotron masses, m_H and m_c, are given by

$$m_H=\mathbf{h}\cdot\mathbf{m}^e\cdot\mathbf{h}, \qquad (2)$$

$$m_c=[\det \mathbf{m}^e/m_H]^{1/2}. \qquad (3)$$

Here $\mathbf{h}$ is the unit vector in the direction of the magnetic field H. The effective-mass tensor $\mathbf{m}^e$ has the form

1098-0121/2009/79(8)/081102(4)

TABLE I. Parameters of the Smith-Baraff-Rowell spectrum (Ref. 8).

Electrons	m_{11}	m_{22}	m_{33}	m_{23}
Orbital mass	0.00113	0.26	0.00443	−0.0195
Spin mass	0.00101	2.12	0.0109	−0.13
Holes		$M_1=M_2$		M_3
Orbital mass		0.07[a]		0.69
Spin mass		0.033		200
$E_g=15.3$ meV			$E_0=38.5$ meV	

[a]Reference 13.

$$\mathbf{m}^e=\begin{pmatrix} m_{11} & 0 & 0 \\ 0 & m_{22} & m_{23} \\ 0 & m_{23} & m_{33} \end{pmatrix}, \tag{4}$$

where axes 1 and 3 coincide with the binary and the trigonal axes, respectively, while axis 2 is along the bisectrix direction. The effective g factor,

$$g^2=4m^2\frac{\mathbf{h}\cdot\mathbf{m}_s^e\cdot\mathbf{h}}{\det\mathbf{m}_s^e}, \tag{5}$$

is defined in terms of a spin-mass tensor $\mathbf{m}_s^e$ that has the form similar to Eq. (4). Within the Lax model the spectrum is also described by formulas (1)–(5), and $\mathbf{m}_s^e$ exactly coincides with $\mathbf{m}^e$. Smith *et al.*[8] admitted that the elements of $\mathbf{m}_s^e$ may differ from the elements of $\mathbf{m}^e$ and that they are free parameters. This is just the generalization proposed in Ref. 8.

Since the spectrum of the holes at point T is parabolic, the Landau levels for them can be easily found,[4]

$$E_0-E=\left(n+\frac{1}{2}\right)\hbar\omega_c+\frac{p_H^2}{2m_H}\pm\frac{1}{2}g\beta_0H, \tag{6}$$

where E_0 is the edge of the hole band at this point of the Brillouin zone. The cyclotron frequency ω_c, the masses m_c and m_H, and the g factor are defined by the same formulas (2), (3), and (5) as for the electrons, but now the tensor of the effective masses for the holes $\mathbf{m}^h$ has the form

$$\mathbf{m}^h=\begin{pmatrix} M_1 & 0 & 0 \\ 0 & M_2 & 0 \\ 0 & 0 & M_3 \end{pmatrix}, \tag{7}$$

and a similar expression is valid for the spin-mass tensor $\mathbf{m}_s^h$. All the parameters in Eqs. (1)–(7) are known for bismuth[8] (see Table I).

In our subsequent discussion we shall denote the Landau levels $E_n(p_H=0)$ as $n_{e,h}^{\mp}$, where n is the quantum number of the level, the subscripts e and h stand for electrons and holes, and the signs $\mp$ correspond to the electron spin directed up and down, respectively. Figure 1 shows the H dependence of these levels for the electrons and holes in bismuth in the case of the magnetic field directed along the trigonal axis. In this figure we also show the H dependence of the Fermi level μ that is found from the equality of the concentrations of the electrons and holes in bismuth. Since the electron levels that are below $\mu(H)$ and the hole levels lying above $\mu(H)$ are filled, one can easily trace the change in the population of the levels with increasing H.

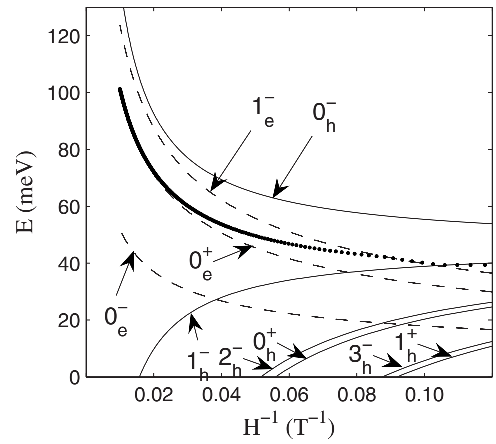

FIG. 1. The H dependence of the Landau levels for the electrons (the dashed lines) at point L and for the holes (the solid lines) at point T in bismuth. The dependence of the Fermi level on H is also shown (the line with dots). The symbols near the lines indicate the Landau-level numbers and the direction of the spin projection on the magnetic field. The subscripts e and h stand for the electrons and holes.

Figure 2 shows the magnetic fields at which the calculated electron and hole Landau levels cross the Fermi energy. This figure also shows the experimental Nernst signal[1,2] for low temperatures $T\sim1$ K. It is seen that the experimental peaks with large amplitudes are caused by the hole ellipsoid, and their positions are well reproduced by our calculation. At the magnetic fields $H<2.5$ T the electron ellipsoids practically do not manifest themselves in the oscillations of the Nernst coefficient due to the low mobility of the electrons as com-

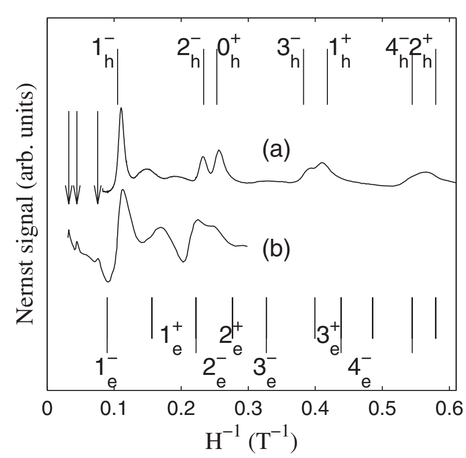

FIG. 2. The Nernst signal in the case of the magnetic field directed along the trigonal axis. Curve (a) reproduces the experimental data of Ref. 1, while curve (b) presents the data of Ref. 2 obtained with the same crystal. The vertical lines mark the calculated magnetic fields at which the appropriate electron and hole Landau levels cross the Fermi energy. The notation of the Landau levels is the same as in Fig. 1. The arrows show positions of the unusual peaks (Ref. 2) seen in curve (b).

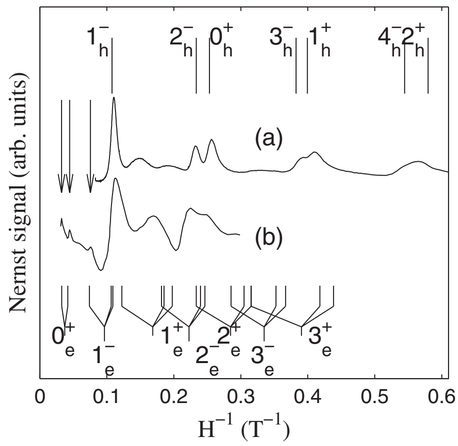

FIG. 3. The same as Fig. 2, but with the magnetic field slightly tilted away from the trigonal axis. Here the magnetic-field direction $\mathbf{h}=(\sin\theta\cos\psi, \sin\theta\sin\psi, \cos\theta)$ is given by $\theta=2.5°$ and $\psi=85°$. We also show the splitting of the electron Landau levels.

pared to the mobility of the holes.[1] Only relatively small maxima seen in the interval $2.5\ \mathrm{T}<H<10\ \mathrm{T}$ can be attributed to the electrons. But the calculated positions of the electron peaks do not agree accurately with the experimental data. Moreover, the positions of the small experimental maxima vary from sample to sample and from experiment to experiment.[14] However, the most essential point is that the calculation does not reveal any peaks at the magnetic fields higher than 11 T. When $H>11\ \mathrm{T}$, the only hole level 0_h^- and the two electron levels 0_e^+ and 0_e^- are filled, and these levels do not cross $\mu(H)$ with increasing H.

Of course, one should keep in mind that the above formulas for the electron Landau levels are not exact. In the case of high magnetic fields corrections to these formulas were studied in Refs. 9 and 10. However, our analysis shows that such corrections can only partly improve the situation, e.g., it is possible to fit the electron energy levels 1_e^+ and 2_e^- so that to describe accurately electron maxima between the hole peaks 1_h^- and 2_h^- in curve (a), but these corrections cannot describe the unusual peaks observed in the magnetic fields above 11 T.

To resolve this problem, we assume that in the experiments[1,2] the magnetic field was slightly tilted away from the trigonal axis. Then, the following explanation of these experimental data is possible: There are three electron ellipsoids in bismuth, and their energy levels coincide only if the magnetic field is directed strictly along the trigonal axis. If the magnetic field begins to tilt away from this axis, each electron Landau level in Fig. 1 splits into two or three levels (this depends on the plane of the tilt). The electron energy level 0_e^+ closely approaches $\mu(H)$ in high magnetic fields (Fig. 1). When the tilt splits this level, the levels resulting from 0_e^+ can intersect $\mu(H)$ in the magnetic fields $H>11\ \mathrm{T}$.

To be specific, consider the case when the magnetic-field direction $\mathbf{h}=(\sin\theta\cos\psi, \sin\theta\sin\psi, \cos\theta)$ is given by the angles $\theta=2.5°$ and $\psi=85°$. In this case each electron level splits into three levels, and the calculated intersections of these split levels with $\mu(H)$ are shown in Fig. 3. Now the two levels resulting from 0_e^+ indeed intersect $\mu(H)$ at the

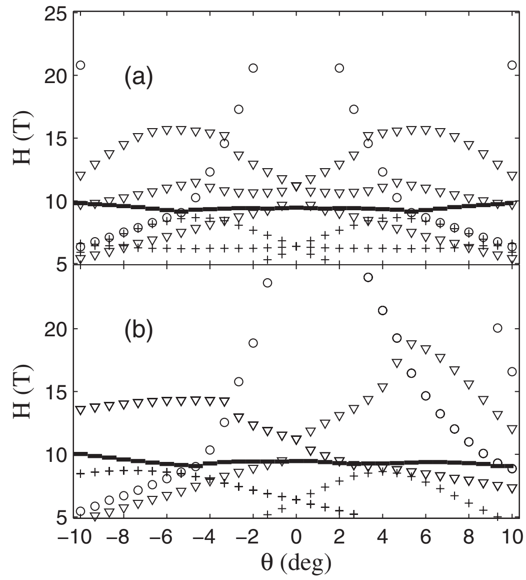

FIG. 4. The calculated angular dependences of the magnetic fields, $H(\theta)$, at which the electron and hole Landau levels cross the Fermi energy; θ is the angle between the magnetic field and the trigonal axis. The magnetic field tilts either (a) toward the binary axis or (b) toward the bisectrix axis. The positions of the hole peak 1_h^- are shown by the thick lines, while positions of the electron peaks 0_e^+, 1_e^-, and 1_e^+ are marked by the circles, triangles, and crosses, respectively.

magnetic fields that are close to the positions of the two unusual peaks seen in curve (b) [the third level does not cross $\mu(H)$]. On the other hand, the intersection of one of the levels 1_e^- practically coincides with the position of the third unusual peak of this curve. Thus, it is quite possible that the unusual peaks can result from the intersection of the chemical potential with the Landau levels split by a tilt of the magnetic field. A small uncontrollable tilt of the magnetic field can also explain why the positions of the electron peaks vary from experiment to experiment.[14] To verify this expla-

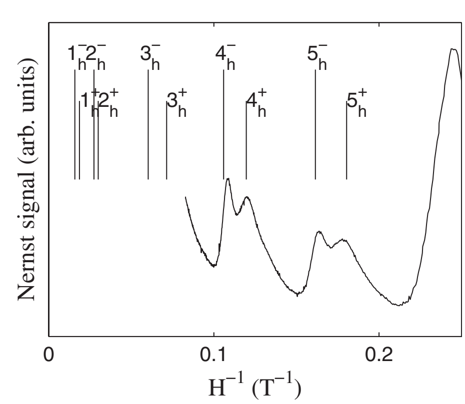

FIG. 5. The Nernst signal in the case of the magnetic field directed practically along the bisectrix axis (Ref. 1). The vertical lines show the calculated magnetic fields at which the appropriate Landau levels of the holes cross the Fermi energy. The magnetic-field direction $\mathbf{h}=(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ with $\theta=92°$, $\psi=85°$ is chosen so that the Landau-level spacing leads to the observed period (Ref. 1) of the oscillations.

nation and to find out which of the unusual peaks are really due to some nontrivial physics, it is necessary to measure angular dependences of their positions.

In Fig. 4 we show intersections of some Landau levels with $\mu(H)$ in the θ-H plane. Interestingly, the upper part of this figure is closely reminiscent of Fig. 3 in Ref. 3 in which experimental data were obtained for the magnetic fields lying in the trigonal-binary plane. In particular, the angular dependences of the magnetic fields at which the Landau levels 0_e^+ and 1_e^- cross the chemical potential $\mu(H)$ are close to the transition lines $H_2(\theta)$ and $H_1(\theta)$ experimentally defined in Ref. 3. These angular dependences are also close to the appropriate dependences recently computed[15] within a tight-binding model of the bismuth spectrum.

We also calculate the Landau levels when the magnetic field is close to the bisectrix direction. The obtained results are presented in Fig. 5. For this geometry in the magnetic fields $H>6$ T all the electrons are in the lowest Landau level, and the oscillations of the Nernst signal[1] shown in Fig. 5 are due to the holes. Note that in the region of high magnetic fields the calculation predicts additional peaks in the Nernst signal which have not been observed yet.

In conclusion, the Smith-Baraff-Rowell model[8] is sufficient to explain the origin of most of the peaks in the Nernst coefficient that were recently observed in bismuth.[1,2] It seems that the positions of some unusual peaks discovered at very high magnetic fields oriented along the trigonal axis can be understood under the assumption that the magnetic field was slightly tilted away from the trigonal axis in these experiments. This assumption can be verified by analyzing the positions of these peaks in tilted magnetic fields. These angular dependences will enable one to select the peaks that are really due to a nontrivial physics. We calculate these angular dependences for the magnetic fields **H** lying in the two principal planes containing the trigonal axis. The results obtained in one of the planes are reminiscent of the recent experimental data.[3] Our calculation also predicts additional high-field peaks in the Nernst signal at the magnetic field oriented along the bisectrix direction.

We thank K. Behnia for useful discussions and for providing us with the experimental data of Figs. 2 and 3. This work was supported by the France-Ukraine program of scientific collaboration “DNIPRO.”

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