## Features of the magnetic susceptibility of semimetals

S. D. Beneslavskii and L. A. Fal'kovskii

L. D. Landau Theoretical Physics Institute, USSR Academy of Sciences (Submitted April 3, 1975) Zh. Eksp. Teor. Fiz. 69, 1063-1071 (September 1975)

The magnetic susceptibility of bismuth and of its alloys with antimony is calculated. Its dependence on temperature and on the magnitude and direction of the magnetic field is found. The resulting features of the susceptibility are determined by the structure of the electron energy spectrum.

PACS numbers: 75.30.C

### INTRODUCTION

The magnetic susceptibility of semimetals of the bismuth type has been studied theoretically and experimentally in many papers. The interest in the magnetic properties of semimetals is explained, firstly, by the fact that the conditions for observing oscillations in their susceptibilities (the de Haas-van Alphen effect) are most favorable by virtue of the small cyclotron masses. Secondly, the constant part of the susceptibility of Bi is an order of magnitude greater than the typical value in metals, given by the Pauli-Landau formula:

$$\chi_0 = \left(\frac{e}{2\pi c}\right)^2 \frac{p_F}{m} \left(\frac{g^2}{4} - \frac{1}{3}\right). \tag{1}$$

(Throughout, we shall use a system of units with  $\hbar = 1$ .) The semimetals are diamagnetic, although their effective g-factor, appearing in (1) and equal to twice the ratio of the spin splitting of the levels to the cyclotron splitting, is close to 2; in this case, it follows from (1) that  $\chi_0 > 0$ .

The correct qualitative explanation of the anomalous diamagnetism of Bi was given by Adams<sup>[1]</sup>, who drew attention to the fact that the nearby filled energy band makes a large contribution

$$\chi \sim -\chi_0 E_0/\gamma, \qquad (2)$$

to the susceptibility, where  $E_0$  is an atomic-scale energy and  $\gamma$  is the small energy gap at the Brillouin-zone boundary. A quantitative calculation of the susceptibility of bismuth and of its alloys with antimony was carried out by Buot and McClure<sup>[2]</sup>. They used the model proposed by Lax for the energy spectrum of the electrons in Bi:

$$\varepsilon \left(1 + \varepsilon/\varepsilon_g\right) = \alpha_{ik} p_i p_k, \tag{3}$$

where  $\alpha_{ik}$  is the tensor of the inverse effective masses,  $\epsilon_g$  is the width of the gap, and the momentum p is measured from the point L of the Brillouin zone. It was found that the susceptibility of the filled band is determined by the electrons with large momenta, when the dispersion law (3) emerges into the linear part  $\epsilon \sim p$ .

In order of magnitude, the susceptibility is

$$\chi \sim \left(\frac{ev}{\pi c}\right)^2 \int \frac{dp}{\varepsilon(p)} \sim -\left(\frac{e}{\pi c}\right)^2 v \ln \frac{E_0}{\varepsilon_s},\tag{4}$$

where v is of the order of the usual velocity of electrons in metals. Buot and McClure<sup>[2]</sup> used the energy  $E_0$ , cutting off the logarithmic integral, and also the quantity  $\epsilon_g$ , as adjustable parameters, achieving agreement with the measured value of  $\chi$  in BiSb alloys<sup>[3]</sup>.

A comparison of their results with those of Adams<sup>[1]</sup> shows that the susceptibility depends essentially on the

behavior of the electron spectrum at large momenta. In Adams' work the cyclotron mass far from the Fermi level is constant, and the corresponding integral (cf. formula (11) below) diverges linearly. In the work of Buot and McClure, at large p the cross-sectional are of a constant-energy surface is  $S \sim p^2 \sim \epsilon^2$  and the mass  $m \sim \partial S/\partial \epsilon \sim \epsilon$ , which leads to the logarithm in formula (4).

The actual form of the spectrum over a wide range of momenta is not known. For this reason, a complete calculation of the susceptibility is impossible. It is of interest to calculate the particular contribution to  $\chi$  due to a small region about the points L, where a certain expansion of the spectrum is valid.

In Lax's model, as can be seen from (4), the susceptibility has a logarithmic singularity in  $\epsilon_g$ . However, the Lax model gives a poor description of the dependence of the electron energy on the momentum component  $p_z$  in the direction of elongation of the electron constant-energy surface. In a paper by Abrikosov and one of the authors<sup>[4]</sup> a theory of the group-V semimetals was constructed, starting from which Abrikosov<sup>[5]</sup> showed that for small spacing between the two bands at the point L the spectrum has the form

$$\left(\varepsilon - \frac{\varepsilon_s}{2} - \frac{p_x^2}{2M_1}\right) \left(\varepsilon + \frac{\varepsilon_s}{2} + \frac{p_z^2}{2M_2}\right) = v_x^2 p_x^2 + v_y^2 p_y^2, \tag{5}$$

where  $M_i$  and  $v_i$  are positive constants and  $\epsilon_g$  depends on the concentration of Sb and the pressure.

It can be seen from (5) that one of the principal values of the tensor  $\alpha_{ik}$  in (3) is equal to zero, while the dependence of the energy on the momentum in the corresponding direction is quadratic. A spectrum of the type (5) was first proposed by Cohen<sup>[6]</sup>, who, in order to describe the experimentally-known large anisotropy of the electron Fermi surface, put  $\alpha_{ZZ} = 0$  in (3) and took the dependence on  $p_Z$  into account by the kp-method.

In the present paper we calculate the magnetic susceptibility of substances of the Bi type in the framework of the theory of<sup>[4]</sup>. It is shown that when the field direction is perpendicular to the trigonal axis, the contribution to the susceptibility of the electrons of the two bands described by Eq. (5) is determined by a small region about the extrema, i.e., does not contain additional unknown constants apart from the parameters in (5). The result depends on the mutual arrangement of the bands-direct ( $\epsilon_g > 0$ ) and inverted ( $\epsilon_g < 0$ ). The treatment is carried out both for weak fields, when the susceptibility does not depend on the field, and for the ultra-quantum limit, which is attainable, e.g., in pure bismuth in fields H > 10 kOe. It turns out that in the latter case the susceptibility is determined by the filled band  $(\chi_{\perp}^{(1)} \sim -H^{-1/4})$  and does not depend on  $\epsilon_g$ . Because of the small size of  $\epsilon_g$ , in a weak field the susceptibility  $\chi_{\perp}^{(1)} \sim -T^{-1/2}$  in a broad range of temperatures.

Besides the closely-spaced bands (5), another filled band figures in the theory of Abrikosov and one of the authors<sup>[4]</sup>, separated from (5) by a distance  $\gamma$  that is large compared with  $\epsilon_g$  but small on the atomic scale. The contribution  $\chi_1^{(2)}$  of this band and the filled bands at the point T is found to be of the order of  $-\chi_0 E_0/\gamma$ (which coincides with Adams' estimate (2)) and depends weakly on the state of the crystal. With a magnetic field parallel to the C<sub>3</sub> axis, the contribution of the bands (5) to the susceptibility  $\chi_{||}$  turns out to be small compared with the susceptibility of the other filled bands, at both the L- and T-points. Therefore, the quantity  $\chi_{||}$ , like  $\chi_1^{(2)}$ , is practically independent of the composition of the alloy, the temperature, etc.

### 1. WEAK-FIELD SUSCEPTIBILITY

The magnetic susceptibility is determined from the dependence of the thermodynamic potential on the magnetic field:

$$\Omega(H) = -\frac{eHT}{4\pi^2 c} \sum_{n,\sigma} \int dp \ln\left[1 + \exp\left(\frac{\mu - \varepsilon_{np}^{(\sigma)}}{T}\right)\right],$$
 (6)

where the summation is performed over the Landau number n and the energy-band index  $\sigma$  (with the spin taken into account), and the integration is performed over the momentum component p along the field direction.

The energy levels  $\epsilon_{np}^{(\sigma)}$  near the point L in a magnetic field were obtained by the authors<sup>[7]</sup> and are determined by the equation

$$S(\varepsilon, p) = 2\pi e H (n + \frac{1}{2} \pm \frac{g}{4})/c, \qquad (7)$$

$$S(\varepsilon, p) = \frac{\pi}{|h_{\varepsilon}| v_{\varepsilon} v_{v}} \left( \varepsilon - \frac{\varepsilon_{\varepsilon}}{2} - \frac{p^{2}}{2M_{i} h_{\varepsilon}^{2}} \right) \left( \varepsilon + \frac{\varepsilon_{\varepsilon}}{2} + \frac{p^{2}}{2M_{z} h_{\varepsilon}^{2}} \right), \qquad (8)$$

where  $h_z$  is the cosine of the angle between H and the direction of elongation of the surface (5). The quantity  $S(\epsilon, p)$  is the section of the surface (5) cut by a plane perpendicular to the magnetic field;  $p \cdot h = p = \text{const.}$ The two signs in (7) correspond to the two spin projections, and the effective g-factor differs from 2 by small quantities of the order of  $\epsilon_g/Mv^2$  ( $M \sim M_i$ ,  $v \sim v_i$ ). The formulas (7) and (8) are valid for  $|h_z| \gg (\epsilon_g/Mv^2)^{1/2}$ . We emphasize that the expressions (7) and (8), being quasi-classical in form, are valid for all n, including n = 0.

In the limit of weak fields, we can calculate to order  $H^2$  using the Euler-MacLaurin formula:

$$\sum_{n=0}^{\infty} F(n) = \int_{0}^{\infty} F(n) dn + \frac{1}{2} F(0) - \frac{1}{12} F'(0).$$
 (9)

Integrating the first term in (9) by parts and using (7), we obtain for the H-dependent correction to  $\Omega$ :

$$\Omega(H) = -\frac{1}{(2\pi)^3} \sum_{\sigma} \int dp \left\{ \int_{\epsilon_{0p}}^{\epsilon_{0p}} de f(e) \left[ S(e, p) \pm \frac{\pi e H}{2c} g \right] + \frac{\pi f(e_{0p}^{(\sigma)})}{6m_{0p}^{(\sigma)}} \left( \frac{eH}{c} \right)^2 \right\}, \quad m_{0p}^{(\sigma)} = \frac{1}{2\pi} \frac{\partial S(e, p)}{\partial e} \Big|_{n=0}$$
(10)

where  $f(\epsilon)$  is the Fermi distribution function.

Differentiating (10) twice with respect to H, summing over the spin and letting  $H \rightarrow 0$ , we find

$$\chi = \frac{1}{8} \left(\frac{e}{\pi c}\right)^2 \left(\frac{g^2}{4} - \frac{1}{3}\right) \sum_{\sigma=1,2} \int dp f(\varepsilon_p^{(\sigma)}) / m_p^{(\sigma)}, \qquad (11)$$

and the dependence  $\epsilon_p^{(\sigma)}$  is determined from the condition

$$S(\varepsilon, p) = 0. \tag{12}$$

From formula (11) we obtain the correct expression (1) for the susceptibility of a free-electron gas. The sign of the susceptibility of substances of the Bi type is explained by the dominant contribution of occupied

states with negative mass  $m_p^{(\sigma)}$  and  $g\approx$  2.

### 2. SINGULAR PART OF $\chi_1^{(1)}$ IN A WEAK FIELD

Using (8) we find the cyclotron mass near the point L:

$$m(\varepsilon, p) = \frac{1}{2\pi} \frac{\partial S(\varepsilon, p)}{\partial \varepsilon} = \left[ \varepsilon + \frac{p^2}{4h_z^2} (M_z^{-1} - M_i^{-1}) \right] / |h_z| v_z v_y.$$
(13)

The condition (12) and formula (8) determine the electron spectrum in the two bands as  $H \rightarrow 0$ :

$$\varepsilon_p^{(1)} = \frac{\varepsilon_d}{2} + \frac{p^2}{2M_1 h_z^2}, \quad \varepsilon_p^{(2)} = -\frac{\varepsilon_d}{2} - \frac{p^2}{2M_2 h_z^2}.$$
(14)

Substituting (14) into (13), we obtain

$$m_{p}^{(1,2)} = \pm \left( \varepsilon_{\varepsilon} + \frac{p^{2}}{2Mh_{z}^{2}} \right) / 2 |h_{z}| v_{z} v_{y},$$

where  $M^{-1} = M_1^{-1} + M_2^{-1}$ .

Summation over the three points L in the Brillouin zone can be performed by going over to integration over  $p/|h_Z|$  in (11). As a result, an expression arises that does not depend on the field direction in the basal plane, and a factor  $\frac{3}{2}$  appears. Neglecting the deviation of g from 2, we obtain

$$\chi_{\pm}^{(1)} = \left(\frac{e}{\pi c}\right)^2 \frac{v_x v_y}{2} \int_0^\infty dp \, \frac{f(e_p^{(1)}) - f(e_p^{(2)})}{e_s + p^2/2M},$$

$$e_p^{(1,2)} = \pm (e_s/2 + p^2/2M_{1,2}).$$
(15)

The expression obtained depends on T,  $\epsilon_g$  and the chemical potential  $\mu$ -quantities which can be varied in an experiment. For T = 0 the integrand in (15) vanishes in regions of p in which carriers are either present or absent in both bands simultaneously:  $f(\epsilon_p^{(1)}) = f(\epsilon_p^{(2)})$ .

Therefore, with the direct arrangement  $(\epsilon_g > 0)$  of the bands and for  $\mu > \epsilon_g/2$  (the current carriers are electrons), we have

$$\chi_{\perp}^{(1)} = -\left(\frac{c}{\pi c}\right)^2 v_z v_y \left(\frac{M}{2\varepsilon_s}\right)^{\frac{1}{2}} \left[\frac{\pi}{2} - \operatorname{arctg}\left(\frac{M_1(\mu - \varepsilon_s/2)}{M\varepsilon_s}\right)^{\frac{1}{2}}\right]. \quad (16)$$

The case  $\mu < -\epsilon_g/2$  (holes) is described by the formula obtained from (16) by replacing  $M_1(\mu - \epsilon_g/2)$  by  $M_2(|\mu| - \epsilon_g/2)$  in the argument of the arctangent.

It can be seen from (16) that as the number of carriers in the bands decreases the diamagnetism increases, attaining the limiting value

$$\chi_{\perp}^{(1)} = -\frac{e^2 v_x v_y}{2\pi c^2} \left(\frac{M}{2e_g}\right)^{\frac{1}{2}}.$$
 (17)

Formula (17) describes the dependence of the susceptibility of semiconducting BiSb alloys at low temperatures in a weak field. The singularity in  $\epsilon_g$  in (17) is stronger than that obtained by Buot and McClure<sup>[2]</sup>.

The current carriers in the bands are paramagnetic, and for large concentrations of them  $(|\mu| > \epsilon_g)$  the diamagnetism decreases with increasing  $\mu$  according to the law (for definiteness, we assume that  $\mu > 0$ ):

$$\chi_{\perp}^{(1)} = -\left(\frac{e}{\pi c}\right)^2 \frac{v_x v_y M}{(2M_1 \mu)^{\frac{1}{2}}}.$$
 (18)

Another interesting case when the final answer can be obtained in explicit form is the limit  $T \gg \epsilon_g$ ,  $\mu$ , which, in alloys with small  $\epsilon_g$  and  $\mu$ , can be attained at moderate temperatures. In this case we obtain

$$\chi_{\perp}^{(1)} = -CT^{-\frac{\nu_{1}}{2}}, \quad C = \left(\frac{e}{4c}\right)^{2} \frac{v_{x}v_{y}}{(2\pi)^{\frac{\nu_{1}}{2}}} \frac{M_{1}M_{2}^{\frac{\nu_{1}}{2}} + M_{2}M_{1}^{\frac{\nu_{1}}{2}}}{M_{1} + M_{2}}.$$
 (19)

With the inverted arrangement of the bands and at T = 0, in the case  $|\mu| < |\epsilon_g|/2$  we obtain from (15)

$$\chi_{\perp}^{(1)} = -\left(\frac{e}{\pi c}\right)^{2} \frac{v_{\pi} v_{\nu}}{2} \left(\frac{M}{2|e_{s}|}\right)^{\frac{1}{2}} \left\{ \ln \left| \frac{M_{1}^{\frac{1}{2}} (|e_{s}|/2+\mu)^{\frac{1}{2}} + |Me_{s}|^{\frac{1}{2}}}{M_{1}^{\frac{1}{2}} (|e_{s}|/2+\mu)^{\frac{1}{2}} - |Me_{s}|^{\frac{1}{2}}} \right|$$

$$+ (M_{1} \rightarrow M_{2}, \quad \mu \rightarrow -\mu) \right\}.$$
(20)

If  $\mu > |\epsilon_{\mathbf{g}}|/2$ , the susceptibility is given by formula (20), in which we need only retain the first term in the brackets, while for  $\mu < -|\epsilon_{\mathbf{g}}|/2$  we need retain only the second. Naturally, (20) goes over into (18) at high electron concentrations  $(|\mu| > |\epsilon_{\mathbf{g}}|)$ .

The susceptibility described by formula (20) as a function of the chemical potential has singularities. Near the point  $\mu = |\epsilon_g|/2$ , we have

$$\chi_{\perp}^{(1)} = -\left(\frac{e}{\pi c}\right)^{2} \frac{\nu_{x}\nu_{y}}{2} \left|\frac{M}{2e_{s}}\right|^{\frac{1}{2}} \left\{\ln\frac{M_{1}^{\frac{1}{2}}+M^{\frac{1}{2}}}{M_{1}^{\frac{1}{2}}-M^{\frac{1}{2}}} + 2\left|\frac{M_{s}(|e_{s}|/2-\mu)}{Me_{s}}\right|^{\frac{1}{2}}\theta\left(\frac{|e_{s}|}{2}-\mu\right)\right\}$$
(21)

and the derivative  $\partial_{\chi}/\partial\mu$  becomes infinite. There is a stronger singularity at the band-intersection point

$$\bar{\mu} = \frac{|\varepsilon_d|}{2} \frac{M_2 - M_1}{M_2 + M_1},$$

near which

$$\chi_{\perp}^{(1)} = -\left(\frac{e}{\pi c}\right)^{2} \left|\frac{M}{2\epsilon_{s}}\right|^{\frac{1}{2}} v_{z}v_{y} \ln\left|\frac{\epsilon_{s}}{\mu-\bar{\mu}}\right|.$$
(22)

The singularities (21) and (22) of  $\chi_{\perp}^{(1)}$  are connected with the topology of the Fermi surface in the absence of a magnetic field: the first, (21), is due to the change in the connectivity of the surface as we pass through the saddle point and is similar to the singularity that we discovered earlier<sup>[7]</sup> in the density of states. The second, (22), arises when the Fermi level passes through the conical point, in the vicinity of which the cyclotron mass is small. The singularities in the susceptibility are smoothed out at finite temperatures; in particular, the magnitude of the logarithm in (22) is of the order of ln ( $|\epsilon_{\rm g}|/T$ ). An analogous role is played by the interaction of the electrons with each other and with impurities.

# 3. SINGULAR PART OF $\chi^{(1)}_{\rm L}$ IN A STRONG FIELD

We shall consider the variation of  $\chi_{\perp}^{(1)}$  with increase of the magnetic-field intensity. So long as the cyclotron frequency  $\omega = eH/cm(\epsilon, p)$  is small compared with  $\mu$ and T, the monotonic part of  $\chi_{\perp}^{(1)}$  is determined by the formulas of Sec. 2, and the oscillating component appearing in the range  $|\mu| > \omega > T$  is given by the Lifshitz-Kosevich formula<sup>[8]</sup>. The monotonic part of the susceptibility is substantially changed when  $\omega \gg |\mu|$ , T,  $|\epsilon_g|$ . Then it is convenient to separate out the contribution of the completely filled band in formula (6), adding (for  $\mu > |\epsilon_g|/2$ ) or subtracting (for  $\mu$ 

 $\mu < -|\epsilon_g|/2$ ) the term with n = 0. The summation over

the levels of this band is conveniently performed using Poisson's formula:

$$\sum_{n} F(n) = \sum_{n=\infty}^{\infty} \int_{0}^{\infty} F(n) e^{2\pi i n v} dn.$$
(23)

If we take into account that, to good accuracy, g = 2, the summation over the spins in formula (6) reduces to the result that each term with  $n \neq 0$  appears twice and the term with n = 0 appears once. The prime in (23) allows for this. Using (23), summing over the spins and integrating the terms with  $\nu \neq 0$  by parts over n we obtain

$$\Omega(H) = \Omega_0 - \frac{eH}{2\pi^2 c} \sum_{\nu=1}^{\infty} \int dp \int_0^{\infty} dn f(\varepsilon_{np}) \frac{\sin 2\pi n\nu}{\pi \nu} \frac{\partial \varepsilon_{np}}{\partial n} - \frac{eH}{4\pi^2 c} \int dp [(\mu - \varepsilon_{0p}^{(1)}) f(\varepsilon_{0p}^{(1)}) - (\mu - \varepsilon_{0p}^{(2)}) (1 - f(\varepsilon_{0p}^{(2)})],$$
(24)

where, of the two spin branches, we choose for  $\epsilon_{np}$  the one which corresponds to the minus sign in front of g in (7);  $\epsilon_{0p}^{(1,2)}$  are given by formula (14);  $\Omega_0$  is the H-

independent potential of the completely filled band and the effect of the magnetic field on this band is taken into account by the sum over  $\nu$ . The derivative  $\partial \epsilon / \partial n$  appearing in (24) is calculated by means of (7) and (8):

$$\frac{\partial \varepsilon_{np}}{\partial n} = -\lambda^2 \left[ \left( \varepsilon_z + \frac{p^2}{2Mh_z^2} \right)^2 + 4\lambda^2 n \right]^{-h},$$
$$\lambda^2 = 2eHv_z v_y |h_z|/c.$$

Formula (11), which we used in a weak field, is obtained if we integrate the second term in (24) by parts and take into account that when  $\epsilon$  is differentiated with respect to n the factor  $\lambda^2/(\epsilon_g + p^2/2Mh_Z^2)^2$ , which is small in a weak field, appears. If  $\lambda \gg |\epsilon_g|$ , T, then  $p \sim (\lambda M)^{1/2}$ are important in the second integral in (24); we can then omit  $\epsilon_g$  and replace the distribution function by unity. We obtain

$$\Omega(H) = \Omega_0 + D |h_z H|^{1/4}$$

$$\frac{eH|h_z|}{3\pi^2 c} \left\{ (2M_1)^{\frac{n}{4}} \middle| \mu - \frac{\varepsilon_d}{2} \middle|^{\frac{n}{4}} \theta \left( \mu - \frac{\varepsilon_d}{2} \right) + (\mu \rightarrow -\mu, M_1 \rightarrow M_2) \right\}, \quad (25)$$

$$D = \left( \frac{e}{c} \right)^{\frac{n}{4}} \frac{M^{\frac{n}{4}} (v_z v_y)^{\frac{n}{4}}}{\pi^{\frac{n}{4}} 2^{\frac{n}{4}}} \Gamma \left( \frac{1}{4} \right) \zeta \left( \frac{7}{4} \right) \cos \frac{\pi}{8}.$$

The numerical coefficient that has appeared here is

$$\tau^{-1/4} 2^{-\frac{1}{4}} \Gamma\left(\frac{1}{4}\right) \zeta\left(\frac{7}{4}\right) \cos\frac{\pi}{8} = 0.0566$$

In formula (25) it is necessary to sum the contributions of the three points L. We recall that  $h_Z$  is the cosine of the angle between the field direction and the direction of elongation of the "ellipsoid" situated at one of the three L-points. The dependence on the field direction, which vanished in a weak field, remains in a strong field. It can be detected, evidently, in measurements of the derivative of the torque with respect to the field direction  $(\partial^2 \Omega / \partial \varphi^2)$ .

In the semiconducting region ( $\epsilon_g > 0$  and  $|\mu| < \epsilon_g/2$ ), the expression in the curly brackets in (25) is absent. The magnetic moment and susceptibility are determined as follows:

$$M_{\perp}^{(1)} = -\frac{7}{4} H^{\nu_{1}} D \sum_{L} |h_{z}|^{\nu_{1}}, \quad \chi_{\perp}^{(1)} = -\frac{21}{16} H^{-\nu_{1}} D \sum_{L} |h_{z}|^{\nu_{1}}. \quad (26)$$

The field-direction dependence contained here is weak:

$$\sum_{L} |h_z|^{1/4} \approx \frac{3}{2}.$$

In the semimetallic region, besides the magnetic moment (26) there is the moment  $\delta M^{(1)}$  due to the

"free" carriers with n = 0, which arises on differentiation of the expression in the curly brackets in (25) with respect to H. For example, with the direct arrangement of the bands ( $\epsilon_g > 0$ ),

$$\delta M_{\perp}^{(1)} = \frac{e}{3\pi^2 c} (2M_1)^{\gamma_h} \left(\mu - \frac{\varepsilon_s}{2}\right)^{\gamma_h} \sum_{L} |h_z| \theta \left(\mu - \frac{\varepsilon_s}{2}\right).$$
(27)

The quantity (27) depends on the field direction, since

$$\sum_{L} |h_{z}| = \sum_{n=0}^{z} \left| \cos \left( \varphi + \frac{2\pi n}{3} \right) \right|$$

where  $\varphi$  is the angle between H and the bisector axis. In addition, the chemical potential  $\mu$  depends on the direction and also on the magnitude of the field. This dependence is determined from the electroneutrality condition. Owing to the large difference in the cyclotron masses of the electrons at L and of the holes at T, there exists a wide range of fields for which the holes at T are in quasi-classical levels and the electrons at L are in ultra-quantum levels. In this case, for  $\mu > \epsilon_{\rm g}/2$ , the electroneutrality requirement gives

$$\frac{e}{c} HM_{1}^{"_{t}} \left( \mu - \frac{e_{s}}{2} \sum_{L} |h_{z}| = \frac{4}{3} m_{\parallel}^{"_{t}} m_{\perp} (E_{T} - \mu)^{"_{t}} \right)$$

where  $E_T - \mu$  is the Fermi-hole energy, reckoned from the bottom of the valence band, and  $m_{\parallel}$  and  $m_{\perp}$ are the cyclotron masses of the holes for H parallel and perpendicular to  $C_3$ .

In the limit of fields that are sufficiently large but for which the condition for the holes to be quasi-classical is still fulfilled, and with neglect of the deviation of the electron g-factor from 2,  $(\mu - \epsilon_g/2)^{1/2} \sim H^{-1}$  and  $\delta M_{\perp}^{(1)} \sim H^{-3}$ . In such fields the contribution of (27) to the susceptibility turns out to be small compared with that of (26):

$$\frac{\delta\chi_{\perp}^{(1)}}{\chi_{\perp}^{(1)}} \sim \left[ \left( \frac{c}{eH} \right)^{3/2} \frac{m_{\parallel}m_{\perp}^{2}(E_{\tau} - \varepsilon_{\theta}/2)^{3}}{Mv} \right]^{\frac{1}{2}}$$

### 4. REGULAR PART OF THE SUSCEPTIBILITY $\chi^{(2)}$

Inasmuch as the spectrum near L in a magnetic field parallel to  $C_3$  is unknown, we shall give an order-ofmagnitude estimate of the contribution of the points L to the susceptibility using (11). Neglecting the 6° declination of the electron "ellipsoid" from the basal plane, and also the difference in the masses  $M_1$  and  $M_2$ , we have for the area of a section of the surface (5):

$$S(\varepsilon, p_{y}) = \frac{2}{v_{x}} \int \left[\varepsilon^{2} - \left(\frac{\varepsilon_{s}}{2} + \frac{p_{z}^{2}}{2M}\right)^{2} - v_{y}^{2} p_{y}^{2}\right]^{\frac{1}{2}} dp_{z}.$$

We are interested in the mass

$$m(\varepsilon, p_{\nu}) = \frac{\varepsilon}{\pi v_{x}} \int \left[ \varepsilon^{2} - \left( \frac{\varepsilon_{g}}{2} + \frac{p_{z}^{2}}{2M} \right)^{2} - v_{\nu}^{2} p_{\nu}^{2} \right]^{-h} dp_{z},$$

calculated with the condition (12). If  $\epsilon_g > 0$ , the section vanishes when  $\epsilon$  has the following relationship with py:

$$\varepsilon^2 = \varepsilon_g^2 / 4 + v_y^2 p_y^2.$$

The corresponding value of the mass is equal to

$$n_{p_{y}} = -\left[\frac{2M}{\varepsilon_{g}}\left(\frac{\varepsilon_{g}^{2}}{4} + v_{y}^{2}p_{y}^{2}\right)\right]^{\frac{1}{2}}v_{x}^{-1}.$$
 (28)

Substituting (28) into (11), we obtain an estimate of the contribution of the points L to  $\chi_{11}$ :

$$\chi_{\parallel,L} \sim \frac{1}{8} \left(\frac{\bar{g}e}{\pi c}\right)^2 \left(\frac{\varepsilon_s}{M}\right)^{\frac{1}{2}} \ln \frac{v\bar{p}}{\varepsilon_s}, \qquad (29)$$

where  $\overline{p} \sim \gamma/v$  is the maximum value of the momentum at which it is still possible to use the expansion (5), and  $\overline{g}$  is the characteristic magnitude of the g-factor for H || C<sub>3</sub>. Since a typical value of the logarithm in (29) is of the order of a few units, the quantity (29) is small compared with (17), principally by virtue of the small size of  $\epsilon_g/Mv^2$ , which in semimetals does not exceed a few per cent.

Besides the states describable by Eq. (5), the deeper levels near the point L, considered earlier<sup>[4]</sup>, can make a contribution to the susceptibility  $\chi_{II^*}$ . This contribution is analogous to the contribution (which we shall estimate using the known spectrum<sup>[4]</sup>) of the deep levels near the point T to the susceptibility  $\chi_{\perp}^{(2)}$ . In the lowest band the area of the section for  $H \perp C_3$  can vanish at  $p_H^2 = [\epsilon^2 - (\gamma + \Delta)^2]/b^2$ , near which

$$S(\varepsilon, p_H) = \frac{\pi}{ab} \left[ \varepsilon^2 - (\gamma + \Delta)^2 - p_H^2 b \right] \left( \frac{\gamma \Delta}{\varepsilon^2 - \gamma^2 - \gamma \Delta} \right)^{1/2},$$

where  $\gamma$ ,  $\Delta$ , a and b are parameters describing the spectrum near T. Differentiating S, we find the mass

$$m_{p_H} \longrightarrow -(\gamma \Delta)^{\nu/h}/ab \quad \text{for } p_H \gg \gamma/b.$$
 (30)

The momentum-independent mass (30) leads to Adams' estimate (2); the quantities  $\gamma$  and  $\Delta$  are of the same order.

The contribution of the lower band at T for  $H \parallel C_3$  is estimated in a similar way. The corresponding section is

$$S(\varepsilon, p_z) = \frac{\pi}{h^2} \left\{ \varepsilon^2 - \Delta^2 - \gamma^2 + a^2 p_z^2 - 2 \left[ \gamma^2 \Delta^2 + (\varepsilon^2 - \gamma^2) a^2 p_z^2 \right]^{\prime h} \right\}$$

and the mass  $m_{p_Z} \rightarrow -\Delta/\pi b^2$  for  $p_Z \gg \gamma/a$ , whence we again obtain the estimate (2) for  $\chi_{||}$ .

Thus, the contribution of the point T to  $\chi_{\perp}$  and  $\chi_{||}$  is determined by the large momenta and therefore depends little on the temperature and the carrier concentration in the vicinity of T.

#### DISCUSSION OF THE RESULTS

The monotonic part of the susceptibility of semimetals of the bismuth type and of the semiconducting alloys based on them can be represented in the form of a sum of two terms. One of these,  $\chi^{(2)}$ , depends little on the temperature, the composition of the alloy and the magnitude of the field. The contribution  $\chi^{(2)}$  is estimated by formula (2) and arises from fairly deep states, both at the T<sub>-</sub> and at the L-points of the Brillouin zone, the relative proportions of these depending on the field direction. The greatest interest lies in  $\chi^{(\bar{1})}$ . This term appears only when  $H \perp C_3$  and is determined by a small region about the points L. The susceptibility  $\chi^{(1)}$  depends on the temperature, the magnitude of the magnetic field and the parameters characterizing the charge carriers at the L-points. An estimate of the ratio  $\chi^{(1)}/\chi^{(2)}$ by means of (2) and (17) shows that in bismuth the regular part and singular part of the susceptibility turn out to be of the same order.

The dependence (26) of  $\chi_{\perp}^{(1)}$  on the field has been observed in the experiment of  $[{}^{[9]}$ . The other singularities of  $\chi_{\perp}^{(1)}$ —the increase as  $\epsilon_{\rm g} \rightarrow 0$  (cf. (17)) and also in the inversion region ((20)—(22))—have not yet been investigated experimentally.

We take the opportunity to thank N. B. Brandt and M. V. Semenov for communicating the results of the experiment before publication.

#### S. D. Beneslavskii and L. A. Fal'kovskii

<sup>1</sup>E. N. Adams, Phys. Rev. 89, 633 (1953).

- <sup>2</sup> F. A. Buot and J. W. McClure, Phys. Rev. B6, 4525 (1972).
- <sup>3</sup>L. Wehrli, Phys. Kondens, Materie 8, 87 (1968).
- <sup>4</sup>A. A. Abrikosov and L. A. Fal'kovskii, Zh. Eksp. Teor. Fiz. 43, 1089 (1962) [Sov. Phys.-JETP 16, 769 (1963)].
- <sup>5</sup>A. A. Abrikosov, J. Low Temp. Phys. 8, 315 (1972).
- <sup>6</sup>M. H. Cohen, Phys. Rev. 121, 387 (1961).
- <sup>7</sup>S. D. Beneslavskiĭ and L. A. Fal'kovskiĭ, Fiz. Tverd.
- Tela 16, 1360 (1974) [Sov. Phys.-Solid State 16, 876 (1974)].
- <sup>8</sup>I. M. Lifshitz and A. I. Kosevich, Zh. Eksp. Teor. Fiz.
- 29, 730 (1955) [Sov. Phys.-JETP 2, 636 (1956)].
- <sup>9</sup>N. B. Brandt and M. V. Semenov, Zh. Eksp. Teor. Fiz. 69, 1072 (1975) [this issue, next article].

Translated by P. J. Shepherd 114