ELECTRONS AND HOLES IN BISMUTH

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Submitted to JETP editor February 1, 1965

J. Exptl. Theoret. Phys. (U.S.S.R.) 49, 265-274 (July, 1965)

The theory [1] is compared with experiment. The values of the parameters of the theory are determined with the aid of an electronic computer from data on cyclotron resonance,[3] magnetic susceptibility,[2] and conductivity [4,7] measurements. The calculated and experimentally measured values are presented in Tables I and II.

THE energy spectrum of electrons and holes in metals with a bismuth-type space lattice was obtained earlier.[1] The investigation in [1] was based on regarding the virtual deformation, through which the simple cubic lattice can be transformed into the lattice of the actual metal, as a small perturbation. The atomic displacements necessary for this purpose constitute approximately $1/20$ of the interatomic distances in the case of bismuth and $1/10$ in the case of arsenic. Near the points at which the degeneracy is lifted, small groups of carriers appear. The holes are located at the intersection of the trigonal axis of the crystal (the C_3 axis) with the boundaries of the Brillouin zone (the points $\mathbf{k}_0$ and $-\mathbf{k}_0$ in the notation of [1]), and their equal-energy surface has D_{3d} symmetry. The electrons are located near the points in which the "former" three-fold symmetry axes cross the boundaries of the zone (the points $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$, $-\mathbf{k}_1$, $-\mathbf{k}_2$, $-\mathbf{k}_3$). The proper symmetry of these points is C_{2h}, and rotations about the C_3 axis transform them into one another (Fig. 1).

We note that the theory enables us to change the places of the electrons and the holes; the arrangement indicated above corresponds to experiment in the sense of the symmetry of the equal-energy surfaces. In all, one hole and three electron sections of the Fermi surface are obtained per zone. The purpose of this paper is a quantitative comparison of the theory of [1] with the experimental data on bismuth, a metal which has been investigated in greatest detail.

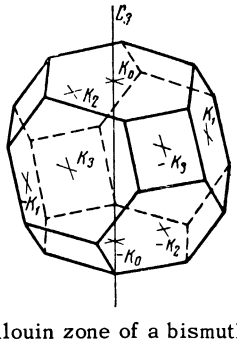

FIG. 1. Brillouin zone of a bismuth-type lattice.

HOLES

The spectrum of the holes is described by the equation

$$(\Omega^2 - \Delta^2 - \gamma^2 - p^2 - q^2)^2 - 4(\gamma^2\Delta^2 + p^2\Delta^2 + p^2q^2) = 0,$$
$$p = ak_z, \quad q = b(k_x^2 + k_y^2)^{1/2} \equiv bk_\perp; \tag{1}$$

where Δ and γ are constants characterizing respectively the spin-orbit coupling and the deformation, referred to above, Ω is the energy variable, and a and b are constants with the dimension of velocity. The origin is located at the point $\mathbf{k}_0$, the z axis is directed along the trigonal axis of the crystal, the x axis along the two-fold symmetry axis (C_2 axis), and the y axis is perpendicular C_2 and C_3. Equation (1) has axial symmetry (that is, a symmetry higher than D_{3d}), owing to the neglect of the terms of next higher order in q.

In the derivation of (1) we took into account four closely lying bands. Therefore Eq. (1) is of fourth degree in Ω. When $p = q = 0$ (the point at which in the case g of Fig. 5 of [1] the extrema of $\Omega(\mathbf{k})$ are realized), we have

$$\Omega_{1,2,3,4} = \pm(\gamma \pm \Delta). \tag{2}$$

The condition for p and q to vary within finite limits (as follows from experiment, the Fermi surface of the holes in bismuth is closed), is written in the form[1)]

[1)]The value of Ω corresponding to the Fermi level will be denoted by the same letter Ω.

Table I. Holes

	Experiment	Theory		Experiment	Theory
$m(0)/m_0$	0.062±0.003 [3] *	0.0585	$n\cdot10^{-17}$, cm^{-3}	2.75 [4]	3.15
$m\left(\frac{\pi}{2}\right)/m_0$	0.195±0.004 [3]	0.196	$\frac{dn}{d\Omega}\cdot10^{-19}$, cm$^{-3}\cdot$ eV^{-1}		3.75
$S(0)\cdot10^{42}$, cgs esu	6.75±0.25 [2] 6.8±0.1 [7]	6.97	ε_Φ, eV	0.011 [4]	0.013
			E_0, eV		0.124
			E_1, eV		0.732
$S\left(\frac{\pi}{2}\right)\cdot10^{42}$, cgs esu	20.5±1.5 [2] 21.2±1.0 [7]	22.7	E_2, eV		0.981
			E_3, eV		0.248

*We used the preliminary data of [3].

$$\Omega^2 < \gamma^2. \tag{3}$$

Our problem is to determine the parameters γ, Δ, Ω, a, and b. The most convenient for this purpose are the data obtained from measurements of oscillations of the magnetic susceptibility [2] and cyclotron resonance [3]. The period of the former, as is well known, is determined by the magnitude of the extremal area (in the direction **n** along the magnetic field) of the section of the Fermi surface; the plane of the section is perpendicular to the vector **n**. We shall denote this quantity by $S(\mathbf{n})$ since it depends on the direction of **n** of the magnetic field relative to the crystallographic axes. The period of the cyclotron oscillations is determined by the cyclotron mass $m(\mathbf{n}) = (2\pi)^{-1}\,\partial S/\partial\Omega$ (its extremal value, or the value on the limit points).

It is easy to see that the area of the section and the mass reach their extrema in the central section of the surface (1). For a definite relation between Ω, γ, and Δ (case h of Fig. 5 in [1]), and in certain directions of **n**, the area can be extremal not only on the central section, whereas the mass has only one extremum.

When **n** is directed along a three-fold axis, we have for the central section ($p = 0$)

$$S(0) = \pi k_\perp^2 = \pi b^{-2}[\Omega^2 - (|\gamma| - |\Delta|)^2], \tag{4}$$

$$m(0) = \Omega / b^2. \tag{5}$$

When **n** is directed along a two-fold axis on the central section ($k_x = 0$) we obtain

$$S\left(\frac{\pi}{2}\right) = \int dk_y dk_z = \frac{2}{ab}\int_0^{x_1} \frac{dx}{1+x^2}\{(1+x^2)[2\Delta^2(\gamma^2+\Omega^2) - (\gamma^2-\Omega^2)^2(1+x^2)] - \Delta^4\}^{1/2},$$

where x_1 denotes the positive value of the variable x_1, at which the expression in the curly brackets in the integral vanishes [under condition (3) there is one such value]. Simple transformations lead to the expression

$$S\left(\frac{\pi}{2}\right) = \frac{2\Delta^2 m}{ab\,\mathrm{sh}\,\psi}\int_0^{\pi/2} d\alpha \frac{\sin^2\alpha(1-\varkappa^2\sin^2\alpha)^{1/2}}{\mathrm{ch}^2\psi/\varkappa^2 - \sin^2\alpha},$$

$$\mathrm{sh}\,\psi = \frac{|\gamma|-|\Omega|}{2|\gamma\Omega|^{1/2}},\quad m = \frac{|\gamma|-|\Omega|}{|\Delta|},\quad \varkappa^2 = (1-m^2)\,\mathrm{ch}^2\psi. \tag{6}*$$

The corresponding value of the mass is

$$m\left(\frac{\pi}{2}\right) = \frac{-|\Delta|}{\pi ab\,\mathrm{ch}\,\psi}[K(\varkappa^2) + (\mathrm{cth}\,\psi - 1)E(\varkappa^2)], \tag{7}†$$

where $K(\kappa^2)$ and $E(\kappa^2)$ are the total elliptic integrals of the first and second kind:

$$K(\varkappa^2) = \int_0^{\pi/2} d\alpha/(1-\varkappa^2\sin^2\alpha)^{1/2},$$

$$E(\varkappa^2) = \int_0^{\pi/2} d\alpha(1-\varkappa^2\sin^2\alpha)^{1/2}.$$

Since bismuth has two atoms per unit cell, the volume occupied by the holes should equal the volume of the electrons. The volume bounded by surface (1) is

$$V = \int d^3k = \frac{2\pi\Delta^2\gamma^2}{ab^2(\gamma^2-\Omega^2)^{1/2}}\Big(\arccos\frac{\gamma^2-\Omega^2-|\Omega\Delta|}{|\gamma\Delta|} - \frac{\gamma^2-\Omega^2+|\Omega\Delta|+2\Delta^2}{3\Delta^2\gamma^2} \times\{(\gamma^2-\Omega^2)[(|\Omega|+|\Delta|)^2-\gamma^2]\}^{1/2}\Big). \tag{8}$$

The experimentally obtained values of the masses and the cross sections are listed in Table I. It remains to determine from (4)–(7) the values of the parameters entering in the hole spectrum (1). This, however, must be done with allowance for the equations pertaining to the electrons, since, first, the constants a, b, γ, and Δ are the same for both, and, second, it is neces-

*sh = sinh; ch = cosh.

†cth = coth.

sary to make the volumes equal. The result of the calculations is listed in Table III. We shall discuss these in greater detail later. We note that the signs of the quantities a, b, γ, and Δ cannot be determined from (4)—(7), since (1) contains their squares.

Using the data of Table III we can calculate by means of (4)—(7) the theoretical value of the experimentally observed quantities. They are listed in the column marked "theory" of Table I. The same Table indicates the distances to the Fermi level $\epsilon_F = \Omega - (-|\gamma| + |\Delta|)$, to the nearest filled band $E_3 = 2|\Delta|$, to the nearest free band $E_1 = 2(|\gamma| - |\Delta|)$, to the following free band $E_2 = 2|\gamma|$, to the "open area" $E_0 = |\Delta|$, all distances being measured from the top of the conduction band (Fig. 2). The fact that all these gaps turn out to be considerably larger than ϵ_F justifies the use for the holes of the "ellipsoidal" approximation

$$-\varepsilon_\Phi = k_z^2/2m_z + k_\perp^2/2m_\perp,$$

which is obtained when one retains in (1) only the terms quadratic in p and q.

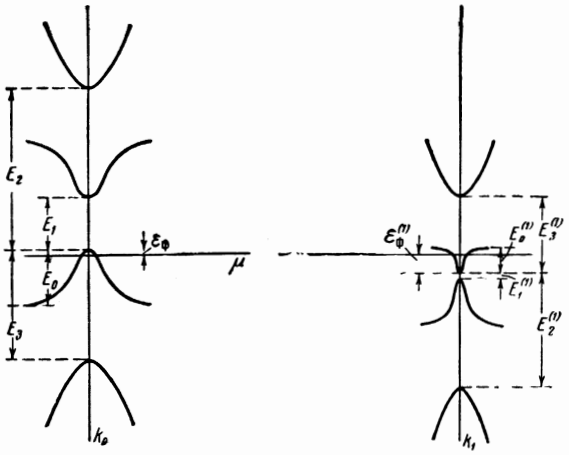

FIG. 2. Diagram of carrier bands in bismuth.

Table I lists also the concentration of the holes in Bi, $n = 2V/(2\pi\hbar)^3$ and the density of states $dn/d\Omega$.

ELECTRONS

The spectrum of one of the three groups of electrons is given by the equation

$$k_1^4 + 2k_1^2(k_2k_3 + D) + (A + k_3^2)(B + k_2^2) + 2\Delta^2k_2k_3 - C = 0;$$

$$k_1 = bk_x, \qquad k_{2,3} = bk_y \pm ak_z;$$

$$A = \gamma_-^2 - \Omega_+^2,$$

$$B = \gamma_+^2 - \Omega_-^2,$$

$$D = \gamma_+\gamma_- - \Omega_+\Omega_- + \Delta^2,$$

$$C = 2\Delta^2(\gamma_+\gamma_- + \Omega_+\Omega_-) - \Delta^4. \tag{9}$$

The parameters γ_+, γ_-, Ω_+, and Ω_- are connected with the quantities $\gamma^{(1)}$, $\delta^{(1)}$, and $\beta^{(1)}$ introduced in [1] and with the energy variable $\Omega^{(1)}$ ($\Omega^{(1)} = \omega - f^{(1)}$) by the relations

$$\gamma_\pm = \gamma^{(1)} \pm \delta^{(1)}, \qquad \Omega_\pm = \Omega^{(1)} \pm \beta^{(1)}.$$

It is important that $\gamma^{(1)} = -\gamma/3$.

Equation (9) is written in terms of the following reference frame: the x axis is chosen along that two-fold axis of the crystal which is the symmetry axis of the surface (9), the z axis makes an angle equal to $\cos^{-1}(1/3)$ with the trigonal axis of the crystal, and the y axis is perpendicular to the x and z axes (see Fig. 3). The symmetry of the surface (9) is actually C_{2h}—it includes the reflection $k_x \to -k_x$ and inversion.

The conditions under which the electron Fermi surface is closed are written in the following fashion

$$A > 0, \qquad B > 0, \qquad D - \Delta^2 > 0. \tag{10}$$

Further, the surface (9), depending on the relations between the parameters which determine it, can either break up into two unconnected parts, or else be connected. The experiment apparently offers evidence in favor of the latter possibility. The requirement for connectivity leads to the condition

$$C - AB > 0. \tag{11}$$

In this case the extrema of $\Omega^{(1)}(\mathbf{k})$ are realized at $\mathbf{k} = 0$. When $\mathbf{k} = 0$, equation (9) has four roots:

$$\Omega_{1,2}^{(1)} = -\gamma^{(1)} \pm [\Delta^2 + (\beta^{(1)} - \delta^{(1)})^2]^{1/2},$$

$$\Omega_{3,4}^{(1)} = \gamma^{(1)} \pm [\Delta^2 + (\beta^{(1)} + \delta^{(1)})^2]^{1/2}. \tag{12}$$

The distance from the origin to the surface (9) in the direction of a two-fold axis is

$$k^{(1)} \equiv k_x(k_2 = k_3 = 0) = [-D + (D^2 + C - AB)^{1/2}]^{1/2}/b. \tag{13}$$

It is known from experiment that the surface (9) is very strongly elongated in a direction lying in the plane $k_x = 0$ and making an angle $\theta_0 = 6°\ 20' \pm 15'$ with the basal plane (the plane perpendicular to the C_3 axis of the crystal). The intersection of the surface (9) with the plane $k_x = 0$, given by Eq. (9), in which one must put $k_1 = 0$, has a rather complicated form:

$$(A + k_3^2)(B + k_2^2) + 2\Delta^2k_2k_3 - C = 0. \tag{14}$$

The smallest distance ρ from the origin to the

curve (14) can be obtained by solving (14) simultaneously with the equation

$$\frac{ak_y}{bk_z}+\frac{k_3(B+k_2^2)+k_2(A+k_3^2)+\Delta^2(k_2+k_3)}{k_3(B+k_2^2)-k_2(A+k_3^2)-\Delta^2(k_3-k_2)}=0. \quad (15)$$

The coordinates of the point closest to the origin are connected with ρ and θ_0 by the obvious relations $k_y = \rho\cos\chi_0$, and $k_z = -\rho\sin\chi_0$, where we introduce for brevity the symbol

$$\chi_0 = \arccos {}^1/_3 \mp \theta_0$$

(see Fig. 3). The ambiguity in the last definition is due to the fact that the angle between the axis and the direction of the elongation can be either $\cos^{-1}({}^1/_3) - \theta_0$ or $\cos^{-1}({}^1/_3) + \theta_0$, depending on whether we look at the electron surface along the direction of the two-fold axis or in the opposite direction.

The area of the central section, for n lying in the yz plane, is given by the expression

$$S^{(1)}(n_{yz})=\frac{1}{|n_z|}\int dk_x dk_y=\frac{4D}{b}(J_+-J_-),$$
$$J_\pm=\int_0^{t_1^\pm} dt\,[-1+st^2\pm(f^2-nt^2)^{1/2}]^{1/2}, \quad (16)$$

where $t_1^\pm$ are the values of the variable for which the integrand vanishes. In the case when t_1 is complex, the corresponding integral need not be written out (the electronic parameters are such that t_1^- is complex for all directions n; the Fermi surface of the electrons has no noticeable dents). If we denote

$$n_{2,3} = an_y \pm bn_z = a\sin\chi \pm b\cos\chi,$$

then the expressions for s, n, and f^2 are of the form

$$s = n_2n_3,\ n = [An_3^2 + Bn_2^2 + 2n_2n_3(D-\Delta^2)]/D,$$
$$f^2 = 1 + (C - AB)/D^2.$$

The integral $J_\pm$ can be expressed in terms of elliptic integrals, but the resultant representation is too cumbersome. The corresponding expression for the mass is

$$m^{(1)}(n_{yz})=\frac{1}{\pi bD}\int_0^{t_1} dt\,\frac{(\Omega_+ + \Omega_-)D\sqrt{f^2-nt^2}+P+Qt^2}{[(f^2-nt^2)(-1+st^2+\sqrt{f_2-nt^2})]^{1/2}},$$
$$P = (\Delta^2 - D)(\Omega_+ + \Omega_-) + A\Omega_- + B\Omega_+,$$
$$Q = D[\Omega_+n_3^2 + \Omega_-n_2^2 + (\Omega_+ + \Omega_-)n_2n_3]. \quad (17)$$

In the case when $f^2 \to 1$, expressions (16) and (17) are simpler. Accurate to $n(f-1)/(n-2s)$, we obtain the following expansions:

$$S^{(1)}(n_{yz})=\frac{\sqrt{2}\,\pi D(f-1)}{b\sqrt{n-2s}}, \quad (18)$$
$$m^{(1)}(n_{yz})=\frac{B\Omega_+ + A\Omega_- + \Delta^2(\Omega_+ + \Omega_-)}{\sqrt{2}\,bD\sqrt{n-2s}}, \quad (19)$$

for which we see that in this region of angles the quantities $S^{(1)}$ and $m^{(1)}$ have the same angular dependence. Namely, their angular dependence is determined by the function

$$\Phi = n - 2s = (An_3^2 + Bn_2^2 - 2\Delta^2 n_2n_3)/D,$$

and the condition that $S^{(1)}(n)$ be minimal for a direction n making an angle θ_0 with the basal plane is written in the form $(d\Phi/d\chi)_{\chi=\chi_0} = 0$, or

$$\operatorname{tg} 2\chi_0 = \frac{2ab(B-A)}{b^2(A+B+2\Delta^2)-a^2(A+B-2\Delta^2)}. \quad (20)^*$$

In this approximation, the minimum value of $S^{(1)}(n_{y,z})$ is connected with ρ and $k^{(1)}$:

$$S^{(1)}_{min} = \pi\rho k^{(1)}.$$

For small values of the function Φ, expressions (18) and (19) are incorrect and we must use the correct expressions (16) and (17).

We now consider the case $n \parallel C_2$. We make first a remark concerning the signs of the electronic parameters. From the inequalities (10) it follows that γ_+ and γ_- have the same sign. Inasmuch as Eq. (9) contains only bilinear combinations of γ_+ and γ_-, the cross sections $S^{(1)}$ and the masses $m^{(1)}$ likewise contain these quantities in bilinear fashion. Therefore knowledge of only the masses and the cross section does not allow us to conclude whether γ_+ and γ_- are both positive or negative. Bearing this in mind, we shall assume, for brevity in notation, that γ_+ and γ_- are positive.

We present an expression for the area and the mass of the central ($k_x = 0$) section:

$$S_x^{(1)} = \int dk_y dk_z = \frac{2\Delta^2 r}{ab\,\mathrm{sh}\,\varphi}\int_0^{\pi/2} d\alpha\,\frac{\sin^2\alpha\sqrt{1-k^2\sin^2\alpha}}{\mathrm{ch}^2\varphi/k^2-\sin^2\alpha}, \quad (21)$$

$$m_x^{(1)} = \frac{\gamma^{(1)}\{(1+l)\,\mathrm{sh}^2\varphi K(k^2)+[1-l(2\,\mathrm{ch}^2\varphi-1)]E(k^2)\}}{\pi abr\,\mathrm{sh}\,\varphi\,\mathrm{ch}^2\varphi};$$
$$r^2 = \frac{(\gamma_+ - \Omega_-)(\gamma_- - \Omega_+)}{\Delta^2}, \quad l = \frac{\Omega_+ + \Omega_-}{\gamma_+ + \gamma_-},$$
$$\mathrm{sh}^2\varphi = \frac{(\gamma_- - \Omega_+)(\gamma_+ - \Omega_-)}{2(\gamma_+\Omega_+ + \gamma_-\Omega_-)}, \quad k^2 = (1-r^2)\,\mathrm{ch}^2\varphi. \quad (22)$$

*tg = tan.

Expressions (21) and (22) are valid when $\gamma_+\Omega_+ + \gamma_-\Omega_- > 0$. The corresponding formulas in the case when $\gamma_+\Omega_+ + \gamma_-\Omega_- < 0$ are obtained from (21) and (22) by making the substitutions $m_x^{(1)} \to -m_x^{(1)}$ and $\Omega_\pm \to -\Omega_\pm$. The condition for the numbers of the electrons and holes to be equal is

$$V = 3V^{(1)}. \tag{23}$$

Here $V^{(1)}$ is a volume bounded by the surface (9):

$$\begin{aligned}
V^{(1)} &= \int d^3k \\
&= \frac{1}{ab^2}\int \frac{dx\,dy}{1+x^2}\{(1+x^2)[C+\Delta^4-2y^2(D-\Delta^2) \\
&\quad - AB(1+x^2)] - (\Delta^2+y^2)^2\}^{1/2} \\
&= \frac{4}{3ab^2}\int_0^{x_1}\frac{dx\,[y_1^2(x)+y_2^2(x)]^{1/2}}{1+x^2} \\
&\quad \times [y_2^2(x)K(q^2) - (y_1^2-y_2^2)E(q^2)]; \\
y_{1,2}^2(x) &= \mp[(D-\Delta^2)(1+x^2)+\Delta^2] \\
&\quad + \{[(D-\Delta^2)(1+x^2)+\Delta^2]^2 \\
&\quad + (1+x^2)[C+\Delta^4 - AB(1+x^2)] - \Delta^4\}^{1/2}, \\
q^2 &= y_1^2/(y_1^2+y_2^2),
\end{aligned} \tag{24}$$

where x_1^2 satisfies the equation $y_1^2(x_1^2) = 0$.

The masses and the cross sections calculated above are known from experiment with sufficient accuracy (see Table II). It has turned out, however, that equations (12)—(17), (21), and (22), together with the information (4)—(7) on the hole surface and the condition for neutrality (23) are still insufficient for an unambiguous determination of the parameters[2]. It became necessary to make use of one more experimentally measured quantity—the distance $E_1^{(1)}$ from the bottom of the conduction band of the electrons to the top of the filled band. According to [4], this distance amounts to 0.0153 eV. Unfortunately, this quantity was not observed directly in [4], but was obtained by computer reduction of experimental data, wherein Smith et al.[4] started from an ellipsoidal model of the electron spectrum

$$E(1+E/E_1^{(1)}) = a_{ik}k_ik_k,$$

which differs noticeably from the spectrum (9).

However, after calculating the electronic parameters it turned out that only two of the four branches of the spectrum (9) are quite close. We can therefore hope that the value of the gap $E_1^{(1)}$ as determined in [4] is close to the real value. On the other hand [see (12)], the value of $E_1^{(1)}$ is determined by the sought parameters:

$$\begin{aligned}
E_1^{(1)} &= |2|\gamma^{(1)}| - [\Delta^2 + (\beta^{(1)}+\delta^{(1)})^2]^{1/2} \\
&\quad - [\Delta^2 + (\beta^{(1)}-\delta^{(1)})^2]^{1/2}|.
\end{aligned} \tag{25}$$

Our task is greatly facilitated by the possibility of using expansions (18) and (19) in calculating the cross section and the mass for those directions of **n** for which $S(\mathbf{n})$ and $m(\mathbf{n})$ are relatively small.

Thus, the system of equations for the unknown parameters a, b, Δ, γ, $\beta^{(1)}$, $\delta^{(1)}$, Ω, and $\Omega^{(1)}$ consists of (4)—(7), (13), and (18)—(25). Of course, none of the equations can be given preference, even if for no other reason than that errors are possible in the interpretation of the experimental data. Among the more weighty reasons are: 1) the accuracy of the approximation in the theory considered amounts to $1/20$ [1]; 2) the bismuth samples with which the experimental data given above were obtained, must have contained impurities. The presence of impurities is particularly important in view of the small amount ($\sim 10^{-5}$

Table II. Electrons

	Experiment	Theory		Experiment	Theory
m_{min}/m_0	0.0080±0.0001 [3]	0.0068	$\frac{dn}{d\Omega}\cdot 10^{-19}$, cm$^{-3}\cdot$eV^{-1}		1.17
m_x/m_0	0.119±0.003 [3]	0.113			
$S_{min}\cdot 10^{12}$, cgs esu	1.30±0.02 [7] 1.34±0.05 [2]	1.2*	$\varepsilon_\Phi^{(1)}$, eV	0.0385 [4]	0.031
$S_x\cdot 10^{12}$, cgs esu	19.5±1.5 [2]	16.1	$E_0^{(1)}$, eV		0.048
θ_0	6°20′±15′ [3]	6°45′			
$k^{(1)}\cdot 10^{21}$, cgs esu	0.54±0.02 [8]	0.64	$E_1^{(1)}$, eV	0.015 [4]	0.013
$k^{(2)}\cdot 10^{21}$, cgs esu		0.6			
$k^{(3)}\cdot 10^{21}$, cgs esu		8.4	$E_2^{(1)}$, eV		0.271
$n\cdot 10^{-17}$, cm^{-3}	0.92 [4]	1.15	$E_3^{(1)}$, eV		0.370

*Calculated with the approximate formula (18).

[2]We are indebted to I. N. Silin, who established this fact with the aid of the JINR computer.

Table III. Values of the Parameters

$\lvert a\rvert\cdot 10^{-8}$, cm/sec	$\lvert b\rvert\cdot 10^{-8}$, cm/sec	$\lvert\Delta\rvert$, eV	Ω, eV	$\lvert\gamma^{(1)}\rvert$, eV	$\lvert\delta^{(1)}\rvert$, eV	$\beta^{(1)}$, eV	$\Omega^{(1)}$, eV
0,390	1.068*	0.1242	—0.3794	0.1635*	0.0853	0.0516	0.00981

*The symbols b and $\delta^{(1)}$ are identical with the symbols a and $\gamma^{(1)}$, respectively.

per atom) of electrons and holes in bismuth. Consequently, we sought such a combination of parameters, which would satisfy in the best manner the entire set of equations. Even the condition of neutrality, which should be satisfied exactly for ideally pure bismuth, was on par with the remaining equations.

The computer solution is shown in Table III. We note that it corresponds to a minus sign in the definition of χ_0. Using these data, we readily obtain the theoretical values of the observed quantities (see Table II). In Table II there are indicated, besides $E_1^{(1)}$, the distances to the next filled band $E_2^{(1)}$, to the next free band $E_3^{(1)}$, to the "open area" $E_0^{(1)}$ [that is, to the value of ω closest to the Fermi level, at which one of the inequalities (10) is violated], and to the Fermi level (see Fig. 2). All these distances are measured from the bottom of the conduction band. The same table gives the concentration and the state density of the electrons. It is seen from Tables I and II that the total density of the carrier states in bismuth is insufficient to explain the large value of the specific heat measured by several workers.[5]

The value of θ_0 calls for an explanation. We calculated it by the same expansion that led to formulas (18) and (19). An error of 1° is quite possible in this calculation. In addition, the figure of (9) is not an ellipsoid. The direction of the elongation, determined from the sections of the surface closest to the origin, does not coincide with the direction of the most remote point. This circumstance was observed by several authors.[2] Figure 3 gives the time of the intersection of the surface (9) and of the plane $k_x = 0$. The curve can be constructed by using the parametric representation of (14):

$$k_y = (\sqrt{B}u + \sqrt{A}v)/2b, \quad k_z = (\sqrt{B}u - \sqrt{A}v)/2a.$$

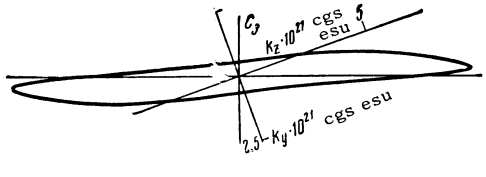

FIG. 3

The quantity u is expressed in terms of v by

$$u = \frac{-\alpha v \pm [\alpha^2 v^2 - (1+v^2)(1+v^2-\beta)]^{1/2}}{1+v^2}$$

where $\alpha = \Delta^2/\sqrt{AB}$, and $\beta = C/AB$.

It is curious that the point of the curve closest to the origin is a saddle point. The distance ρ to it amounts to 0.57×10^{-21} cgs esu, which differs appreciably from the value $(0.76 \pm 0.03) \times 10^{-21}$ determined by A. P. Korolyuk in experiments on the absorption of ultrasound. V. F. Gantmakher indicates for this quantity a range 0.68×10^{-21}—0.84×10^{-21} (this is the width of the size-effect line observed in the study of the surface impedance). To be sure, all that is known about the value obtained in the experiment is that it is half the extremal dimension of the curve. The dimension is measured along a perpendicular to a direction inclined approximately 6° to the basal plane. This quantity, as can be seen from Fig. 3, can correspond to 0.57×10^{-21} as well as to 0.60×10^{-21}. The distance 8.4×10^{-21} to the most remote point agrees best with the value $(7.6 \pm 0.3) \times 10^{-21}$ obtained by Korolyuk.

The most noticeable is the discrepancy between the experimentally measured values of the cyclotron mass and those calculated from (17), although the angular dependence agrees with experiment in general outline. The minimum value of the mass, determined from the values of the parameters of Table II, is $0.0068\ m_0$, while the experimental value [3] is $0.0081 m_0$. The maximum value is $0.086\ m_0$ but that calculated from (17) is $0.18\ m_0$. In [6] a value $0.11\ m_0$ is given for this quantity, which apparently pertains to the limit point.[3] It is possible that the discrepancy is due to the fact that the maximum of (17) is very sharp, such that a 2° inclination of the magnetic field reduces the mass by one half. It must also be borne in mind that in the determination of the parameters the value of m_{max} was not taken into account, and this value is determined by a small combination of the parameters. This constitutes the main difficulty, since it follows from experiment that the Fermi surface of the electrons is quite anisotropic, while for equation (9) none of the directions is preferred, provided only one does not require, for example, that the coefficient A

be accidently small compared with B. Analogously, the requirement that the Fermi surface be close to an ellipsoid leads to smallness of the quantity $(C - AB)/D^2$. Thus, small combinations of the parameters γ_+, γ_-, Ω_+, Ω_-, and Δ become important, whereas the approximation in question, strictly speaking, makes it possible to determine the parameters themselves with accuracy $1/20$. For this reason, the agreement between theory and experiment, reflected in Tables I and II, is satisfactory.

The authors are grateful to E. G. Shustin for help in the calculations, V. F. Gantmakher, V. S. Édel'man, and A. P. Korolyuk for reporting the experimental results prior to publication, and A. A. Abrikosov for a discussion of the work.

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Translated by J. G. Adashko
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