

Shape of the electron Fermi surface of bismuth

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Quantum oscillations of the resistance at a frequency ~ 2.5 MHz and a temperature $\sim 0.1^\circ\text{K}$ are investigated in perfect bismuth single crystals characterized by a carrier residual relaxation time of 2–5 nsec. The sections of the Fermi surface in two crystallographic planes are measured with an accuracy to ~ 0.2 – 0.3% . Inversion of the data with a computer is performed and the shape of the electron Fermi surface is determined. The volume of the electron surface is calculated and found to be $(14.66 \pm 0.01) \times 10^{-68} \text{ g}^3\text{cm}^3/\text{sec}^3$. A comparison of the total volume of the three electron surfaces with the obtained volume $(43.99 \pm 0.05) \times 10^{-68} \text{ g}^3\text{cm}^3/\text{sec}^3$ of the hole surface, and a comparison of the results of calculation of the effective masses in the limiting points with those measured experimentally, show that the proposed empirical model quantitatively describes the shape of the electron Fermi surface for bismuth. The accuracy of determination of the momenta from the model is ~ 0.1 – 1% , depending on the direction relative to the crystal lattice. The spin splitting of the Landau levels for the major crystal directions and its anisotropy in the plane of the trigonal and bisector axes are measured.

Deviations of the shape of the electron Fermi surface (FS) of bismuth from ellipsoidal has been observed in a number of studies^[1]. Although these deviations amount to only several percent, they can apparently lead to appreciable effects. For example, a difference by as much as 35% was observed between the electron masses on the central section and at the limiting point.^[2] In addition, an investigation of cyclotron waves has revealed a discrepancy, by a factor of two, between the calculated and the experimentally observed values of the wave velocity^[3].

The known numerous investigations of quantum oscillations in bismuth have not made it possible to establish the values of the extremal cross sections with an accuracy sufficient for a quantitative analysis of the deviations of the shape of the FS from ellipsoidal. This is connected with singularities, which will be considered below, in the spectrum of the carriers in bismuth. Quantum oscillations are observed in fields satisfying the condition

$$2\pi^2 k(T + T_D) mc / ehH \ll 1$$

(T_D is the Dingle temperature). From the quantization condition $nehH/c = S \approx \pi p_F^2$ and from the estimate of the effective mass $m \approx p_F/v_F$ we obtain for the number of observed oscillations $n \approx v_F p_F / 4\pi^2 k(T + T_D)$. For bismuth, p_F is smaller by a factor of 10^2 than for ordinary metals, while v_F is of the same order, so that the values of n are smaller by a factor $\sim 10^2$ and amount to ~ 10 – 30 at $T + T_D \approx 2^\circ\text{K}$, depending on the sensitivity of the measurements. The accuracy with which the period of the oscillations is measured is several percent. The presence of magnetic-field directions for which the spin splitting in bismuth is equal to half the distance between the Landau levels reduces greatly the measurement accuracy for these directions.

Large FS sections are observed at $T \approx 1^\circ\text{K}$ in the range of fields in which the Fermi level depends on the magnetic field, and therefore the oscillations of the small period cease to be periodic in the reciprocal field^[1], and the measurement accuracy of the large cross sections decreases to $\sim 10\%$.

These difficulties can be avoided by performing the measurements with perfect single crystals at $T + T_D \ll 1^\circ\text{K}$.

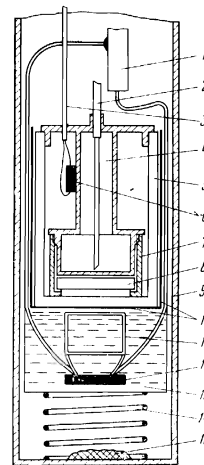
EXPERIMENTAL PROCEDURE

Production of low temperatures. We used a dissolution cryostat^[5] to obtain a temperature $\sim 0.1^\circ\text{K}$. The construction of the dissolution bath with the sample holder is shown in Fig. 1. The dissolution bath is a vacuum-tight volume 4, in the upper part of which are sealed-in the heat-exchange capillaries 2. A holder with a freely-lying sample 8 is threaded on the outside of the bath.

To produce thermal contact between the sample and the dissolution bath, $\sim 0.5 \text{ cm}^3$ of ^3He was condensed through capillary 3 into a cavity bounded by a teflon cartridge 5, so as to produce a liquid layer between the bottom of the bath and the sample. At room temperature, the cartridge 5 could be slipped on tightly on the silicone-lubricated rim of the dissolution bath. After cooling, owing to the large coefficient of thermal expansion of the teflon, the junction became vacuum tight. This ensured thermal insulation of the cold part of the instrument from the screen 9, the temperature of which was 0.4°K . After 1–2 cycles of cooling from room to helium temperature, irreversible deformations of the bath 4 and of the cartridge 5 took place and broke the seal. It was then necessary to replace the cartridge 5.

Since the outside diameter of the cartridge 5 was 22

FIG. 1. Construction of low-temperature part of the instrument: 1—coaxial inlet, 2—heat-exchanger capillaries, 3—capillary for the admission of ^3He , 4—dissolution bath, 5—teflon cartridge, 6—resistance thermometer, 7—sample holder, 8—sample, 9—screen at temperature 0.4°K , 10—caprone cloth, 11—coil of tuned circuit, 12—capacitor, 13—epoxy compound, 14—screen, 15—activated charcoal.



mm, and the inside diameter of the screen was 23 mm, it was impossible to keep them from touching. To decrease the heat influx through the mechanical contact, which could become appreciable if the silicone lubricant were to find its way to the contact, the teflon cartridge was wrapped with caprone cloth 10 (from a stocking). The operation of the dissolution cryostat was monitored with a carbon resistance thermometer 6, the current leads to which passed through capillary 3 to the cap.

The dissolution bath was made of MB copper with 1% pure aluminum¹⁾. In comparison with the known technical materials, this alloy contains practically no ferromagnetic impurities of superconducting inclusions capable of distorting the magnetic field in the sample. Its resistivity at helium at room temperatures is of the same order. Owing to the relatively large resistance, the heat produced by the eddy currents during the course of variation of the magnetic field is small and estimated by us at $10^{-9} - 10^{-10}$ W.

All the seals of the dissolution bath were made with copper-silver solder, to prevent possible distortions of the magnetic field or thermal effects when the superconductivity is destroyed by the magnetic field, as would occur if soft solder were to be used. The volume of each seal was ~ 0.1 mm³, and the seals were located ~ 4 cm away from the sample. The sample temperature 0.1°K could be maintained for 5–6 hours before the ³He in the bath cooling the condensation-pump walls^[5] was completely evaporated.

A magnetic field of intensity up to 10 kOe was produced with the aid of an electromagnet that could be rotated in the horizontal plane through 360° and inclined $\pm 4^\circ$ in two mutually perpendicular directions. The angle of rotation in the horizontal plane was read with accuracy $\sim 5'$ against the scale of the magnet and with accuracy $\sim 0.5'$ against the scale of a theodolite mounted on the upper plate of the magnet. The orientation of the theodolite relative to the laboratory was maintained constant when the magnet was rotated, by observing the reflection from a flat mirror fastened on the theodolite using an AKT-250 autocollimation tube. Since the rotation axes of the theodolite and of the magnet did not coincide, the range of angles that could be read by this method was 45–60°. The angle of inclination of the magnet was measured accurate to $\sim 15''$ with a Talyvel goniometer.

The stabilization and time sweep of the magnetic field were carried out using a Hall pickup. The output voltage of which was compared with a voltage with a time variation $U \propto 1/(T + t_0)$. This yielded a field variation $H^{-1} \propto t$. The voltage $U(t)$ was picked off a fixed resistor fed through a rheostat (PPML 20-k multiturn potentiometer) the shaft of which was driven by a synchronous motor. The frequency of the alternating current fed to the motor was maintained by a quartz oscillator and a frequency divider IK3-15, making it possible to vary the field sweep velocity in a calibrated manner and to obtain part of the recording at increased velocity to shorten the measurement time. The total time required to cover the established range of fields could be varied from ~ 1 hour to ~ 5 minutes.

The measurement results were registered with an EZ-4 automatic recorder. To determine the field, each recording was calibrated at several points against a nuclear-resonance signal with the aid of a running-water magnetometer.^[6] The long-period field instability de-

termined from the nuclear resonance was $\sim 0.01\%$, the integral nonlinearity of the scale was $\sim 1-2\%$, and the accuracy with which the field was determined against the calibration marks on the experimental plot was $\sim 0.05\%$.

The homogeneity of the magnetic field in the field range 1000 Oe–10 kOe was $\sim 0.01\%$ in the volume of the sample. The differences in the readings of the magnetometer did not exceed $\sim 0.01\%$ when a feeler gauge was placed in the center of the magnet at the location of the sample and at the location it occupied during the measurement (~ 20 mm from the center). In the construction of the instrument, care was taken to keep magnetic materials and superconductors far from the sample. During the time of the measurements, at a field ~ 600 Oe, an intense NMR signal of width ~ 6 Oe on protons was observed, apparently from the epoxy compound in which the measuring circuit was potted. The center of the NMR line coincided with accuracy ~ 0.5 Oe with the value of the field determined from the magnetometer outside the cryostat. Thus, the accuracy with which the absolute value of the field was determined in the sample was not worse than $\sim 0.1\%$.

The oscillations were registered by measuring the surface resistance of the bismuth at the frequency ~ 2.5 MHz by a frequency-modulation method.^[7] The changes of the surface resistance of the sample led to change in the parameters of the circuit coil, which was located as shown in Fig. 1.

It is usually assumed that to obtain high sensitivity it is necessary to increase the filling factor of the coil by placing the sample inside the coil^[8]. This opinion is justified by the calculation of the value of the useful signal. However, no account is taken here of the fact that when the filling factor is increased the Q of the circuit is decreased and the noise increases accordingly. The signal/noise ratio increases in this case relatively slowly. When choosing the filling factor it is apparently necessary to see to it that the additional losses introduced by the sample be of the same order of magnitude as the losses in the circuit without the sample. Using our replacement of the sample and of the coil, the Q of the circuit with the sample was lower by a factor 2–3 than without the circuit, and ranged with changing field from ~ 50 (in zero field) to ~ 25 at helium temperatures.

To decrease the microphone effect and to increase the stability, the KSO capacitor (12) of the circuit, from which the plastic housing was removed to replace the tinned leads with copper leads, was placed alongside the coil 11, and the entire circuit was potted in a compound based on epoxy resin P. The circuit was connected to the generator with a coaxial cable with an inside constant wire of 0.15 mm diameter and insulating beads of foamed polystyrene. Since the capacitor of the circuit was alongside the coil, the coaxial cable did not make a noticeable contribution to the circuit losses, in spite of its large resistance.

The circuit was part of a Pound oscillator with a feedback loop to stabilize the generation level as the magnetic field was varied. The amplitude of the oscillations at the circuit was 2–3 mV, corresponding to a power dissipation $\sim 10^{-8} - 10^{-9}$ W in the sample.

The magnetic field applied to the sample was modulated at a frequency 12.5 Hz synchronized with the utility network. The periodic changes in the sample re-

sistance led to frequency modulation of the generator, which was registered in analogy with the procedure used in [7]. The modulation field could be applied both parallel and perpendicular to the constant magnetic field, so that we could observe isotropic and anisotropic effects separately [9], and the analysis of the result was made easier.

Samples in the form of disks of 18 mm diameter and 2 mm thickness were grown from the melt by the method described in [10]. Cyclotron resonance measurements on bismuth single crystals grown by a similar method have previously established that the residual relaxation time is ~ 2 nsec for electrons and $\sim 4-5$ nsec for holes [11].

Quantum oscillations in two samples were investigated. In one sample the direction of the normal to the flat surface coincided within $2-3^\circ$ with the trigonal axis C_3 . The magnetic field, when working with this sample, was applied in the basal plane with accuracy $\pm 5'$, this being accomplished by inclining the magnet to minimize the period of the hole oscillations when the field was parallel to the binary axes. The directions of the latter in the plane of the sample were determined from the minimum period of the electron oscillations, with accuracy $\pm 0.5'$.

For the other samples, the direction of the normal to the flat surface coincided within $\sim 1^\circ$ with the binary axis C_3 . The magnetic field was applied to a plane containing the bisector axis C_1 and the C_3 axis. The adjustment of the inclination of the field was based on the splitting of the oscillations from the two ellipsoids, which should have identical cross sections in the bisector plane (Fig. 2). It was observed that the direction of the magnetic field makes an angle $2' \pm 30''$ with the plane of rotation of the magnet. The magnet was therefore set in such a way that at $H \parallel C_3$ the field was in the bisector plane with accuracy $30''$, and when the magnet was rotated the field vector moved over the surface of a cone tangent to the bisector plane near the C_3 axis. Rotation of the magnet in the interval $\pm 90^\circ$ from this direction caused no splitting of the signal of the quantum oscillations for the two ellipsoids inclined 60° to the plane of the rotation of the magnet. The direction of the C_3 axis for this sample was established with accuracy $\sim 0.5'$ by computer reduction of the experimental results. Since the sample was not clamped, mechanical jolts caused by adding helium to the cryostat could rotate the sample through $10-20'$. Each measurement was therefore preceded by control experiments for the purpose of establishing the sample position. The measurements performed in different days were mutually reconciled with accuracy $0.5-1'$ by means of this effect.

Reduction of measurement results. The periods of the oscillations in the reciprocal field ΔH^- were determined from plots analogous to that shown in Fig. 3. In strong fields, the oscillations took the form of narrow well-resolved lines split in accordance with the two spin directions. The line shape coincided as a rule with the calculated value (see Fig. 3) obtained by differentiating three times, with respect to the field, the well known expression for the oscillations of the thermodynamic potential [13]

$$\Phi = 2kT \left(\frac{eH}{2\pi\hbar} \right)^{3/2} \left(\frac{\partial^2 S}{\partial p_z^2} \right)^{-1/2} \sum_{n=1}^{\infty} \frac{\exp(-2\pi^2 n k T / \hbar \Omega)}{n^{1/2} \operatorname{sh}(2\pi^2 n k T / \hbar \Omega)} \times \cos \left(\frac{n\pi g m}{m_0} \right) \cos \left[\left(\frac{cS}{e\hbar H} - \gamma \right) n \pm \frac{\pi}{4} \right]. \quad (1)$$

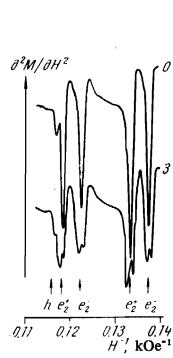


FIG. 2

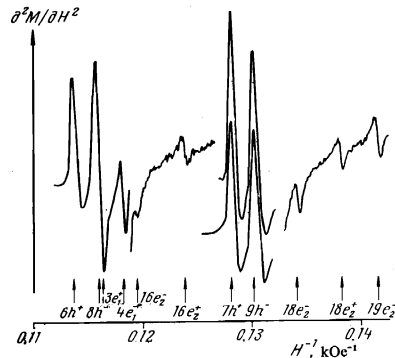


FIG. 3

FIG. 2. Surface-resistance oscillations from two equivalent electron ellipsoids (e_2) at $H \perp C_2$ and an angle $6^\circ 20'$ between H and C_3 . The plus and minus signs correspond to different directions of the spin. The curves are marked with the angles of inclination of the magnetic field to the bisector plane. The signal from the hole oscillations (h) was suppressed by using transverse modulation.

FIG. 3. Oscillations of surface resistance at $H \perp C_2$ and an angle $-14^\circ 26'$ between H and C_3 . h —holes, e_1 —electrons for which the binary axis of the FS is perpendicular to H , e_2 —two other sections of the FS of the electrons, the sections of which in the investigated bisector plane were identical. The plus and minus signs correspond to different spin directions. The oscillations marked e_2 were obtained with the gain increased sixfold. Upper curve—experiment, lower ($7h^+9h^-$)—calculated line shape for $T + T_D = 0.2^\circ K$. The oscillations are numbered in accordance with [12].

The quantity ΔH^- was measured in the following manner:

A. The experimental data were used to determine the value of H^- for oscillations corresponding to the same spin direction and located at the edges of the dynamic range of field variation. Owing to the oscillations of the Fermi level and the strong fields, the observed lines, as shown by experiment and calculation, could shift from the position they should have occupied if the quasiclassical condition were satisfied for all sections of the FS; this shift reaches in some cases $10-20\%$ of ΔH^- . Since we are interested in the quasiclassical value of ΔH^- , the oscillatory change of the Fermi level could be taken into account by introducing corrections³⁾ to H^- . The correction was calculated by us in the quasiclassical approximation using the formulas of I. Lifshitz and Kosevich [13], with simultaneous allowance for all the FS regions whose sections were chosen in accordance with the described experiments, while the effective masses were taken from [2]. The possibility of introducing the corrections was verified at $H \parallel C_1$ and $H \parallel C_2$ for the hole oscillations and at $H \parallel C_2$ for the short-period electron oscillations. The deviations from periodicity in the "corrected" scale were decreased thereby one order of magnitude.

B. The phase of the line located in the stronger field was determined, as was the magnitude of the spin splitting relative to the distance between the Landau levels. The obtained values were used to calculate the value of γ in formula (1). In all the investigated cases (~ 100) a constant value $\gamma = \pi \pm 10\%$ was obtained for both electrons and holes.

C. Taking into account the results obtained in Item B and using formula (1), the phase (reckoned from $H^- = 0$) of some characteristic section of the oscillations in the weak field was determined (including the case when the oscillations was sinusoidal). It was assumed here that

$\gamma = \pi$. The correction to the field, which decreased rapidly with increasing H^{-1} , never exceeded $\sim 1\%$, and was not introduced if it amounted to $< 0.1\%$. The period ΔH^{-1} was determined by dividing H^{-1} by the corresponding value of the phase. The accuracy with which ΔH^{-1} was determined, with allowance for the errors in the measurement of the absolute value of the field and for the assumption made with respect to γ , is estimated at $0.2-0.3\%$. In all cases the corrected value of ΔH^{-1} differed from the preliminary value determined in Item A by not more than 0.5% .

The values of the central sections and the values of the relative spin splitting for field directions along the principal axes of the electron and hole ellipsoids are given in Table I. Figure 4 shows the anisotropy of the spin splitting for the electrons in the binary plane.

Determination of the shape of the electron Fermi surface. As is well known (see [15]), the shape of a convex FS having an inversion center can be reconstructed from the central sections. These conditions are satisfied by the FS of bismuth [1]. Mueller [16] has proposed a simple method for the inversion of the data on the de Haas-Van Alphen effect, based on the relation

$$A_{n,m}^{+,-} = \pi P_n(0) B_{n,m}^{+,-}, \quad (2)$$

where P_n are Legendre polynomials of order n ; $A_{n,m}^{+,-}$ and $B_{n,m}^{+,-}$ are the coefficients of the expansion of the central sections $S(\theta, \varphi)$ and of the squared momenta $p^2(\theta, \varphi)$ in the spherical harmonics $\cos(m\varphi)P_n^m(\cos\theta)$ and $\sin(m\varphi)P_n^m(\cos\theta)$, and P_n^m are associated Legendre polynomials. We investigated a modification of Mueller's method [16], proposed by Ketterson and Windmiller [17] for FS with near-ellipsoidal shape. As the first approximation for the FS shape we used an ellipsoid described by the equation

$$p_1^2 / p_{10}^2 + p_2^2 / p_{20}^2 + p_3^2 / p_{30}^2 = 1, \quad (3)$$

where the indices 1, 2, and 3 pertain to the principal axes of the ellipsoid, the 2 axis coincides with the binary axis C_2 , the 1 axis lies in the bisector plane and is inclined $6^\circ 23' \pm 1'$ to the basal plane, $p_{20} = 0.564 \times 10^{-21}$, and $p_{30} = 0.743 \times 10^{-21}$ g-cm/sec. The presented ellipsoid parameters were determined by least squares using all (~ 130) obtained values of the periods of the oscillations. The rms error in the determination of the cross sections, with the FS approximated by an ellipsoid, amounted to 1.26% , which greatly exceeds the measurement error $0.2-0.3\%$.

To determine more precisely the shape of the FS, the experimental values of $S(\theta, \varphi)$ were approximated by a series of spherical functions

$$Y_{n,m}(\theta, \varphi) = \begin{cases} \cos(m\varphi)P_n^m(\cos\theta), & m \text{ odd} \\ \sin(m\varphi)P_n^m(\cos\theta), & m \text{ even} \end{cases} \quad (4)$$

with $n = 0, 2$, and 4 . The angle φ is reckoned from the 2 axis in the plane of the axes 1 and 2, while the angle θ is reckoned from the 3 axis. The system of functions (4) was chosen in accordance with the symmetry of the electron FS (inversion plus symmetry plane) [1]. The values of the associated Legendre polynomials were calculated with formula (8.735.2) of [18].

The approximation by means of the system with functions (4) was carried out, in analogy with [17], in a coordinate system transformed in accordance with the relations

$$\begin{aligned} p_1' &= p_1, \quad p_2' = p_2 p / p_{20} = \alpha p_2, \\ p_3' &= p_3 p / p_{30} = \beta p_3. \end{aligned} \quad (5)$$

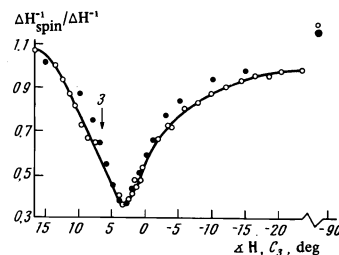


FIG. 4. Anisotropy of relative spin splitting for electrons in the bisector plane: O—experiment, ●—calculated from the ellipsoid parameters given in [12] for the effective and spin masses. The arrow shows the direction of the axis 3.

TABLE I

	$S, 10^{-42} \text{ g}^2 \cdot \text{cm}^2 / \text{sec}^2$			$\Delta H^1_{\text{spin}} / \Delta H^1$	
	Experiment	Empirical model	[*]	Experiment	[**]
Electrons					
$H \parallel 1^*$	1.300 ± 0.003	1.300	1.27 ± 0.01	1.09 ± 0.01	1.07
$H \parallel 2$	$19.23 \pm 0.05^{**}$	19.27	20 ± 1.1	0.25 ± 0.1	0.35
$H \parallel 3$	$14.48 \pm 0.04^{***}$	14.35	15.3 ± 0.7	0.53 ± 0.03	—
Holes					
$H \parallel C_1$	22.49 ± 0.02	—	23.6 ± 1	< 0.2	< 0.01
$H \parallel C_2$					
$H \parallel C_3$					

*1, 2, 3—directions of principal axes of the ellipsoid, the axis 1 lying in the bisector plane and inclined $6^\circ 23'$ to the basal plane, and the axis 2 parallel to C_2 . The positive direction of the angles is from C_3 to the nearest direction of 3.

** $\angle H, 2 = 15^\circ, H \perp 3$.

*** $\angle H, 3 \cong 7^\circ, H \perp 1$.

TABLE II. Coefficients of the expansion of $S(\theta, \varphi)$ in the spherical harmonics (4) in a coordinate system transformed in accordance with the relations (5), their variance σ_i^2 , and the correlation matrix ρ_{ik}

n	0			2			4			
	0	1	2	0	1	2	3	4		
m	0	1	2	0	1	2	3	4		
$A_{n,m} \cdot 10^{-42} \text{ g}^2 \cdot \text{cm}^2 / \text{sec}^2$	184.7	4.86	1.91	3.20	-2.51	-0.12	-0.25	0.069	-0.022	
$\sigma_i^2 \cdot 10^{-92} =$	1.05	$\rho_{12} \cdot 100 = 40$	-19	80	80	17	81	-18	16	
		1.3	-23	20	-40	23	58	-23	7	
			2.5	1	26	-98	-4	99	-14	
				0.17	-60	-3	67	2	22	
					4.4	-25	-83	26	9	
						2.6	1	-98	13	
							0.023	-2	-15	
								0.071	-15	
									$5.5 \cdot 10^{-5}$	

Unlike in [17], the value of p was not set equal to p_{10} , but was varied to obtain the minimum residual sum of the squares. This made it possible to decrease the rms error by approximately one-half.

It was observed during the course of the calculations that the data obtained for two crystallographic planes do not suffice to construct the FS model. This was manifest in the fact that in the transformed coordinate system in the plane of the axes 3 and 2 the values of the momentum differed from the mean value by an amount reaching $\sim 10\%$, i.e., the FS contour in this plane differed from an ellipse. At the same time, according to previously obtained results [2, 19], these differences cannot exceed $\sim 1-2\%$. The experimental data were therefore supplemented with 30 cross section values that varied in accordance with the ellipsoidal law, with the field rotated through 3° in the plane of the axes 2 and 3. The weights for these points were chosen to be smaller by one order of magnitude than for the experimentally determined points. Calculations performed with the additional set of points have shown that the rms approxi-

mation error remained practically unchanged, and the anisotropy of both the cross section and of the momenta in the plane of the axes 3 and 2, for the approximating surface, differed from an ellipse by not more than $\sim 0.1\%$.

The best approximation of the sections with the system of functions (4) and with the relative rms error 0.2% was obtained at $\alpha = 13.04$ and $\beta = 9.88$. The expansion coefficients $A_{n,m}$, their variances σ_i^2 , and their correlations ρ_{ijk} are given in Table II. Figure 5 demonstrates the degree of approximation in the basal plane and in a plane perpendicular to C_2 , for an ellipsoid whose major axis lies in this plane.

DISCUSSION OF RESULTS

The results obtained in the preceding section solve the problem of constructing a model describing the shape of the electron FS. In its construction we used no theoretical representations whatever of the FS of bismuth, apart from its symmetry^[1]. The proposed model can therefore be called empirical.

It is of interest to compare the empirical model both with the results of our measurements and with the known theoretical models of the FS of bismuth. Using the obtained values of $A_{n,m}$ and formulas (2) we calculated the values of the Fermi momenta. The contours of the intersection of the FS by planes containing the axes 1, 2, and 1, 3 are shown in Fig. 6. In the plane of the axes 2 and 3, in the coordinate system transformed in accordance with (5), the section coincides with a circle within $\sim 0.1\%$. The extremal values of the momenta in Table III are set in correspondence with those known from experiments.

Taking into account the smallness of all the coefficients $A_{n,m}$ in comparison with $A_{0,0}$ and the orthogonality of the spherical harmonics, it is easy to calculate the volume of the FS of the electrons with the aid of the relation

$$V_e = \frac{4\pi}{3} \left(\frac{A_{00}}{\pi} \right)^{3/2} \left[1 + \frac{3}{32} \sum_{n=2,4} \sum_{m=0}^n \frac{A_{n,m}^2}{A_{0,0}^2 \rho_n^2(0)} \frac{(m+n)!}{(2n+1)(n-m)!} \right]. \quad (6)$$

Substitution of the values of $A_{n,m}$ in (6) shows that the second term is $\sim 0.1\%$ of the first, and

$$V_e = (14.66 \pm 0.01) \cdot 10^{-63} \text{ g}^3 \cdot \text{cm}^3 / \text{sec}^3,$$

The summary volume of the three electron surfaces is

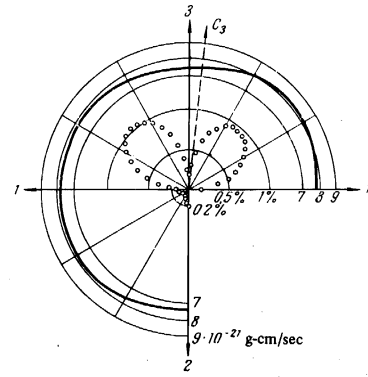


FIG. 6. Shapes of the intersections of the FS of bismuth with planes containing the axes 1, 3 and 1, 2 in the transformed coordinate system. The real surface is compressed in the direction of the 3 axis by a factor 9.88, and by a factor 13.04 in the direction of the 2 axis. The direction of C_3 axis in the real coordinate system is shown dashed. Thick curves—values of p_F calculated using formula (2), points—error in the determination of p_F . The values of $A_{n,m}$, σ_i^2 , and ρ_{ijk} given in Table II were used in the calculation.

TABLE III. Extremal values of the electron momenta ($p \cdot 10^{21}$, g-cm/sec)

Axis	Empirical model	[20]	[21]	[22] *
1	$0.740 \pm 0.2\%$	0.54 ± 0.015	0.76 ± 0.03	0.79 ± 0.06
2	$0.559 \pm 0.2\%$		0.55 ± 0.02	0.545 ± 0.01
3	$7.88 \pm 0.2\%$		7.6 ± 0.2	7.95 ± 0.2

*And also private communication from H. U. Müller.

$(43.98 \pm 0.4) \times 10^{-63} \text{ g}^3 \text{cm}^3 / \text{sec}^3$, and the electron concentration is $3.015 \times 10^{17} \text{ cm}^{-3}$.

Using the values given in Table I for the sections of the holes, and taking the FS of the holes to be an ellipsoid, we obtain

$$V_h = (43.99 \pm 0.05) \cdot 10^{-63} \text{ g}^3 \cdot \text{cm}^3 / \text{sec}^3,$$

which coincides with $3V_e$.

The principal curvature radii of the FS in the directions of the 2 axis and near the 3 axis, calculated in accordance with the model, are (accurate to $\sim 1\%$) 177×10^{-21} , 0.983×10^{-21} , and respectively 163×10^{-21} , 0.422×10^{-21} g-cm/sec. Using the values of the Fermi velocity obtained in^[10], and refined in accordance with our values of the curvature (10.25×10^7 and 7.85×10^7 cm/sec), we obtain for these directions, at the limiting point, the effective masses $(0.141 \pm 0.03) m_0$ and $(0.117 \pm 0.03) m_0$, which coincides within the limits of errors with the previously measured^[2,3] values $(0.138 \pm 0.02) m_0$ and $(0.117 \pm 0.04) m_0$.

An analysis of the FS shape obtained in the present paper shows that the non-quadratic non-ellipsoidal model of the spectrum of bismuth^[23] can describe the real FS better than the ellipsoidal model, since it contains an additional parameter. However, it cannot, first, describe the asymmetry of the FS (see Figs. 5 and 6) and, second, the large curvature radii along the 2 and 3 axes should differ in Cohen's model by a factor 1.32, whereas they differ only by 7%. Thus, Cohen's model^[23] can hardly be used to advantage for a quantitative description of the FS of bismuth.

Another known theoretical model of the bismuth spectrum, that of Abrikosov and Fal'kovskii, contains a large

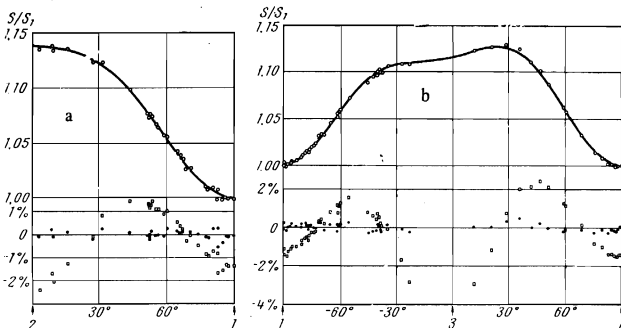


FIG. 5. Anisotropy of the central sections in a coordinate system transformed in accordance with relations (5): a—in the basal plane, b—in the bisector plane; \circ —experiment, \square —deviation from ellipsoidal model, \bullet —residual difference. Solid line—approximation by a sum of the functions (4) with the coefficients given in Table II.

number of additional parameters, and by choosing the latter it is apparently possible to obtain satisfactory agreement with experiment. However, the presently known set of constants in this model^[24] leads to a discrepancy of $\sim 10\%$ between theory and experiment. A refinement of the parameters of the Abrikosov-Fal'kovskii model on the basis of the results obtained here is beyond the scope of the present paper.

The spin splitting in the quasiclassical approximation was calculated by Fal'kovskii^[1]. The qualitatively predicted behavior of the g-factor or for the electrons (see Fig. 8b in^[1]) agrees with the experimentally measured value (Fig. 4). It is possible that allowance for the term $-\mu_0\sigma H$, and also the use of spectrum parameters that give a better agreement with experiment for the FS, will result also in quantitative agreement. Such calculations are all the more interesting since the solution will apparently describe the spectrum of the electrons also at small quantum numbers. This conclusion can be drawn also by comparing our results with those of Smith et al.^[12], in which information on the spin splitting was obtained at values of the quantum number on the order of unity (Fig. 4).

Thus, by improving the experimental procedure it became possible to improve the accuracy of the measurement of the central sections of the FS bismuth by more than one order of magnitude. This has made it possible not only to observe the deviations of the electron FS from an ellipsoid, but also to describe them quantitatively. Using a BESM-6 computer, we performed calculations that resulted in the construction of an empirical model of the electron FS, expressed analytically in the form of an expansion in spherical harmonics. The obtained model agrees well with such geometry-dependent experimental characteristics of the FS as the extremal values of the momenta and the effective masses at the limiting points. The concentration of the electrons on the holes turned out to be the same with accuracy $\sim 0.1\%$. The results can be used to refine the theoretical model of the carrier spectrum in bismuth.

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¹An alloy of this composition for use at low temperatures was proposed by V. M. Pudalov.

²In the frequency-modulation method one measures the derivative of the inductance of the circuit, and the changes in the inductance are determined either by the differential susceptibility or by the oscillations of the conductivity of the sample. Both quantities are proportional to the second derivative of Φ [3].

³This correction is not connected with the magnetic interaction in the de

Haas-Van Alphen effect [14] which, as shown by estimates, is negligibly small. The difference between these effects becomes particularly clearly manifest in the fact that in our case the correction depends on the type of the considered carriers, and it has not only different values in the same field but also different signs for electrons and holes.

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