THE FERMI SURFACE OF LEAD

N. E. ALEKSEEVSKII and Yu. P. GAĬDUKOV

Institute for Physics Problems, Academy of Sciences, U.S.S.R.

Submitted to JETP editor March 22, 1961

J. Exptl. Theoret. Phys. (U.S.S.R.) **41**, 354-362 (August, 1961)

A detailed study of the galvanomagnetic properties of single crystal lead is carried out. From the experimental data the Fermi surface could be established and is found to be double sheeted: one part of the Fermi surface is an open surface of the "fluted cylinder net" type, the axes of the cylinders being parallel to the [111] crystallographic axis; the other part is a closed surface. The volumes of the open and closed surfaces are equal and opposite in sign (the closed surface corresponds to "hole" conductivity). The model proposed for the Fermi surface of lead is compared with the experimental results on the de Haas–van Alphen effect, known from the literature.

A preliminary study of the anisotropy of the resistivity of single crystals of lead in the range of large magnetic fields showed that lead has an open Fermi surface.[1,2] An open Fermi surface for metals with cubic lattice symmetry can only be a surface of the "fluted cylinder space net" type, with axes parallel to rational axes of the reciprocal lattice. Such surfaces were found in copper,[3] gold and silver.[2,4]* It would be expected that the Fermi surface of lead would also be a "space net." The anisotropy of the galvanomagnetic properties would then be similar to that in gold, silver and copper. However, on the polar diagram of the resistance of lead in a magnetic field there are wide angular ranges with quadratic growth of resistance, and saturation of the resistivity in a magnetic field is only found in some selected directions. (This behavior of the resistivity of lead single crystals is the opposite of the resistance behavior of gold, silver and copper.)

It was established previously that the quadratic resistance growth in a wide range of directions for tin single crystals is connected with the compensation of the "electron" and "hole" volumes of the Fermi surface.[6] An analogous "compensation" can therefore be expected for the Fermi surface of lead.

The purpose of the present work was to determine the topology of the Fermi surface of lead. Lead is also of interest in that the de Haas–van Alphen effect has been studied in most detail for this metal.[7 8] It was therefore possible to compare the results of two different methods of studying the Fermi surface of metals.

SPECIMENS AND MEASUREMENTS

The lead single crystals, grown by the Czochralski method, were 20 — 30 mm long and 2 — 3 mm in diameter. In some cases specimens of the required orientation were in plate form. Such specimens were cut by electro-erosion from a large single crystal obtained by the Obreimov-Shubnikov method. The orientation of the round single crystals was determined optically with an accuracy of 1°. The orientation of the plates was determined by x rays. The resistivity change of the specimens from room temperature to 4.2° K was $\rho_{300}/\rho_{4.2} = 6{,}000 - 10{,}000$, so that measurements could be made in large effective fields, starting at about 1 koe ($\rho_{4.2}$ was determined by extrapolating the $\rho_{4.2}(H)$ dependence to zero magnetic field).

The measurements were carried out at 4.2° K with a potentiometer system having a sensitivity of 10^{-9} v. The angular dependence of the resistivity and the Hall e.m.f. were determined in a field of 23 koe. The magnetic field was rotated in a plane perpendicular to the specimen axis. The Hall e.m.f. was measured both on the plates and on the round specimens. In the latter case the Hall e.m.f. was taken off at two pairs of mutually

*We must point out that we are discussing the topological features, and not the form of the Fermi surface, which are not the same at all.[5] For example, the Fermi surface of copper is a system of cubes, the vertices of which intersect in such a way that the "openness" arises in the [001] and [110] directions as well as [111]. For galvanomagnetic properties, the topology of such a surface is equivalent to a "fluted cylinder space net" with axes parallel to the directions [111], [110] and [001]. These are precisely the topological features that show up in the galvanomagnetic properties of gold, silver and copper.

Specimen Pb	Orientation* φ; ϑ', deg	$\rho_{300}/\rho_{4.2}$	Position of the minima and maxima (in degrees) on the $\rho_H(\vartheta)$ diagrams**
1	[001]	8000	[010] (13) ***; [110] (1)
2	0; 10		0 (6); ± 41 (1.1); ±43 (1.5); ± 45 (1); ± 47 (1.5); ±49 (1.1); ± 90 (5.5)
3	0; 14		0 (4); ± 44 (1,2); ± 47 (1.5); ±49 (1); ±90 (5)
4	0; 20		0 (3.7); ± 30 (2); ±40 (2.3); ±52 (1); $\overline{90}$ (4.5)
5	0; 27	7150	0 (6); ± 25 (3.2); ± 38 (4); ± 51 (1); ± 90 (7.5)
6	0; 31		0 (4.3); ± 3 (4.5); ± 19 (3.2); ± 53 (1); ± 90 (6.6)
7	0; 35		0 (1.6); ± 16 (3.2); ± 52 (1); ± 90 (5)
8	[011]	9400	[0$\bar{1}$1] (1); ± 20 (10.5); [2$\bar{1}\bar{1}$] (1); [100] (15.5)
9	45; 6		0 (1.2); ± 45 (6); ± 90 (1)
10	45; 10	9900	0 (1); ± 3 (4); ± 6 (2); ± 45 (17); ± 90 (1.3)
11	45; 16		0 (6.5); ± 2 (8.5); ± 9 (4); ± 43 (20); ± 90 (1)
12	45; 37	10800	0 (8); ± 5 (8.5); ± 23 (3); ± 48 (9); ± 60 (8); ± 72 (9); ± 90 (1)
13	45; 41	8500	0 (8); ± 15 (9); ± 25 (2.5); ±32 (5.5); ± 36 (4); ± 40 (9.5); ± 90 (1)
14	40; 45	6050	0 (5); + 14 (5.8); + 27 (2); + 34 (3.5); + 36 (2.7); + 48 (6); — 86 (1); — 44 (6); — 23 (1.4); — 10 (5.5):
15	[111]		[112] (4.5); ± 16 (5.5); [011] (1)
16	43; 64		0 (4.8); + 12 (5.5); + 22 (3); + 26 (3.5); + 34 (1.3); + 88 (1)
17	45; 80	10800	0 (12.5); ± 34 (1); ± 72 (8); ± 90 (1)

*φ and ϑ' are the polar coordinates of the specimen axes: φ is measured from the (010) or (100) plane; ϑ' is the angle between the [001] axis and the specimen axis.

**The direction of the line of intersection of the plane of rotation of the magnetic field with the plane passing through the specimen axis and the [001] axis is chosen as $\vartheta = 0$.

***The ratio of the resistance for the given direction to the resistance in the deepest minimum is given in parentheses.

perpendicular contacts, placed on a transverse section of the specimen. The table shows data on the specimens.

EXPERIMENTAL RESULTS*

Some characteristic angular dependences of the resistance $\rho_H(\vartheta)$, where ϑ is the angle of rotation of the magnetic field, are shown in Fig. 1. The $\rho_H(\vartheta)$ dependence for the specimen Pb-1 was given previously.[2] One can gain a qualitative idea of the nature of the resistance anisotropy from the table.

Figure 2 shows characteristic examples of the behavior of the resistance in a magnetic field for different directions. A marked anisotropy is also observed in the behavior of the Hall e.m.f. (Fig. 3), and on the $E_x(\vartheta)$ diagrams narrow maxima, which are observed for H ∥ [110] are characteristic. The principal variations of Hall e.m.f. with magnetic field are shown in Fig. 4.

As mentioned above, a quadratic growth of resistance in a magnetic field is observed over a wide range of angles [broad maxima on the $\rho_H(\vartheta)$ diagrams]. Saturation of the resistance is only observed in special directions, for example for H ∥ [110], H ∥ [112] with I ∥ [011]. For these magnetic field directions narrow deep minima appear on the $\rho_H(\vartheta)$ diagrams. All the directions for which narrow minima are observed are plotted on the stereographic projection (Fig. 5). The depth of the narrow minima of resistance (except those corresponding to H ∥ [110]) depends on the current orientation. For example, with I ∥ [111] a broad maximum of resistance is found in the region of the [112] direction, and $\rho \sim H^2$. This made it essential to make an analysis of current diagrams, which enabled the cause of the quadratic growth and saturation of the resistance to be explained, and made it possible to determine the direction of the open sections of the Fermi surface.

As has already been noted,[6] three types of current diagram $\rho_H(\alpha)$ are possible in the general case; α is the angle between the current and the mean direction of the open sections of the Fermi surface or of some crystallographic direction (I ⊥ H).

1. If in some direction of the magnetic field there are no open sections of the Fermi surface, but there is compensation of the "electron" and "hole" volumes of the Fermi surface, $V_{el} = V_{hole}$, then for any angle α the resistance increases quadratically with field: $\rho \sim H^2$.

2. If for some direction of H there are no open sections of the Fermi surface, but $V_{el} \neq V_{hole}$, then the resistance in a magnetic field reaches

*The authors thank A. P. Kir'yanov who made the measurements on a number of specimens.

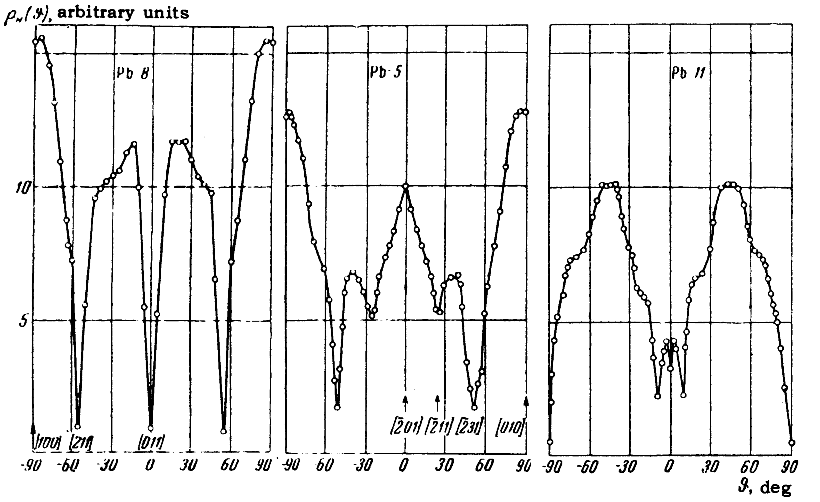

FIG. 1. The anisotropy of the resistance of single crystals of lead; H = 23 koe, T = 4.2°K.

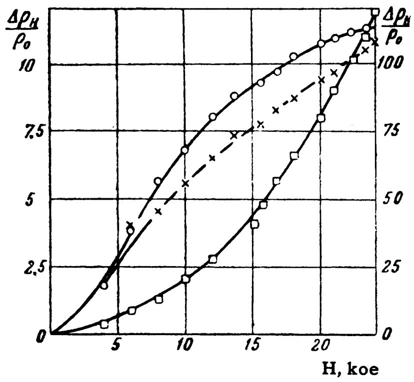

FIG. 2. The change of resistance in a magnetic field for specimen Pb-8 for various values of the angle ϑ: ○ – $\vartheta = 0°$, × – $\vartheta = 55°$ (left ordinate scale); □ – $\vartheta = 90°$ (right ordinate scale).

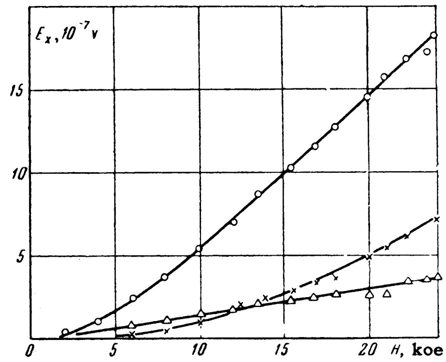

FIG. 4. Dependence of the Hall e.m.f. on the magnitude of the magnetic field for a fixed angle ϑ for specimen Pb-8 (I = 3 amp): ○ – $\vartheta = 0°$, × – $\vartheta = 55°$, Δ – $\vartheta = 90°$.

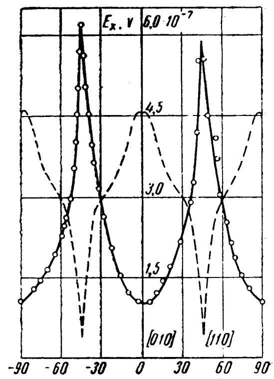

FIG. 3. Anisotropy of the Hall e.m.f. for specimen Pb-1 (specimen diameter 1.8 mm); H = 22 koe, T = 4.2°K, I = 1 amp. For comparison, the angular dependence of the resistance is shown in the figure (dashed curve).

saturation for any α (the resistance behaves in a similar way if there are open sections with a different mean direction).

3. If for a given direction of the magnetic field, there is a layer of open sections of the Fermi surface with a single mean direction, then

$$\rho_H(\alpha) = AH^2\cos^2\alpha + B.$$

An analysis of the experimental angular dependences $\rho_H(\vartheta)$ shows that a current diagram of the first type is met in wide ranges of directions of the magnetic field, grouped round the [001] and [111] axes. The second type of current diagram only occurs for the [110] direction. For direction of **H** lying in the (111) planes, for which an analysis could be carried out, the current diagrams had a form close to a $\cos^2\alpha$ dependence.

It is natural to suggest that any direction of the magnetic field lying in the (111) planes (except directions near [110]) will have this property. This is borne out by the fact that the narrow minima of resistance lie mainly in the (111) planes. We can thus consider that the directions of the narrow minima are those field directions for which open sections of the Fermi surface exist. The stereographic projection of the narrow minima is, therefore, in fact the projection of the singular directions of the magnetic field for an open Fermi surface of lead. This projection is shown in the upper part of Fig. 5. The dimensions of the two dimensional regions around the [110] direction could be determined very approximately from the disappearance of the minima of resistance in the

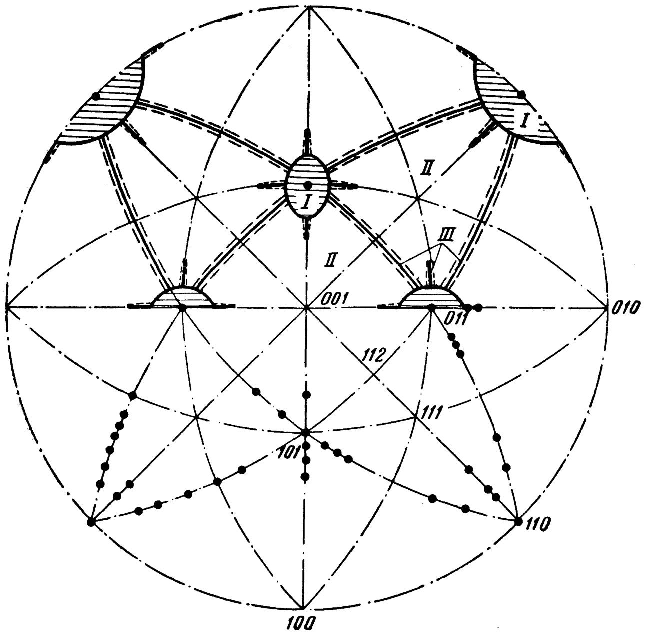

FIG. 5. Stereographic projection of the directions of the narrow minima of resistance (lower half) and of the singular magnetic field directions for the Fermi surface of lead (upper half). Region I – double regions of magnetic field directions for which open sections exist (the thickness of the layer of open sections is zero at the edges of the regions I and in the direction [110]); there are no open sections for regions II, but there is compensation of the "electron" and "hole" volumes: $V_{el} = V_{hole}$; there are considerably drawn out closed sections for the regions III. Open trajectories are only found for those directions of the magnetic field which lie on the "whiskered" lines.

(111) planes as the plane of the magnetic field approached the [110] direction: the diameter of the region is $(20 \pm 2)°$ in the (001) plane; $(14 \pm 2)°$ in the (110) plane; in the (001) and (110) planes the minima of resistance exist at distances somewhat greater than the dimensions of the double region. This feature, which has been studied in detail earlier,[6] is connected with the fact that for rational planes, open sections of the Fermi surface can exist beyond the limits of the double region. There are, therefore, "whiskers" on the projections of the singular directions of **H** for open sections of the Fermi surface of lead. The ends of the "whiskers" are 15° from the center of the double region.

THE FERMI SURFACE OF LEAD

The stereographic projection of the singular magnetic field directions (Fig. 5) corresponds to a Fermi surface of the "fluted cylinder space net" type, with axes parallel to the [111] directions. Such a surface is one of the simplest possible for metals with cubic lattice symmetry. The diameter of the "cylinders" (assuming that there is some mean constant diameter[9]) can be calculated from the dimensions of the double region on the projection. This "diameter" is (0.18 ± 0.03)b, where b is the period of the reciprocal lattice of lead in the [001] direction, $b = 2(2\pi/a)$, $a = 4.9$ A.

In order to explain the compensation of volumes, which is observed when the magnetic field direction lies in the regions II of the stereographic projection, it must be assumed that the Fermi surface of lead is double sheeted, and it must consist of at least two parts equal in volume and opposite in sign. There are, in general, two possibilities: either both parts are open surfaces, or one is open and the other closed. The second possibility is more likely, since the combination of two open surfaces could hardly give such a simple stereographic projection of the singular magnetic field directions as was found for lead.

Taking one of the surfaces to be closed, we can decide whether it refers to holes or to electrons. For this purpose the sign of the Hall constant for **H** ∥ [110] must be determined. The sign of the Hall constant is in this case determined by the sign of the closed surface. The sign of the Hall constant found experimentally corresponds to a "hole" surface. The open surface is, correspondingly, electronic.

Some mean diameter d_m of the "fluted cylinders," which form the open Fermi surface of lead, can be determined from the value of the Hall constant R in the [110] direction. For this we use equations (33) and (34) of the paper by Lifshitz and Peschanskii.[9] For the present case the equations can be written in the following form:

$$R_{[011]} = 1/\Delta nec,$$
$$\Delta n = 2h^{-3}(V_{tot} - 0.7b^2 d_m),$$
$$V_{tot} = V_{el} - V_{hole}.$$

As $V_{el} = V_{hole}$ for the Fermi surface of lead, $\Delta n = \pm 1{,}4 h^{-3} b^2 d_m$. The Hall constant $R_{[110]} = 4.3 \times 10^{-3}$ cgs emu, determined from experiment, leads to the value $d_m \approx 0.16$b, which agrees well with the value found before from the dimensions of the double region of the stereographic projection.

Knowing d_m, the volumes of the open and closed parts of the Fermi surface of lead can be found. With d = 0.17 b, the volume of the open surface $V_{el} = 0.11 b^3$. Assuming that the closed surface is a sphere, the radius of this sphere $r \approx 0.3$ b. A model of the surface of lead, which does not contradict the experimental results is shown in Fig. 6.

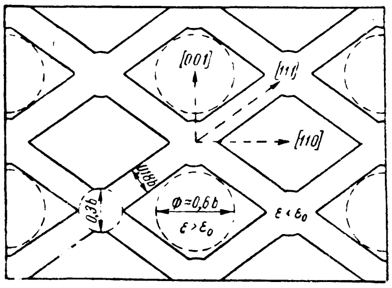

FIG. 6. Section of the Fermi surface of lead by the (110) plane (schematic).

COMPARISON OF THE RESULTS OBTAINED WITH DATA FROM THE DE HAAS–VAN ALPHEN EFFECT

Shoenberg first observed the de Haas–van Alphen effect in lead, using a pulse method to measure the susceptibility in high magnetic fields.[7] Gold later studied the effect in detail.[8]* He was able to propose a model of the Fermi surface from the results obtained, which consists of several parts. One part of the surface is open and other parts of the surface are closed. However, the open surface does not have open sections, and cannot therefore accord with the galvanomagnetic properties of lead. It is thus interesting to analyze Gold's experimental data directly and compare them with the model of the Fermi surface derived from the data of the present work.

Figure 7 shows the periods of oscillation of the susceptibility, observed in Gold's experiments. It can be seen that the periods fall into three groups: α, β, and γ. Gold notes that the short-period α oscillations show insignificant anisotropy of the period for all directions of the magnetic field: the β oscillations have weak anisotropy, roughly the same for all planes containing the [001] axis. The disappearance of the β oscillations for an inclination of the magnetic field 25° from the [001] axis is a characteristic here. The long period group of γ oscillations consists of several branches, showing considerable anisotropy of periods.

Comparing these results with the Fermi surface shown in Fig. 6, it is natural to relate the β oscillations with the closed "hole" surface, as does Gold. The closed surface has, in fact, the largest area of diametral section. The oscillations connected with the closed surface must, therefore, have the shortest period (since the period of the oscillations $P = \Delta(1/H) = 4\pi e/chS_m$, where S_m is the extremal cross-section of the Fermi surface). Knowing the mean dimensions of the closed surface, we can deduce that the corresponding period of the susceptibility oscillations will be $P_\alpha \approx 0.54 \times 10^{-8}$ oe^{-1}, which is in good agreement with Gold's data: $P_\alpha = 0.56 \times 10^{-8}$ oe^{-1}.

*We should also point out that Harrison[10] has recently studied the Fermi surface of lead theoretically.

The β and γ oscillations can be related to the maximal and minimal sections respectively of the open Fermi surface of lead. The region where four "cylinders" cross one another has the maximal section. When the magnetic field is inclined to the [001] axis these sections increase, leading to a reduction in the corresponding period of oscillations. For some angular distance from the [001] axis, the oscillations of this type disappear. This occurs near those directions of the magnetic field for which open sections of the Fermi surface occur (the thick lines in Fig. 5).

For example, if the magnetic field lies in the (001) plane, the maximal closed section (and, correspondingly, the β oscillations) disappear for an angle of 30° between the field and the [001] axis. There is thus qualitative agreement with Gold's results. It is, however, difficult to make a quantitative calculation for this case. We only note that if the volume of a sphere is deduced from the period of the β oscillations (diameter ~ 0.3 b), then this volume agrees approximately with the volume of the region where the "cylinders" of the open Fermi surface cross.*

The γ oscillations can be ascribed to the minimal sections of the open Fermi surface, i.e., to the sections of the four "cylinders" parallel to the [111] direction. In the general case four sections of different area are possible. All four sections coincide for **H** || [001]. Taking the diameter of the cylinders equal to 0.17 b, we find that $P_{\gamma[001]} \approx 3.6 \times 10^{-8}$ oe^{-1}. According to Gold's data $P_{\gamma[001]} = 4.1 \times 10^{-8}$ oe^{-1}. Assuming that these periods coincide for [001], we can compare the form of the anisotropy of the γ oscillations with the periods of the oscillations possible for the minimal sections of the "cylinders." The behavior of the anisotropy of the periods of the

*We must point out two facts. 1) One concludes from the model of the Fermi surface of lead that β oscillations should exist in the region of the [111] direction as well as the [001] direction (the former direction is also far from directions which lead to open sections). In Gold's work there is no indication of oscillations in this region with a period close to the period of the β oscillations. 2) As soon as open sections of the Fermi surface arise, new closed "hole" sections also arise. It can easily be seen from Fig. 6 that the area of these sections exceeds not only the areas of the sections connected with the β oscillations, but also the areas referring to the α oscillations. Gold's data to not indicate the existence of such large sections.

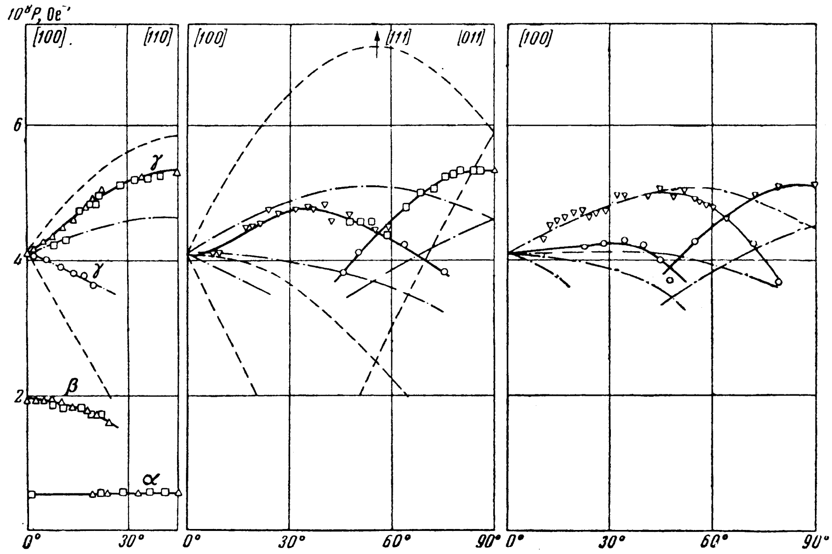

FIG. 7. Periods of oscillations of the susceptibility of lead, found by Gold.[8] The continuous lines are drawn through Gold's experimental points. Case a – H‖(001), b – H ‖ (0$\bar{1}$1), c – the field parallel to the plane, the normal to which has the orientation [φ = 30°, ϑ = 90°]. The periods for the α and β oscillations are not shown for cases b and c.

oscillations corresponding to the open Fermi surface of lead is shown by the dotted line (these curves are not shown in Fig. 7c). It can be seen from the figure that there is some qualitative agreement in behavior of the calculated and observed periods of the γ oscillations.

The collapse in the γ oscillations (and also of the β oscillations) for some directions of the magnetic field, associated with the appearance of open sections, is most characteristic. It must be remarked, nevertheless, that there are great quantitative discrepancies in the behavior of the anisotropy of the calculated and observed periods of the γ oscillations. This is not surprising, however, since it was assumed in the calculation that the open Fermi surface is formed by right cylinders. If we make the natural assumption that the cylinders are corrugated, we can obtain better agreement with Gold's data. For example, for corrugation of the cylinders produced by part of an ellipsoidal surface of revolution with axes in the ratio 3 : 2 (the long axis parallel to the [111] axis), the picture of the behavior of the anisotropy of the γ oscillations is shown in Fig. 7 by the dashed line.

In conclusion, we consider it a pleasure to thank Academician P. L. Kapitza for his constant interest in this work.

[1] N. E. Alekseevskii and Yu. P. Gaĭdukov, JETP **36**, 447 (1959), Soviet Phys. JETP **9**, 311 (1959).

[2] N. E. Alekseevskii and Yu. P. Gaĭdukov, JETP **37**, 672 (1959), Soviet Phys. JETP **10**, 481 (1960).

[3] A. B. Pippard, Phil. Trans. Roy. Soc. **A250**, 325 (1957).

[4] Yu. P. Gaĭdukov, JETP **37**, 1281 (1959), Soviet Phys. JETP **10**, 913 (1960).

[5] J. R. Klauder and J. E. Kunzler, Phys. Chem. Solids **18**, 256 (1961).

[6] Alekseevskii, Gaĭdukov, Lifshitz, and Peschanskii, JETP **39**, 1201 (1960), Soviet Phys. JETP **12**, 837 (1961).

[7] D. Shoenberg, Physica **19**, 791 (1953).

[8] A. V. Gold, Phil. Trans. Roy. Soc. **A251**, 85 (1958).

[9] I. M. Lifshitz and V. G. Peschanskii, JETP **35**, 1251 (1958), Soviet Phys. JETP **8**, 875 (1959).

[10] W. A. Harrison, Phys. Rev. **118**, 1190 (1960).

Translated by R. Berman
70