ELECTRON IN A PERIODIC ELECTRIC AND HOMOGENEOUS MAGNETIC FIELD, II.

G. E. ZIL'BERMAN

Submitted to JETP editor January 7, 1957; resubmitted May 9, 1957

J. Exptl. Theoret. Phys. (U.S.S.R.) **33**, 387-396 (August, 1957)

The energy spectrum of an electron in a magnetic field is considered in the case in which its trajectory in **k**-space (i.e., the intersection of the Fermi surface by a plane perpendicular to the magnetic field) is an open periodic. In this case, equidistant or quasi-equidistant discontinuities appear in the continuous spectrum. The distance between them is of the same order as that between levels in a discrete spectrum [$\sim \epsilon^2$, Eq. (3)], while the width, which is usually exponentially small or of order ϵ^4, may be of the order of ϵ^3 or ϵ^2 in individual cases. The results that are obtained are applied to the theory of the de Haas-van Alphen effect.

THE present paper is a continuation of the research of Ref. 1, in which the energy levels of an electron in a crystal in a magnetic field were found in the quasi-classical approximation for the case in which the trajectory in **k**-space is closed and is located entirely within a single cell of the reciprocal lattice. In this case the energy is determined from the equations obtained in the work of Lifshitz and Kosevich:[2]

$$S(E, k_3) = (2\pi eH/\hbar c)(n+\gamma) \equiv (2\pi/\alpha_0^2)(n+\gamma). \tag{1}$$

Here $S(E, k_3)$ is the area of the intersection of the surface of constant energy in **k**-space by a plane perpendicular to **H**, while γ, as shown in Ref. 1, is equal to $\frac{1}{2}$ for almost all closed trajectories.

It was shown in Ref. 1 that if the closed surfaces in neighboring cells of **k**-space come close to one another, the discrete levels $E = E(n, k_3)$ [which are obtained from Eq. (1)] broaden out into narrow bands. This broadening is small if the trajectories are closed. If the trajectory of the electron is an open periodic, then the broadening is so great that one no longer speaks of broadening but rather of discontinuities in a continuous spectrum.

Let us consider open periodic trajectories obtained in the intersection of open, isoenergetic surfaces of the "corrugated cylinder" type by planes which pass through the axis of the cylinder. When **H** lies in one of the principal crystallographic planes, as is usually the case for experimental investigations of the de Haas-van Alphen effect, the plane perpendicular to **H** is located in precisely this fashion.

1. THE LIMITING CASE OF A "WEAKLY CORRUGATED CYLINDER"

If the surface $E(k_1, k_2, k_3) = \text{const}$ is a cylinder (whose axis we identify with the k_2 axis), then the intersection of such a surface with a plane passing through the axis of the cylinder (we shall consider this plane perpendicular to the k_3 direction) will consist of two parallel lines $k_1 = \pm k_0 = \text{const}$.

As was shown in Refs. 1 and 2, $\alpha_0^2 k_1$ plays the role of the momentum relative to the "coordinate" k_2. Constancy of the classical momentum denotes free motion of a particle with a continuous energy spectrum. Continuity of the spectrum in our case follows from the following considerations.

In the absence of a magnetic field, let the energy spectrum of the electron be expressed by the equation

$$E(k_1, k_2, k_3) = \sum_{\mathbf{n}} A_{\mathbf{n}} e^{i\mathbf{k}\mathbf{n}}. \tag{2}$$

Then, as was shown in Ref. 1, the energy levels E in a magnetic field, and the eigenfunctions of the electron in **k**-space [under the condition that $\epsilon \ll 1$, where

$$\varepsilon = a/\alpha_0, \quad \alpha_0 = \sqrt{\hbar c/eH} \tag{3}$$

a = lattice constant; if $a = 2.5 \times 10^{-8}$ cm, then $\epsilon = 10^{-2}$ for $H = 10^4$ Oe] are determined by the

equation*

$$\hat{E}g \equiv \mathrm{E}(\hat{\varkappa}_1, k_2, k_3)\, g = \sum_{\mathbf{n}} A_{\mathbf{n}} \exp\left(i\,\mathbf{kn} - i\,\frac{n_1 n_2}{2\alpha_0^2}\right) g\left(k_2 - \frac{n_1}{\alpha_0^2}\right) = Eg; \tag{4}$$

$$\hat{\varkappa}_1 = k_1 - (i/\alpha_0^2)\,\partial/\partial k_2. \tag{5}$$

If the surface $\mathrm{E}(\kappa_1, \mathrm{k}_2, \mathrm{k}_3) = \mathrm{const}$ is a cylinder (with axis k_2), then $A_{n_1 n_2 n_3} = 0$ $(n_2 \neq 0)$ in Eq. (2), and Eq. (4) is satisfied by a plane wave, which it is appropriate to write in the form

$$g(k_1, k_2, k_3) = \exp\{i\alpha_0^2 (p_1 + k_1) k_2\},$$

so that

$$E = \sum_{\mathbf{n}} A_{\mathbf{n}}\, e^{i(p_1 n_1 + k_3 n_3)},$$

i.e., a continuous spectrum exists.

If a weak periodicity ("corrugation," Fig. 1) appears on the energy surface, then the classical momentum κ_1 becomes a periodic function of k_2. For a quadratic dependence of E on κ_1, this would mean motion in a weak periodic potential field. The eigenfunction is obtained in this case by multiplication of a plane wave by a modulating periodic function.

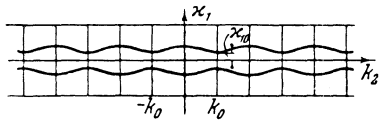

FIG. 1

Narrow discontinuities appear in the energy spectrum, and the continuous spectrum breaks up into bands which represent strongly broadened levels.

Considering terms with $n_2 \neq 0$ in Eq. (4) as a small perturbation, we can find the energy spectrum both close to the discontinuity and far from it. The discontinuities are obtained for those values of k_1 which satisfy the condition $\mathrm{k}_1 = a_2 n/2\alpha_0^2$ (n = interger, a_2 is the lattice constant in the k_2 direction). This means that the areas of the intersections (in a single cell) appropriate to the middle of the level, are equal to $S = 2k_1(2\pi/a_2) = (2\pi/\alpha_0^2)(n + \frac{1}{2})$, i.e., they are again determined by Eq. (1).

The width of the n-th discontinuity in the spectrum is determined by the equation

$$E(k_1) = E^0(k_1) \pm \left[\sum_{n_1 n_2 m_1 m_2} A_{n_1 n n_3} A_{m_1 n n_3} \exp\left\{i a_2 n \frac{m_1}{\alpha_0^2} + i k_3 (n_3 + m_3)\right\}\right]^{1/2}, \tag{6}$$

where $\mathrm{k}_1 = a_2 n/2\alpha_0^2$. The width of the discontinuity can be changed both monotonically and non-monotonically for a change in the number n or the magnetic field (α_0).

In the approximation considered, the discontinuities in the energy spectrum are quasi-equidistant, and have the order of magnitude ϵ^2. Such large discontinuities can take place only in those cases in which the corresponding coefficient A_{n_2} is different from zero. However, even if there is a finite number of terms in the expansion (2), exponentially small discontinuities exist in every case.

As was shown in Ref. 1 (see Mathematical Appendix 3),† Eq. (4) together with the nondiagonal terms corresponding to other energy bands, is written in the form

$$\hat{E}_r g_r - E g_r = \alpha_0^{-2} \sum_s \sum_{\mathbf{m}} D_{\mathbf{m}rs}\, e^{i\mathbf{km}}\, g_s\left(k_2 - \frac{m_1}{\alpha_0^2}\right).$$

The nondiagonal terms give discontinuities in the spectrum of order ϵ^3, in which the number of such discontinuities is equal to the number of coefficients $D_{m_1 m_2 m_3}$ not equal to zero $(m \neq 0)$ (the coefficients $D_{\mathbf{m}}$ are the coefficients of the Fourier expansion $\Sigma D_{\mathbf{m}} e^{i\mathbf{km}}$ of the integral of some bilinear combination of eigenfunctions in the absence of a magnetic field: $\psi_{\mathbf{ks}}$, $\psi_{\mathbf{kr}}$).

*This equation was obtained in Ref. 1 from the Schrödinger equation for an electron in a periodic electric and homogeneous magnetic field. For lack of space, we have not carried through this derivation, which demonstrates that we can obtain this Hamiltonian if we postulate the substitution in Eq. (2) of the corresponding non-commuting operators for the components of k, carrying out the operation of total symmetrization, i.e., arbitrary products of $\hat{\mathrm{k}}_i^n$ and $\hat{\mathrm{k}}_s^m$ are taken in all possible combinations.

†We take the opportunity to observe that there was an error [in Eq. (8) of Appendix 2] in that paper which has no effect on the subsequent conclusions.

In all the cases considered in the present section, the discontinuities in the spectrum arise for those values of the energy for which the area of the intersection of the isoenergetic surface is given by $S = 2\pi n/\alpha_0^2$, and the mean of the broadened level corresponds to an area of intersection $S = (2\pi/\alpha_0^2)(n + \frac{1}{2})$, precisely the same as for the discrete levels of the closed trajectory.

In the following sections we shall consider cases in which the discontinuities in the spectrum are sufficiently large that a noticeable de Haas-van Alphen effect appears. In such a case, we shall not make use of the approximation of a "weakly corrugated cylinder," since it requires too large an anisotropy of the coefficients, expressed by the relation

$$A_{n_1 n_2 n_3} \ll \varepsilon^2 A_{n_1 0 n_3}. \tag{7}$$

Such an anisotropy obviously does not occur in real cases ($\epsilon^2 \lesssim 10^{-4}$).

2. SOLUTION OF THE PROBLEM OF MOTION IN A PERIODIC FIELD, USEFUL FOR SMALL VALUES OF THE MOMENTUM ON THE CELL BOUNDARIES

In the case of closed trajectories which are divided into large regions of imaginary momentum, the broadening associated with a periodicity in the direction k_2 (Fig. 2) is exponentially small (in this case, however, as was shown in Refs. 1 and 5, there is an additional broadening, of order ϵ^4 and connected with the non-equivalence in the crystal of the different positions of the "center of rotation" of the electron). Such a picture holds for the motion of a particle in a periodic potential field at low energy levels, when the regions of imaginary momentum are large (level A in Fig. 2). The bands in this case are so narrow that they can be regarded as narrow levels. When the closed trajectories are divided into small regions (level B in Fig. 2), the broadening becomes significant. In this case, we must use a method analogous to the method of "strongly coupled electrons" for the calculation of the broadening.

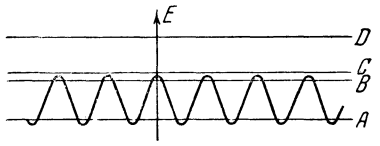

FIG. 2

If the trajectories are open and the momentum is large (which corresponds to the level D), the discontinuities are small.

We now consider the case in which the momentum in the vicinity of some point (we shall assume that it is located on the cell boundary) takes on a small value (level C).

We analyze several neighboring elementary cells in the region shown in Fig. 3. While the momentum κ_1 is large in regions I, III, V, and the quasi-classical approximation can be used, the momentum is small in regions II and IV, and we can obtain an exact solution. A similar division into different regions follows in the case in which κ_1 or κ_1' has a discontinuity for some $k_2 = b$ (Fig. 3). Our considerations will apply to both cases.

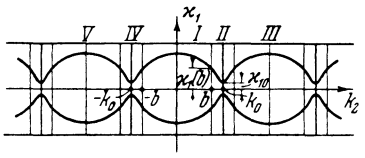

FIG. 3

We write the eigenfunctions for regions I, III, V in the form of linear combinations of quasi-classical wave functions.

The second quasi-classical approximation for these functions, obtained in Ref. 1, has the form:

$$g(k_1 k_2 k_3) = e^{i\alpha_0^2 k_1 k_2} f(k_2), \quad f(k_2) = \left|\frac{\partial E}{\partial \kappa_1}\right|^{-1/2} \exp\left\{-i\alpha_0^2 \int_0^{k_2} \kappa_1 \, dk_2\right\}, \tag{8}$$

while the next (third) approximation, which we employ in the present paper, is

$$f(k_2) = \left|\frac{\partial E}{\partial \kappa_1}\right|^{1/2} \exp\left\{-i\alpha_0^2 \int_0^{k_2} \kappa_1 \, dk_2\right\} \left(1 - \frac{i}{2\alpha_0^2} \int_0^{k_2} F(k_2)\, dk_2\right), \tag{9}$$

where

$$F = Q\left(\frac{3}{4}\frac{P'^2}{P^3} - \frac{P''}{2P^2}\right) - \frac{Q'P'}{2P^2} + \frac{Q''}{4P} + \frac{R\kappa_1''}{12P}; \quad P = \frac{\partial E}{\partial \kappa_1}, \quad Q = \frac{\partial^2 E}{\partial \kappa_1^2}, \quad R = \frac{\partial^3 E}{\partial \kappa_1^3}.$$

We write the eigenfunction in regions II, IV in the form $f = Af_1 + Bf_2$, where f_1 and f_2 are the even

and odd solutions, respectively, in these regions. From the condition of equality of the eigenfunctions and their derivatives on the boundaries of the regions, we get the equation (p is a new, continously variable quantum number corresponding to a quasimomentum in a periodic field):

$$\cos p = \left\{f_1' f_2 + f_1 f_2' + f_1 f_2 \frac{P'}{P} - \frac{\Phi}{\alpha_0^4}\left[\frac{1}{2}(f_1 f_2)' \frac{P'}{P\varkappa_1} + \frac{f_1' f_2'}{\varkappa_1} + f_1 f_2\left(\frac{P'^2}{4P^2\varkappa_1} - \alpha_0^4 \varkappa_1\right)\right]\right\} \frac{1}{D} \cos \frac{\alpha_0^2 S(b)}{2}$$

$$- \left\{\frac{P'}{2P\varkappa_1}(f_1 f_2)' + \frac{f_1' f_2'}{\varkappa_1} + f_1 f_2\left(\frac{P'^2}{4\varkappa_1 P^2} - \alpha_0^4 \varkappa_1\right) + \Phi\left[(f_1 f_2)' + f_1 f_2 \frac{P'}{P}\right]\right\} \frac{1}{\alpha_0^2 D} \sin \frac{\alpha_0^2 S(b)}{2}. \quad (10)$$

Here

$$S(b) = 2\int_{-b}^{b} \varkappa_1 dk_2, \quad D = f_1 f_2' - f_1' f_2, \quad \Phi = \int_0^b F dk_2, \quad P = \frac{\partial E}{\partial \varkappa_1}, \quad (11)$$

and the values of all quantities are referred to the point $k_2 = b$.

This equation defines the possible values of the areas of intersection, i.e., it gives the possible values of the energy in implicit form. We write Eq. (10) for the case in which $\kappa_1 = \kappa_{10}$ is small on the cell boundary (for $k_2 = k_0$).

We expand $E(\kappa_1, k_2, k_3)$ in a series about the point (κ_{10}, k_0) (retaining only the terms we have written down):

$$E(\varkappa_1, k_2, k_3) = E(\varkappa_{10}, k_0, k_3) + (\varkappa_1 - \varkappa_{10})\frac{\partial E}{\partial \varkappa_{10}} + \frac{1}{2}(\varkappa_1 - \varkappa_{10})^2 \frac{\partial^2 E}{\partial \varkappa_{10}^2} + \frac{1}{2}(k_2 - k_0)^2 \frac{\partial^2 E}{\partial k_0^2} + \cdots \quad (12)$$

Here the terms of first degree in $k_2 - k_0$ are absent in view of the obvious [following from Eq. (2)] vanishing of the corresponding coefficients: $\partial E/\partial k_0$ and $\partial^2 E/\partial \kappa_1 \partial k_0$.

We shall consider that the expansion (12) is sufficiently accurate up to the point $k_2 = b$; in the opposite case, we can keep the succeeding terms of the expansion (which would naturally make the subsequent calculations more involved). Inasmuch as the expansion (12) refers to points on a curve of constant energy, it determines the dependence $\kappa_1(k_2)$. In our case, this dependence has a hyperbolic form, the equation of which is written:

$$\varkappa^2 = \varkappa_0^2 + (\varkappa_0 / R) a_2^2 (k_2 - k_0)^2. \quad (13)$$

Here, $\kappa = a_1 \kappa_1$, $\kappa_0 = a_1 \kappa_{10}$ is the value of κ on the boundary of the cell (Fig. 3). R is the dimensionless radius of curvature of the curve $\kappa_1(k_2)$ at the point k_0. Replacing κ by the operator (5), we get a second-order differential equation:

$$\partial^2 f / \partial x^2 + (\lambda + x^2) f = 0. \quad (14)$$

Here

$$x = a_2 (k_2 - k_0) / \varepsilon (R/\varkappa_0)^{1/4}, \quad \lambda = (\varkappa_0 / \varepsilon)^2 \sqrt{R/\varkappa_0}. \quad (15)$$

As is evident from (10), we are interested in the values of the function f and its derivatives at the point $k_2 = b$, for which $\kappa \gg \kappa_0$ and, consequently, in accordance with Eqs. (13) and (15),

$$\varkappa^2 \approx (\varkappa_0 / R) a_2^2 (b - k_0)^2 = \varepsilon^2 x^2 \sqrt{\varkappa_0 / R}.$$

Making the substitution

$$z = -ix^2, \quad f = e^{-z/2} u(z), \quad (16)$$

in Eq. (14), we get an equation for u(z):

$$zu'' + u'(1/2 - z) - \frac{\lambda + i}{4i} u = 0, \quad (17)$$

from which it follows that u is a degenerate hypergeometic function.[4] This allows us to write the exact solution of Eq. (14). The two independent solutions, the even f_1 and the odd f_2, have the form

$$f_1 = e^{-z/2} F(\alpha, \gamma, z), \quad f_2 = e^{-z/2} z^{1/2} F(\alpha - \gamma + 1, 2 - \gamma, z), \quad \alpha = (\lambda + i)/4i, \quad \gamma = 1/2. \quad (18)$$

Here

$$F(\alpha, \gamma, z) = \frac{\Gamma(\gamma)}{\Gamma(\gamma-\alpha)}(-z)^{-\alpha} G(\alpha, \alpha-\gamma+1, z) + \frac{\Gamma(\gamma)}{\Gamma(\alpha)} e^z z^{\alpha-\gamma} G(\gamma-\alpha, 1-\alpha, -z),$$

where

$$G(\alpha, \beta, z) = \frac{\Gamma(1-\beta)}{2\pi i}\int_C \left(1-\frac{t}{z}\right)^{-\alpha} t^{\beta-1} e^t\, dt, \tag{19}$$

and the integration is carried out over the contour C surrounding the point $t = 0$ and extending on both branches along the real axis to $-\infty$. The function $G(\alpha, \beta, z)$ can be represented in the case of large z by an asymptotic series:

$$G(\alpha, \beta, z) = 1 + \frac{\alpha\beta}{z} + \frac{\alpha(\alpha+1)\beta(\beta+1)}{z^2} + \cdots \tag{20}$$

We assume that the expansion (12) [and that also means Eq. (14)] remains valid up to such large values of κ_1 (b) (Fig. 3) for which Eq. (9) for the quasi-classical solution is also valid. The corresponding approximation for the exact solution will be such for which we keep only the first and second terms. The functions (18) in this approximation take on the form

$$f_1 = \mathrm{Re}(BF),\quad f_2 = \mathrm{Re}(CF),\quad B = \Gamma\left(\frac{1}{2}\right)\Big/\Gamma\left(\frac{1}{4}+i\frac{\lambda}{4}\right),\quad C = e^{-i\pi/4}\Gamma\left(\frac{3}{2}\right)\Big/\Gamma\left(\frac{3}{4}+i\frac{\lambda}{4}\right),$$

$$F = \exp\left\{-\frac{1}{2}\ln x - \frac{\pi i}{8} + i\frac{\lambda}{2}\ln x + i\frac{x^2}{2}\right\}\left(1-\frac{3i+4\lambda-i\lambda^2}{16x^2}\right) \tag{21}$$

Computing the brackets in Eq. (10) [by means of (21)] and making use of the properties of the Γ functions, we transform (10) to the form

$$\cos p = \sqrt{1+e^{-\pi\lambda}}\left\{\cos\frac{\alpha_0^2}{2}S + \frac{\lambda^3-6}{8x^2}\sin\frac{\alpha_0^2}{2}S\right\}. \tag{22}$$

Here S is the area of intersection (in one cell) of the surface $E = \text{const}$ with the plane $k_3 = \text{const}$, $x^2 = (\kappa/\epsilon)^2\sqrt{R/\kappa_0}$, λ is from (15), κ_0 is the dimensionless momentum on the boundary of the cell, κ, that on the boundary of regions I — II (Fig. 3). Expansion (20), and therefore (21) also, is valid for $\lambda \ll x$.

The boundary of region II is that point $k_2 = b$ where the dispersion laws (12) or (13) are still valid. It is assumed that at this point, the quasi-classical approximation (9) is also valid ($\kappa \sim \epsilon^{1/2}$ usually satisfies both these conditions). If the quadratic expansion (12) takes place even for κ larger than $\sim \epsilon^{1/2}$, then we must take the point with the largest possible κ as the boundary for the region, since the larger the κ, the more accurate both the asymptotic expansion (20) and the quasi-classical solution (9) will be.

Initially, we throw away the small terms ($\sim x^{-2}$) in (22). For $\lambda \ll 1$, we then obtain $\cos p = \sqrt{2} \times \cos(\alpha_0^2 S/2)$. Thus, for very low levels, the allowed and forbidden intervals are identical, with accuracy up to the discarded terms. Upon increase in λ, the width of the forbidden intervals decreases; for $\lambda \gg 1$, the forbidden intervals are already determined by terms $\sim x^{-2}$ and also, generally speaking, decrease with increase in energy.

The smaller the ratio R/κ_0, the larger the number of levels located in regions of those values of λ for which the square root $\sqrt{1-e^{-\pi\lambda}}$, is still significantly different from unity.

If we keep terms $\sim x^{-4}$ in (22), then, as is shown, this reduces not only to the addition of similar terms to the coefficient of the sine in (22), but also to the appearance in (22) of a new component of the form $x^{-4}e^{-\pi\lambda/2}\sin(\alpha_0^2 S(b)/2)$ [S(b) is the area within the boundaries (−b, +b)]. The chief peculiarity here is the fact that the frequency with which it oscillates (for a change in the energy or magnetic field), differs little from the frequency of the basic terms of (22). This leads to a non-monotonic change in the width of the forbidden intervals for a change in the magnetic field. A similar phenomenon has already been pointed out in Sec. 1.

3. CASE IN WHICH THE MOMENTUM OR ITS DERIVATIVE HAVE DISCONTINUITIES

Let the momentum κ_1 or its derivative $\kappa_1' = d\kappa_1/dk_2$ have a discontinuity at $k_2 = b$ (three individual cases are drawn in Fig. 4). For the functions f_1 and f_2, we use the quasi-classical expression (8), which is valid in those cases when the momentum κ nowhere takes on too small a value ($\kappa \gg \epsilon$).

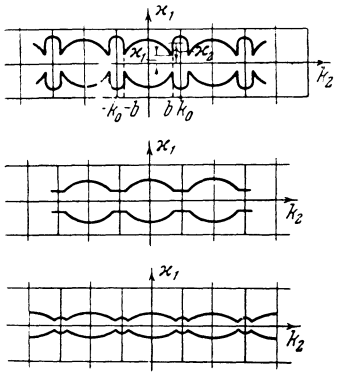

FIG. 4

We introduce the notation

$$y = \frac{\alpha_0^2}{2} S/2, \quad y_1 = y - y_b, \quad y_b = \alpha_0^2 S(b)/2, \quad P_1 = \partial E/\partial \varkappa_1, \quad P_2 = \partial E/\partial \varkappa_2, \tag{23}$$

κ_1 and κ_2 are the values of κ on the two sides of the discontinuity. We denote the derivaties with respect to k_2 by primes. With this notation, Eq. (10) takes on the form

$$\cos p = \cos y - \frac{(\varkappa_1 - \varkappa_2)^2}{2\varkappa_1\varkappa_2} \sin y_b \sin y_1 + \frac{P_2' P_1 - P_1' P_2}{2\alpha_0^2 P_1 P_2}\left(\frac{1}{\varkappa_1}\sin y_b \cos y_1 + \frac{1}{\varkappa_2}\cos y_b \sin y_1\right) + (P_1' P_2 - P_2' P_1)^2 \sin y_b \sin y_1 / 8\alpha_0^4 \varkappa_1 \varkappa_2 P_1^2 P_2^2. \tag{24}$$

If the momenta on the boundaries of the regions, κ_1 and κ_2, are small and we can apply there the quadratic dispersion laws $E = Q\kappa^2/2 + \varphi(k_2)$, then $P_1 = Q_1\kappa_1$, $P_2 = Q_2\kappa_2$ (Q_1 and Q_2 are constants) and the equation is simplified. We consider two particular cases:

1. $\kappa_1 \neq \kappa_2$, $\kappa_1' = \kappa_2'$. To abbreviate the expressions in this case from the general formula (24), we omit all terms except the first two (generally, the remaining terms are of much higher order of smallness; however, in special cases they can be large, and must then be retained). Returning to the earlier notation, we have:

$$\cos p = \cos\frac{\alpha_0^2}{2} S - \frac{(\varkappa_1 - \varkappa_2)^2}{2\varkappa_1\varkappa_2} \sin\frac{\alpha_0^2}{2} S(b) \cdot \sin\frac{\alpha_0^2}{2}[S - S(b)]. \tag{25}$$

2. $\kappa_1 = \kappa_2$, $\kappa_1' \neq \kappa_2'$. In this case, we get

$$\cos p = \cos\frac{\alpha_0^2}{2} S + \frac{\varkappa_2' - \varkappa_1'}{2\alpha_0^2 \varkappa_1^2} \sin\frac{\alpha_0^2}{2} S + \frac{(\varkappa_1' - \varkappa_2')^2}{8\alpha_0^4 \varkappa_1^4} \sin\frac{\alpha_0^2}{2} S(b) \cdot \sin\frac{\alpha_0^2}{2}(S - S(b)). \tag{26}$$

There are terms in Eqs. (25) and (26) which have a frequency different from the frequency of the fundamental term. As will be evident from what follows, their presence leads to fluctuations in the width of the levels upon change in the magnetic field or the energy.

Let us find what value one ought to expect for the derivative κ' at the discontinuity of κ and what value for the derivative κ'' one ought to expect for the discontinuity in κ'. The answer to this question furnishes the requirement (see Ref. 1) that in the expansions applied in the quasi-classical method (in powers of ϵ^2) each successive term would be much smaller than the preceding. Investigation shows that if at each point the inequality

$$\varkappa' \ll \varepsilon^{-2}\varkappa, \quad \varkappa'' \ll \varepsilon^{-4}\varkappa^4, \quad \varkappa'' \ll \varepsilon^{-2}\varkappa', \tag{27}$$

is not satisfied, then we must expect that a discontinuity occurs (either in κ or in κ') at this point.

4. APPLICATION TO THE THEORY OF THE DE HAAS-VAN ALPHEN EFFECT

In a previous paper,[5] starting from the approximations of electrons that are weakly and strongly coupled, it was shown that the broadening of the levels (if it does not change monotonically with change in energy and magnetic field H) leads to the phenomenon of "beats" on the curves of the dependence of the magnetic susceptibility and other physical quantities on H. In the approximation of weakly coupled electrons (in the anisotropic case) just such open trajectories occur about which we spoke in the preceding sections. In almost all cells, the curve $\kappa_1(k_2)$ is an ellipse and is sharply distorted only at the boundary.

In the present section the phenomenon of "beats" is again considered but outside the framework of the approximation of weakly or strongly coupled electrons. In Secs. 1 — 3 we considered a series of equations

which determine the energy levels and contain terms of different frequency, which produce oscillation of the levels. We investigate the simplest of these — Eq. (25) [Eq. (26) is entirely similar].

Using the notation

$$\alpha_0^2 S/2 = y, \quad (\alpha_0^2/2)(S - S(b) = \gamma y, \quad (\varkappa_1 - \varkappa_2)^2/2\varkappa_1\varkappa_2 = 2\beta, \tag{28}$$

we write (25) in the form:

$$\cos y - 2\beta \sin \gamma y \cdot \sin y (1 - \gamma) = \cos p. \tag{29}$$

Since γ and β do not depend on the magnetic field, it is possible to assume them constant and consider that only y changes. Let γ satisfy the inequality $\gamma \ll 1$. We consider two cases: $\beta \ll 1$ and $\beta \gg 1$. It is expedient to rewrite (29) in the form

$$\sqrt{1 + 4\beta(1+\beta)\sin^2 \gamma y}\cos(y + \varphi_1) \equiv R\cos(y+\varphi_1) = \cos p; \ \sin\varphi_1 = \frac{\beta \sin 2\gamma y}{R}. \tag{30}$$

For $\beta \ll 1$, the left side of (30), as well as the function $\varphi = y + \varphi_1$, has the form shown in Fig. 5.

It is not difficult to show from (30) that the area of intersection in Fig. 5, corresponding to the center of the level will be

$$S = \frac{2\pi}{\alpha_0^2}\left(n + \frac{1}{2} - \frac{\beta}{\pi}\sin 2\pi\gamma\left(n + \frac{1}{2}\right)\right). \tag{31}$$

The connection between S, n and p inside the level is expressed by the formula

$$n = \frac{\alpha_0^2 S}{2\pi} + \frac{\beta}{\pi}\sin\gamma\alpha_0^2 S - \frac{1}{\pi}\arccos(\cos p / R), \tag{32}$$

and the width of the level is equal to

$$\Delta y = \pi - 4\sqrt{\beta \sin^2 \pi n\gamma}. \tag{33}$$

The width of the level changes periodically with the change in the number of the level, n.

The effect of broadening on the de Haas-van Alphen effect can be studied by computing the partition function

$$Z(E, H) \sim \int dp \sum_{n=0}^{n_{max}} k_3 = \sum_{q=-\infty}^{+\infty} \int dp \int dn e^{2\pi i q n} k_3(n, p).$$

We transform the inner integral to the form $\int dp \int dk_3 e^{2\pi i n(k_3, p)}$ and substitute for n from Eq. (32). We then obtain

$$-4\pi\beta |q| \cos[\alpha_0^2 S_m + 2\beta \sin(\alpha_0^2 S_m \gamma)] \sin^2\left(\gamma \frac{\alpha_0^2 S_m}{2}\right) \tag{34}$$

(S_m is the extremum area of intersection with the plane k_3 = const.)

Terms of such form all enter into the expression for the magnetic susceptibility instead of the simple $\cos(\alpha_0^2 S_m + \delta)$ which is obtained in the absence of level broadening. It is evident that the broadening reduces to (1) a decrease in the amplitude of oscillation by a factor β, (2) the appearance of a factor $\sin^2(\gamma\alpha_0^2 S_m/2)$ which leads to beats, and (3) the appearance of an additional small oscillating term under the sign of the cosine.

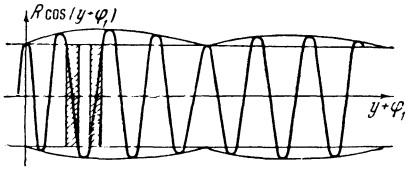

FIG. 5

The beats are not necessarily expressed by a factor similar to that used in (34) and capable of completely absorbing the oscillations (at absolute zero). This factor has another form in the case $\beta \gg 1$, when we get, in place of (34),

$$\cos\left[(1-\gamma)\alpha_0^2 S_m - \frac{1}{A}\cos\frac{\alpha_0^2}{2}\gamma S_m\right] I_0(2/A), \quad A = \beta\sin\frac{\alpha_0^2}{2}\gamma S_m + \sin\frac{\alpha_0^2}{2}\gamma(1-\gamma)S\ . \tag{35}$$

Here I_0 is the Bessel function of order zero. Equation (35) is valid in the region in which the argument I_0 remains < 1. Therefore, I_0 does not vanish, but oscillates slightly, similar to what is obtained in the approximation of weakly coupled electrons (considered in Ref. 5). Thus we have made it clear that both

complete and incomplete beats of oscillating physical quantities are possible (Fig. 6).

Both these forms of beats are encountered in experiment.[6,7] The beats can also be connected with the presence of two groups of electrons having neighboring parameters. If the beats are connected with the broadening of the levels, the period of oscillation of the curve $\chi(H^{-1})$ ought, generally speaking, to be much less than in the case in which these beats are produced by the existence of two electron groups.

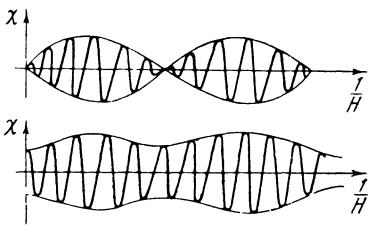

FIG. 6

Both beat mechanisms account equally well for the great sensitivity of the beats of the angle made by H with one of the crystalline axes (but the large sensitivity to the arrangement of the crystal, i.e., to the emergence of H from the fundamental crystallographic plane, is better accounted for by the mechanism described here). The vanishing of the beats on increase in temperature is also equally well explained. If we expand (34) into monochromatic components, then each of them (after integration with the Fermi distribution function in the calculation of the thermodynamic potential from the partition function) will have its own temperature factor. For sufficiently low temperatures, these factors are all close to unity, but upon elevation of the temperature, one of the factors remains significantly greater than the others and the beats disappear.

The dispersion law (34), can lead, for certain values of the parameters, to the "crescent-shaped" character of the change of the amplitude of oscillation of physical quantities observed in experiments.[6,7]

In this work we have not considered the interesting case in which the equation for $\kappa_1(k_2)$ is more than double-valued (for examples, quadruple valued). Such trajectories are frequently encountered.[8] In the dispersion equation for such trajectories, there appear terms with a large number of different frequencies. Corresponding to this case the oscillations of the physical quantities can have a more complicated character than is shown in Fig. 6.

The author takes this occasion to express his sincere gratitude to Professor I. M. Lifshitz for his attention to the present research and for his discussions.

[1] G. E. Zil'berman, J. Exptl. Theoret. Phys. (U.S.S.R.) **32**, 296 (1957); Soviet Phys. JETP **5**, 208 (1957).

[2] I. M. Lifshitz and A. M. Kosevich, J. Exptl. Theoret. Phys. (U.S.S.R.) **29**, 730 (1955); Soviet Phys. JETP **2**, 636 (1956); Dokl. Akad. Nauk SSSR **96**, 963 (1954).

[3] Lifshitz, Azbel', and Kaganov, J. Exptl. Theoret. Phys. (U.S.S.R.) **30**, 220 (1956); Soviet Phys. JETP **3**, 143 (1956).

[4] L. D. Landau and I. M. Lifshitz, Квантовая механика (Quantum Mechanics), Pt. 1 (Moscow-Leningrad, 1948), p. 557.

[5] G. E. Zil'berman, J. Exptl. Theoret. Phys. (U.S.S.R.) **30**, 1092 (1956); Soviet Phys. JETP **3**, 835 (1957).

[6] B. I. Verkin and I. F. Mikhailov, J. Exptl. Theoret. Phys. (U.S.S.R.) **25**, 471 (1953).

[7] D. Shoenberg, Paper at the Conference on the Physics of Magnetic Phenomena, Moscow, May, 1956.

[8] G. E. Zil'berman and Ia. E. Aizenberg, Физика металлов и металловедение (Phys. of Metals and Metal Research) **4**, 216 (1957).

Translated by R. T. Beyer
77