DYNAMICS OF CONDUCTION ELECTRONS UNDER MAGNETIC BREAKDOWN CONDITIONS

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Submitted February 6, 1967

Zh. Eksp. Teor. Fiz. 53, 767–783 (August, 1967)

The dynamics of conduction electrons with a complex dispersion law is considered for conditions of interband magnetic breakdown. A general method is proposed, which yields for the main breakdown characteristics simple analytic expressions that are valid for arbitrary magnetic field strengths and directions. It is found, in particular, that the exponential dependence of the breakdown probability on 1/H is valid for all values of H. Closed analytic expressions are derived and investigated for the energy spectrum under magnetic breakdown conditions. The treatment is carried out for an arbitrary dispersion law without application of any model concepts. These results are obtained after a preliminary analysis of various possible types of energy spectrum (for H = 0) with a small interband energy gap. It is demonstrated that along with the usual type of spectrum, such as that encountered in the Harrison model, a characteristic feature of many metals is that the interband gap vanishes on a whole line in **p**-space. In the latter case magnetic breakdown results in the formation in **p**-space of a narrow layer of open trajectories; the thickness of the layer depends on H. It is shown that the existence of such a layer results in sharp anomalies in the galvanomagnetic phenomena. In some cases the anomalies are manifest as "giant magnetic breakdown" oscillations of the electric conductivity with respect to the magnetic field, similar to those observed by Stark.[3]

1. INTRODUCTION

It is well known[1] that interband tunnel transitions of conduction electrons in metals placed in a strong magnetic field $\mathbf{H} = \{0, 0, H\}$ lead under definite conditions to a complete realignment of the electronic energy spectrum. This effect, called "interband magnetic breakdown," is strongly manifest in most kinetic and thermodynamic phenomena occurring in metals[2-5].

Magnetic breakdown was analyzed in [6-8] for the limiting cases of weak fields, when the probability of interband transition $W \to 0$, and for very strong field $H \to \infty$ ($W \to 1$). The methods proposed by the authors of these papers have a limited region of applicability and do not make it possible to investigate interband tunnel transitions in the intermediate case of arbitrary finite values of H.

We investigate in this paper the dynamics of the conduction electron with due allowance for quantum interband transitions in a magnetic field satisfying the quasiclassical condition

$$\varkappa = \hbar\Omega_0/\varepsilon_0 \ll 1 \tag{1}$$

(Ω_0—characteristic value of the Larmor frequency of the electron ε_0—characteristic energy on the order of the width of the band). Condition (1) imposes practically no limitations on the magnitude of the field, since this condition is satisfied by all realistically attainable values $H \ll 10^8 - 10^9$ Oe. To solve the problem of magnetic breakdown we shall formulate below a general method which essentially makes use of the smallness of the quasiclassical parameter. This method makes it possible to find the main characteristics of the breakdown and to obtain closed analytic expressions which determine the stationary wave functions and the electronic energy spectrum for arbitrary values and orientations of H.[1)] In particular, it will be shown that the breakdown probability is determined by the following universal formula, which is valid for arbitrary H:

$$W = \exp(-\bar{H}/H), \quad \bar{H} > 0 \tag{2}$$

($\bar{H}$ does not depend on the magnetic field. In accordance with the universally accepted concept of charged quasiparticles—carriers of conductivity in the metal—the analysis is carried out without involving any model representations, in terms of an arbitrary law of quasiparticle dispersion $\varepsilon_s(\mathbf{p})$ (ε—energy, **p**—quasimomentum, s—number of band). The method of solving the magnetic-breakdown problem and the main quantitative results are formulated in Secs. 2 and 3; in Sec. 4 we consider quantitatively certain macroscopic effects connected with magnetic breakdown.

2. TWO TYPES OF ELECTRONIC SPECTRUM WITH SMALL INTERBAND ENERGY GAP

In the classical approximation, the dynamics of a charged quasiparticle acted upon by a constant and homogeneous magnetic field is determined completely by the conservation laws

$$\varepsilon_s(\mathbf{p}) = E, \quad p_z = p_{z0}. \tag{3}$$

Here E—energy, p_{z0}—projection of quasimomentum on the direction of **H**. Quantum effects lead to tunnel transitions between the trajectories $\varepsilon_s(\mathbf{p}) = E$, $p_z = p_{z0}$ with identical E and p_{z0} and with different values of the band number (it is assumed that the energy lies in the band-overlap region $\min\{\varepsilon_2(\mathbf{p})\} < E < \max\{\varepsilon_1(\mathbf{p})\}$).

[1)] A preliminary communication concerning this method was published by the author in [9].

From the general properties of the quasiclassical wave function of the electron in a magnetic field it follows that the probability of tunneling (W) through classically forbidden regions is proportional to $\exp(-|B|p_{min}^2/\sigma)$ ($|B| \sim 1$, $\sigma = e\hbar H/c$), where p_{min} is the smallest distance between trajectories participating in the magnetic breakdown. As seen from the foregoing estimate, the probability W is not small when $p_{min} \lesssim \sqrt{\sigma} \ll b$ (b—fundamental period of the reciprocal lattice). Such an approach of the trajectories becomes possible if curves (3) pass through sections of $\mathbf{p}$-space in which the difference $\Delta(\mathbf{p}) = |\varepsilon_1(\mathbf{p}) - \varepsilon_2(\mathbf{p})| \ll \varepsilon_0$ (1, 2—numbers of bands participating in the breakdown). In the $\mathbf{p}$-space regions with small $\Delta(\mathbf{p})$, the electronic spectrum has a number of singularities that determine the entire specific behavior of the interband transitions in the magnetic field. It follows therefore that to solve the problem of interband magnetic breakdown it is necessary to analyze first the structure of the spectrum with small interband energy gap. The results of this analysis, which we shall perform in the present section, will be extensively used subsequently in the formulation of the general method of the problem.

To investigate the dispersion near a certain point $\mathbf{p}'$, where $\Delta(\mathbf{p}') \ll \varepsilon_0$, we write down the single-particle Schrödinger equation with H = 0 in the following form

$$\hat{\mathcal{H}}_0(\mathbf{p})u_{\mathbf{p}}^{(s)}(\mathbf{r}) = \varepsilon_s(\mathbf{p})u_{\mathbf{p}}^{(s)}(\mathbf{r}),$$
$$\hat{\mathcal{H}}_0(\mathbf{p}) = \exp\{-i\mathbf{p}\hat{\mathbf{r}}/\hbar\}\hat{\mathcal{H}}_0\exp\{i\mathbf{p}\hat{\mathbf{r}}/\hbar\}. \quad (4)$$

Here $\hat{\mathcal{H}}_0$ is the Hamiltonian of the quasiparticle at H = 0, $u_{\mathbf{p}}^{(S)}(\mathbf{r})$ is the Bloch factor (which is periodic in $\mathbf{r}$) in the stationary wave function $\psi_{\mathbf{p}}^{(S)} = u_{\mathbf{p}}^{(S)}(\mathbf{r})\exp\{i\mathbf{p}\cdot\mathbf{r}/\hbar\}$; $\mathbf{p}$ enters in (4) as a parameter, and different branches of the dispersion law $\varepsilon_S(\mathbf{p})$ represent discrete terms of the Hamiltonian $\hat{\mathcal{H}}_0(\mathbf{p})$. Since the $u_{\mathbf{p}'}^{(S)}(\mathbf{r})$ constitute a complete set of orthonormal functions, the following relations are satisfied for all values of $\mathbf{p}$

$$u_{\mathbf{p}}^{(s)}(\mathbf{r}) = \sum_{s'} R_{ss'}(\mathbf{p}|\mathbf{p}')u_{\mathbf{p}'}^{(s')}(\mathbf{r}), \quad R_{ss'}(\mathbf{p}|\mathbf{p}') = \langle u_{\mathbf{p}}^{(s)}|u_{\mathbf{p}}^{(s')}\rangle. \quad (5)$$

From the definition of $R_{SS'}$ and $\hat{\mathcal{H}}_0(\mathbf{p})$ it follows that for small $\delta\mathbf{p} \equiv \mathbf{p} - \mathbf{p}'$ the following relations are approximately valid:

$$R_{ss'}(\mathbf{p}|\mathbf{p}') \sim 1 \quad (s, s' = 1, 2), \quad R_{ss'}(\mathbf{p}|\mathbf{p}') = O(|\delta\mathbf{p}|/b) \quad (s, s \neq 1, 2);$$
$$\hat{\mathcal{H}}_0(\mathbf{p}) = \hat{\mathcal{H}}_0(\mathbf{p}') + \hat{\mathbf{v}}(\mathbf{p}')\delta\mathbf{p} + O[(|\delta\mathbf{p}|/b)^2],$$
$$\hat{\mathbf{v}}(\mathbf{p}) = \exp\{-i\mathbf{p}\hat{\mathbf{r}}/\hbar\}\hat{\mathbf{v}}\exp\{i\mathbf{p}\hat{\mathbf{r}}/\hbar\}, \quad (6)$$

where $\mathbf{v}$ is the quasiparticle velocity operator. Substituting (5) and (6) in the Schrödinger equation (4) and solving the resultant system of equations

$$\sum_{s''=1}^{2}\{(\varepsilon_{s''}(\mathbf{p}') - E)\delta_{s's''} + \mathbf{v}_{s's''}(\mathbf{p}')\delta\mathbf{p}\}R_{ss''}(\mathbf{p}|\mathbf{p}') = 0,$$
$$E = \varepsilon_s(\mathbf{p}), \quad (s, s' = 1, 2), \quad \mathbf{v}_{s's''}(\mathbf{p}) = \langle u_{\mathbf{p}}^{s'}|\hat{\mathbf{v}}(\mathbf{p})|u_{\mathbf{p}}^{(s'')}\rangle, \quad (7)$$

it is easy to obtain the unitary matrices $R_{SS'}$ and to determine the spectrum near the point $\mathbf{p}'$

$$\varepsilon_{1,2}(\mathbf{p}) = \frac{1}{2}\sum_{s'=1}^{2}\varepsilon_{s'}(\mathbf{p}') + \mathbf{A}\delta\mathbf{p} \pm \left[\frac{(\Delta + \mathbf{B}\delta\mathbf{p})^2}{4} + |\mathbf{C}\delta\mathbf{p}|^2\right]^{1/2},$$
$$\Delta = \Delta(\mathbf{p}') = \varepsilon_1(\mathbf{p}') - \varepsilon_2(\mathbf{p}'),$$
$$\mathbf{A} = \frac{1}{2}\sum_{s'=1}^{2}\mathbf{v}_{s's'}(\mathbf{p}'), \quad \mathbf{B} = \mathbf{v}_{11}(\mathbf{p}') - \mathbf{v}_{22}(\mathbf{p}'), \quad \mathbf{C} = \mathbf{v}_{12}(\mathbf{p}') = \mathbf{v}_{21}^*(\mathbf{p}'). \quad (7a)$$

The smallness of the parameter Δ in formula (7a) denotes that in the vicinity of $\mathbf{p}'$ the dispersion laws $\varepsilon_S(\mathbf{p})$ and the Bloch factors $u_{\mathbf{p}}^{(S)}$ corresponding to them) are "sharp" functions of the argument $\mathbf{p}$: the characteristic interval of their variation is $\lesssim (\Delta/\varepsilon_0)b \ll b$.

The space groups of the crystal lattice of all the metals contain inversion. It is shown in the Appendix that the invariance of the Hamiltonian $\hat{\mathcal{H}}$ against space inversion denotes reality of $\mathbf{C}(\mathbf{p})$ at all points of $\mathbf{p}$-space. In considering the spectrum with Im $\mathbf{C}(\mathbf{p}) = 0$, it is necessary to single out two topologically different cases.

(a) $\mathbf{B}(\mathbf{p}') \parallel \mathbf{C}(\mathbf{p}')$. In this case we have everywhere near $\mathbf{p}'$ the difference $\Delta(\mathbf{p}) \neq 0$, with min $\Delta(\mathbf{p})$ reached not at an isolated point, but on the plane $\mathbf{B}\delta\mathbf{p} = -\Delta|\mathbf{B}|^2(|\mathbf{B}|^2 + 4|\mathbf{C}|^2)^{-1}$ passing near $\mathbf{p}'$. It follows therefore that in case (a) the points where $\Delta(\mathbf{p}) \ll \varepsilon_0$ are concentrated near a certain surface of closest approach of the bands; on the surface itself (denoted later by the letter M) and near it we have $\Delta(\mathbf{p}) \neq 0$. The energy spectrum near the surface M, as seen from (7a), is determined by the formula

$$\varepsilon_{1,2}(\mathbf{p}) = \frac{1}{2}\sum_{s'=1}^{2}\varepsilon_{s'}(\mathbf{p}_M) + \frac{1}{2}\sum_{s'=1}^{2}\mathbf{v}_{s's'}^{(n)}\delta p_n \pm \left[\frac{\Delta^2(\mathbf{p}_M)}{4} + (\delta p_n v_{12}^{(n)})^2\right]^{1/2},$$
$$\delta p_n = \mathbf{n}(\mathbf{p} - \mathbf{p}_M). \quad (8)$$

Here $\mathbf{n}$ is a unit vector normal to M, the point $\mathbf{p}_M$ lies on the M-surface, $\mathbf{v}_{S'S'}^{(n)}$ are matrix elements of the n-component of the velocity operator at the point $\mathbf{p}_M$; $\mathbf{v}_{12}(\mathbf{p}_M) = \mathbf{n}v_{12}^{(n)} + O(\Delta_M v_0/\varepsilon_0)$, Δ_M is the characteristic value of $\Delta(\mathbf{p})$ on the M-surface, v_0—characteristic value of the velocity, $|\mathbf{v}_{11}(\mathbf{p}_M) - \mathbf{v}_{22}(\mathbf{p}_M)| \sim \Delta_M v_0 \varepsilon_0$. The functions $\varepsilon_{1,2}(\mathbf{p}_M)$ (and the corresponding $u_{\mathbf{p}_M}^{(1,2)}(\mathbf{r})$) depend smoothly on $\mathbf{p}_M$ (the characteristic interval of their variation on the M surface is $\sim b$).

As follows from (8), the smallest distance between the trajectories $\varepsilon_1(\mathbf{p}) = E$, $p_Z = p_{Z0}$ and $\varepsilon_2(\mathbf{p}) = E$, $p_Z = p_{Z0}$ is reached at the points where these trajectories cross the M-surface, with $p_{min}(E, p_{Z0}) \sim \Delta_M b/\varepsilon$ being a smooth function of E and p_{Z0}.

The spectrum corresponding to case (a) is the basis for the analysis of the experimental data and the starting point of the theoretical investigation in all the papers on magnetic breakdown known to the author. This spectrum is realized, in particular, by the Harrison model (the model of almost free electrons), first applied to magnetic breakdown by Cohen and Falicov.[1] In this model the M-surface is formed by planes that are boundaries of Brillouin zones. Of course, other mechanisms for the occurrence of the spectrum of type (a) are possible, for example doubling of one of the periods of the lattice of the metal as a result of a displacement of its atoms.[10]

(b) A spectrum that differs qualitatively from that considered above occurs in the case when the vectors $\mathbf{B}$ and $\mathbf{C}$ are not parallel. In case (b) the difference $\Delta(\mathbf{p})$ vanishes on the line of intersection of the planes $\Delta + \mathbf{B}\cdot\delta\mathbf{p} = 0$ and $\mathbf{C}\cdot\delta\mathbf{p} = 0$ passing near $\mathbf{p}'$. Thus, a spectrum of the type (b) is characterized by the fact that there exists in $\mathbf{p}$-space a line of points $\mathbf{p}_0$ (henceforth called the $\mathbf{p}_0$-line) at which $\Delta(\mathbf{p}_0) = 0$ and the energy level $\varepsilon_1(\mathbf{p}_0) = \varepsilon_2(\mathbf{p}_0) = \varepsilon(\mathbf{p}_0)$ is doubly degenerate. To each value of $\mathbf{p}_0$ there corresponds a two-dimen-

sional linear space of eigenvectors of the operator $\hat{\mathcal{H}}_0(\mathbf{p}_0)$, belonging to the eigenvalue $\varepsilon(\mathbf{p}_0)$. It is possible to introduce in this space hermitian operators $\hat{V}_x$, $\hat{V}_y$, and $\hat{V}_z$ acting on the vectors of the arbitrary orthonormal bases $u_{\mathbf{p}_0}^{(1)}$ and $u_{\mathbf{p}_0}^{(2)}$ in accordance with the formulas

$$\hat{V} u_{\mathbf{p}_0}^{(s)} = \sum_{s'=1}^{2} v_{ss'}(\mathbf{p}_0)\, u_{\mathbf{p}_0}^{(s')} \qquad (s = 1, 2), \tag{9}$$

where $v_{ss'}(\mathbf{p})$ is defined in (7).

To investigate the structure of a spectrum of type (b) near the point $\mathbf{p}_0 = \{p_0^{(x)}, p_0^{(y)}, p_0^{(z)}\}$, let us ascertain the dependence of the terms of the Hamiltonian $\hat{\mathcal{H}}_0(\mathbf{p})$ on p_x for fixed $p_{y,z} = p_0^{(y,z)}$ (the direction of the x axis is arbitrary). Substituting in formulas (5)–(7) in lieu of $u_{\mathbf{p}}^{(1,2)}$ the eigenvectors of the operator $\hat{V}_x$ (we shall denote them by $e_x^{(1,2)}$; $\hat{V}_x e_x^{(1,2)} = V_x^{(1,2)} e_x^{(1,2)}$), we find that the terms of the Hamiltonian $\hat{\mathcal{H}}_0(\mathbf{p})$ are determined by the following expressions:

$$\bar{\varepsilon}_{1,2}(p_x, p_0^{(y)}, p_0^{(z)}) = \varepsilon(\mathbf{p}_0) + V_x^{(1,2)} \delta p_x, \qquad \delta\mathbf{p} = \mathbf{p} - \mathbf{p}_0. \tag{10}$$

As seen from (10), the terms $\bar{\varepsilon}_{1,2}$ and the corresponding eigenvectors of the operator $\hat{\mathcal{H}}_0(\mathbf{p})$, denoted below $\bar{u}_{p_x, p_0^{(y)}, p_0^{(z)}}^{(1,2)}(\mathbf{r})$ ($u_{\mathbf{p}_0}^{(1,2)} = e_x^{(1,2)}(\mathbf{p}_0)$), are functions that are analytic in p_x, and are distinguished thereby from the "true" dispersion laws $\varepsilon_s(\mathbf{p})$ and Bloch factors $u_{\mathbf{p}}^{(s)}$. The connection between $\bar{\varepsilon}_s(\mathbf{p})$, $\varepsilon_s(\mathbf{p})$ and $\bar{u}_{\mathbf{p}}^{(s)}$, $u_{\mathbf{p}}^{(s)}$ is very simple:

$$\varepsilon_{1,2}(p_x, p_0^{(y)}, p_0^{(z)}) = \theta(\delta p_x)\bar{\varepsilon}_{1,2}(p_x) + \theta(-\delta p_x)\bar{\varepsilon}_{2,1}(p_x),$$
$$u_{p_x, p_0^{(y)}, p_0^{(z)}}^{(1,2)}(\mathbf{r}) = \theta(\delta p_x)\bar{u}_{p_x}^{(1,2)} + \theta(-\delta p_x)\bar{u}_{p_x}^{(2,1)}; \quad \theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases}. \tag{11}$$

On the basis of formulas (7a), the expression for the energy spectrum can be represented in a form invariant to the choice of the basis:

$$\varepsilon_{1,2}(\mathbf{p}) = \varepsilon(\mathbf{p}_0) + \frac{1}{2}\sum_{i=1}^{3} \operatorname{Sp} \hat{V}_i \delta p_i$$
$$\pm \frac{1}{2}\left[\sum_{i,k=1}^{3} \{2 \operatorname{Sp}(\hat{V}_i \hat{V}_k) - \operatorname{Sp} \hat{V}_i \operatorname{Sp} \hat{V}_k\}\, \delta p_i \delta p_k\right]^{1/2}, \tag{12}$$

It follows from (12) that the equal-energy surface $\varepsilon_s(\mathbf{p}) = E$ near $\mathbf{p}_0(E)$ ($E = \varepsilon(\mathbf{p}_0)$) is an elliptic cone defined by the equation:

$$A_1 \delta p_1^2 + A_2 \delta p_2^2 + A_3 \delta p_3^2 = 0, \qquad \delta\mathbf{p} = \mathbf{p} - \mathbf{p}_0(E). \tag{13}$$

Equation (13) is written in a coordinate system in which the tensor $A_{ik} = \operatorname{Sp} \hat{V}_i \operatorname{Sp} \hat{V}_k - \operatorname{Sp}(\hat{V}_i \hat{V}_k)$ is diagonal, A_i are the eigenvalues of the tensor A_{ik}, and the axis 3 is directed along the axis of the cone. The cavities of the cone, separated by the point $\mathbf{p}_0(E)$, correspond to the equal-energy surfaces of the first and second zones. Thus, each surface $\varepsilon_s(\mathbf{p}) = E$ crossed by the p_0-line has a conical point $\mathbf{p}_0(E)$.

The spectrum of type (b) can be the result of the so-called "forced" degeneracy[11] due to a definite type of symmetry of the crystal lattice of the metal. In particular, such a situation takes place in all metals whose crystal group contains a nontrivial helical axis or slip plane;[11] examples are metals with hexagonal close packing (Zn, Cd, Mg, etc.). It can be shown that a spectrum of type (b) is stable against small lattice deformations that conserve the center of symmetry of the first lattice. It follows therefore that for a number of metals there can occur a "random" degeneracy not connected with the symmetry properties.

In concluding this section we note that for both types of spectrum under consideration (formulas (8) and (12)) the trajectories $\varepsilon_{1,2}(\mathbf{p}) = E$, $p_z = \text{const}$ on the closest-approach section are different branches of one hyperbola. (These branches are shown in Fig. 1, where the solid lines are the asymptotes of the hyperbola and the dashed lines and the ± signs pertain to the text of Sec. 3).

3. FORMULATION OF THE METHOD AND GENERAL SOLUTION OF THE PROBLEM

Let us first formulate the problem in a manner common to both types of spectrum, without specifying concretely the form of the dispersion law in the regions of $\mathbf{p}$-space with small $\Delta(\mathbf{p})$.

In the regions of $\mathbf{p}$-space where the interband transitions can be neglected, the stationary Schrödinger equation can be written, in the first approximation in the parameter κ, in the form:[12]

$$\varepsilon_s\left(P_x + \frac{i\sigma\partial}{\partial P_y}, P_y, P_z\right) f_s(\mathbf{P}) = E f_s(\mathbf{P}), \quad \sigma = e\hbar H/c, \tag{14}$$

where $f_s(\mathbf{P})$ are the coefficients of the expansion of the stationary wave function Ψ in the functions

$$\tilde{\psi}_{\mathbf{p}}^{(s)} = u_{P_x + eHy/c,\, P_y,\, P_z}^{(s)}(\mathbf{r}) \exp\{i\mathbf{P}\mathbf{r}/\hbar\},$$

$\mathbf{P}$ is the generalized momentum (we shall henceforth call the expansion in $\mathbf{r}$ the P, s representation). The quasiclassical solution of Eq. (14), corresponding to classical motion along the trajectories $\varepsilon_s(\mathbf{p}) = E$, $p_z = P_{z0}$, will be written in the following fashion:

$$f_s^{(\pm)}(\mathbf{P}) = \sum_{\nu} f_{s,\nu}^{(\pm)}(P_y)\, \delta(P_x - P_{x0})\, \delta(P_z - P_{z0}),$$
$$f_{s,\nu}^{(\pm)}(P_y) = c_{s,\nu}^{(\pm)} \exp\left\{\frac{i}{\sigma}\left(P_{x0} P_y - \int^{P_y} p_x^{(s,\nu)}(P_y)\, dP_y'\right)\right\} \Big/ \sqrt{|\partial\varepsilon_s/\partial p_x|}, \tag{15}$$

$$\varepsilon_s(p_x^{(s,\nu)}(P_y), P_y, P_{z0}) = E. \tag{15a}$$

The indices ± pertain here to the "quasiclassical" regions of the values of P_y separated by a small interval (with characteristic dimension $\Delta P_y \ll b$), inside of which the interband transitions are significant and Eqs. (14) and (15) are not valid; the interval ΔP_y is designated schematically by the dashed lines of Fig. 1; the quasiclassical regions are designated on the same figure by the ± symbols; the index ν denotes one of the solutions of (15a); $c_{s,\nu}^{(\pm)}$ are constant coefficients related by the linear equations

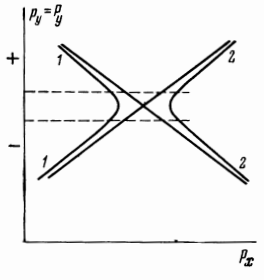

FIG. 1.

$$c_{s,\nu}^{(+)} = \sum_{s'=1}^{2} \tau_{ss'}^{(\nu)} c_{s,\nu}^{(-)} \quad (s = 1,2). \tag{16}$$

Thus, an investigation of the dynamics of the quasiparticle under conditions of magnetic breakdown actually reduces to a determination of the "joining" matrices τ, which depend on $\mathbf{H}$ and which conserve the quantities E, P_{Z0}, and the main parameters of the problem, which determine the behavior of the dispersion law inside the region of the small values of $\Delta(\mathbf{p})$. Knowing the matrices $\hat{\tau}$, we can construct the stationary wave functions and the electronic energy spectrum in all the cases of physical interest.

In order to find $\hat{\tau}$ it is necessary to investigate Schrödinger's equation inside the aforementioned region of strong magnetic breakdown, and to join the obtained solution with the quasiclassical functions $f_S^{(\pm)}(P_y)$. The solution of the "joining" problem will be obtained in two stages: we first construct the effective Hamiltonian, which determines the dynamics of the electron in the non-quasiclassical region (ΔP_y) with allowance for the interband transitions, and then investigate the eigenfunctions of this Hamiltonian and find the matrices $\hat{\tau}$.[2)] Cases (a) and (b) will be considered below separately.

1) In the case of a spectrum of type (a) it can be assumed, without loss of generality, that the M-surface is a plane passing through the origin. We choose the coordinate system such that the x axis is parallel to the M-plane; the z axis, which is parallel to $\mathbf{H}$, is at an angle θ to the M-plane; no limitations are imposed on the magnitude of this angle. The plane P_z = const crosses the M-plane along a straight line $P_y = \bar{p}_y = P_z \operatorname{tg}\theta$ parallel to the x axis.

The functions $\tilde{\psi}_{\mathbf{p}}^{(S)}(\mathbf{r})$ are not suitable for an investigation of the dynamics of the quasiparticle in a small vicinity of p_y, owing to the "sharpness" of the Bloch factors with respect to the argument P_y, as noted in Sec. 2. It is more expedient to use in lieu of $\tilde{\psi}$ the function

$$\chi_{\mathbf{p}}^{(s)}(r) = u_{P_x+eHy/c,\ \bar{p}_y,\ P_z}^{(s)}(\mathbf{r}) \exp\{i\mathbf{Pr}/\hbar\}, \quad \bar{p}_y = \bar{p}_y(P_z) \equiv P_z \operatorname{tg}\theta, \tag{17}$$

in which the dependence on P_y enters only in the exponential, and the dependence of χ on the argument $P_x + eHy/c$ is smooth, since the x axis is parallel to the M-plane.

With small values of $\delta P_y - \bar{p}_y$, the following relations, which serve as the basis of further application of the function $\chi_{\mathbf{p}}^{(S)}$, are valid:

$$\hat{\mathcal{H}}\chi_{\mathbf{P}}^{(s)}(\mathbf{r}) = \exp\{i\mathbf{Pr}/\hbar\}\,\hat{\mathcal{H}}(\mathbf{P})\, u_{\mathbf{P}M}^{(s)}(\mathbf{r}) = \varepsilon_s(\mathbf{P}_M)\chi_{\mathbf{P}}^{(s)} + \sum_{s'=1}^{2} v_{ss'}^{(y)}(\mathbf{P}_M)\delta P_y \chi_{\mathbf{P}}^{(s')}, \tag{18}$$

$$\hat{\mathcal{H}}(\mathbf{P}) = \exp\{-i\hat{\mathbf{Pr}}/\hbar\}\,\hat{\mathcal{H}}\exp\{i\hat{\mathbf{Pr}}/\hbar\} = \hat{\mathcal{H}}(P_x, \bar{p}_y, P_z) + \hat{v}_y\delta P_y + O[(\delta P_y/b)^2]; \tag{19}$$

$$\tilde{\psi}_{\mathbf{P}}^{(s)}(\mathbf{r}) = \sum_{s'=1}^{2} R_{ss'}(p_x, P_y, P_z \mid P_M)\,\chi_{\mathbf{P}}^{(s')}(\mathbf{r}); \quad P_M = \{p_x, \bar{p}_y, P_z\},\ p_x = P_x + eHy/c. \tag{20}$$

$\hat{\mathcal{H}}$ is the total Hamiltonian of the charged quasiparticle in the magnetic field, $v_{SS}^{(y)}$, the matrix elements of the y-component of the velocity operator $\hat{v}_y = i[\hat{\mathcal{H}}_0\hat{y}]/\hbar$ in the representation of the functions $\tilde{\psi}_{\mathbf{P}}^{(S)}$, and $R_{SS'}(\mathbf{p}|\mathbf{p}')$ are matrices defined by formulas (5)–(7). Relation (18) is ensured by the smooth dependence of $u_{\mathbf{P}}^{(S)}$ on P_x and is satisfied accurate to first-order quantities in $\kappa \ll 1$.[3)] Equation (20) follows directly from the definition of $\tilde{\psi}_{\mathbf{P}}^{(S)}$ and $\chi_{\mathbf{P}}^{(S)}$ and from formulas (5) and (6).

We introduce the quantities $\beta_S(\mathbf{P})$—the coefficients of expansion of the stationary wave function Ψ in the function $\chi_{\mathbf{P}}^{(S)}$—and take (18) into account. Then, after simple transformations accurate to quantities $\sim\kappa$, we find that the stationary Schrödinger equation in the χ-representation has the following form

$$\sum_{s'=1}^{2}\left\{\left[\varepsilon_s\left(P_x + i\sigma\frac{\partial}{\partial P_y}, \bar{p}_y, P_z\right) - E\right]\delta_{ss'} + \delta P_y v_{ss'}^{(y)}\left(P_x + i\sigma\frac{\partial}{\partial P_y}, \bar{p}_y, P_z\right)\right\}\beta_{s'}(\mathbf{P}) = 0. \tag{21}$$

Comparison of (21) with formula (7) shows that Eqs. (21) are obtained from the system (7) (which determines the electronic spectrum near the M-plane when H = 0) with the aid of the corresponding principle:

$$\delta\mathbf{p} \to \{0, \delta P_y, 0\}, \quad p_x \to P_x + i\sigma\partial/\partial P_y, \quad \mathbf{p}' \to \{P_x + i\sigma\partial/\partial P_y, \bar{p}_y, P_z\}.$$

The smallness of the parameter κ allows us to seek the solution of (21) in the form

$$\beta_s(\mathbf{P}) = \sum_{\nu} \varphi_s^{(\nu)}(P_y) \exp\left\{\frac{i(P_{x0} - \bar{p}_x^{(\nu)})}{\sigma}\right\}\delta(P_x - P_{x0})\,\delta(P_z - P_{z0}),$$
$$\frac{1}{2}\sum_{s'=1}^{2}\varepsilon_{s'}(\bar{p}_x^{(\nu)}, \bar{p}_y(P_{z0}), P_{z0}) = E, \tag{22}$$

where $\varphi_{\mathbf{X}}^{(\nu)}(P_y)$ are functions that vary little over distances $\sim\sigma/b$ (this circumstance will be confirmed below), $\bar{p}_{\mathbf{X}}^{(\nu)}(E, P_{Z0})$ is represented by the second equation of (22), and the index ν has the same meaning as in (15a). Substituting (22) in (21) and taking the aforementioned property of $\varphi_S^{(\nu)}(P_y)$ into account, we obtain, in first approximation in κ, the following system of differential equations:

$$i\sigma\bar{v}_x^{(\nu)}d\varphi_1^{(\nu)}/dP_y + (\bar{v}_y^{(\nu)}\delta P_y - \bar{\Delta}_\nu)\varphi_1^{(\nu)}(P_y) + \delta P_y\bar{v}_{12}^{(\nu)}\varphi_2^{(\nu)}(P_y) = 0,$$
$$i\sigma\bar{v}_x^{(\nu)}d\varphi_2^{(\nu)}/dP_y + (\bar{v}_y^{(\nu)}\delta P_y + \bar{\Delta}_\nu)\varphi_2^{(\nu)}(P_y) + \delta P_y\bar{v}_{12}^{(\nu)}\varphi_1^{(\nu)}(P_y) = 0,$$
$$\bar{\Delta}_\nu = \varepsilon_1(\bar{\mathbf{p}}_\nu) - \varepsilon_2(\bar{\mathbf{p}}_\nu);$$
$$\bar{\mathbf{p}}_\nu = \{\bar{p}_x^{(\nu)}, \bar{p}_y, P_{z0}\}; \quad \bar{v}_{12}^{(\nu)} = v_{11}^{(y)}(\bar{\mathbf{p}}_\nu) = v_{21}^{(y)}(\bar{\mathbf{p}}_\nu),$$
$$\bar{v}_{x,y}^{(\nu)} = v_{11}^{(x,y)}(\bar{\mathbf{p}}_\nu) = v_{22}^{(x,y)}(\bar{\mathbf{p}}_\nu). \tag{23}$$

[2)] The problem of "joining" the quasiclassical solutions arises also when intraband breakdown is considered, that is, tunnel transitions occurring with conservation of the number of the band (Azbel' [17], Zil'berman [18]). In the case of intraband "joining" the question of the construction of the effective Hamiltonian in the non-quasiclassical region does not arise at all, since the dynamics of the electron within the limits of the band (including also tunneling through classically forbidden section of p-space) is completely described by (14). This essentially distinguishes the intraband breakdown from the interband breakdown, the investigation of which is impossible without the construction of an effective Hamiltonian which takes into account the nonconservation of the band number s.

[3)] Formula (18) is verified with the aid of a Hamiltonian describing the motion of the "ordinary" electron in a periodic electric and constant magnetic field.

In writing down (23) we took account of the fact that the relation $|v_{11}(\bar{p}_\nu) - v_{22}(\bar{p}_\nu)| \sim \Delta_M v_0/\varepsilon_0$ is satisfied at the point $\bar{p}_\nu$ lying on the M-plane (see Sec. 2). Introducing the functions $\Phi_{1,2}(z)$ defined by the formulas

$$\Phi_{1,2}(z(P_y)) = \exp\{i\delta P_y^2 \bar{v}_y/\sigma\bar{v}_x\}(\varphi_z(P_y) \pm \varphi_2(P_y)), \quad z = \delta P_y |\bar{v}_{12}/\sigma\bar{v}_x|^{1/2}, \tag{24}$$

we can easily obtain for $\Phi_{1,2}(z)$ a system of equations of the type (A.2) (see the Appendix), in which the parameter $\gamma = \bar{\Delta}^2/\sigma\,|\bar{v}_x\bar{v}_{12}|$. As seen from (24) and (A.4), the function $\varphi_S(P_y)$ changes appreciably over an interval $\gtrsim \sqrt{\sigma}$, thus proving the aforementioned statement concerning the properties of φ_S.

In order to "join" with the classical functions $f_S^{\pm}(P_y)$ and to determine the matrices τ, it is necessary to go over from the χ representation to the **P**, s representation, making use of the fact that the region of applicability of expressions (15) ($|\delta P_y| \gg \sqrt{\sigma}$) and the region where the system (23) is valid ($|\delta P_y| \ll b$) overlap. In the overlap region, this transition is effected by means of the following formula, which can be derived from (20), (15), and the definition of β_S after simple calculations that are accurate to $\sim\kappa$:

$$\beta_s(P_y) = \sum_{\nu}\sum_{s'=1}^{2} R_{s's}(p_x^{(s',\nu)}(P_y)P_y, P_{z0}|p_x^{(s',\nu)}, \bar{p}_y, P_{z0}) f_{s,\nu}^{(\pm)}(P_y). \tag{25}$$

The signs ± over f_S depend on the sign of δP_y, and the dependence $p_x^{(S,\nu)}(P_y)$ in $R_S{}'s$ and $f_S^{\pm}$ is determined by (15a), where the dispersion laws for $|\delta P_y| \ll b$ are specified by expression (8).

In the coordinate system chosen by us, the elements of the matrix $\hat{R}$ have for $b \gg |\delta P_y| \gg \Delta_M b/\varepsilon_0$ the following form:

$$R_{11} = R_{22} = 1/\sqrt{2}, \quad R_{12} = -R_{21} = \operatorname{sign}\delta P_y/\sqrt{2}.$$

Using these equations and the asymptotic form of the functions $\Phi_{1,2}$ as $z \to \pm\infty$, we obtain with the aid of (A.4), (25), (15), and (8) a final expression for the "joining" matrices:

$$\hat{\tau_\nu} = \begin{pmatrix} \tau_\nu e^{i\omega_\nu}, & -\rho_\nu \\ \rho_\nu, & \tau_\nu e^{-i\omega_\nu} \end{pmatrix},$$
$$\tau_\nu^2 + \rho_\nu^2 = 1, \quad \rho_\nu = \exp(-\pi\gamma_\nu/2),$$
$$\omega_\nu = \operatorname{sign}\bar{v}_x^{(\nu)}\left[\frac{\pi}{4} + \frac{\gamma_\nu}{2} - \frac{\gamma_\nu}{2}\ln\frac{\gamma_\nu}{2} + \arg\Gamma\left(\frac{i\gamma_\nu}{2}\right)\right]; \tag{26}$$
$$\gamma_\nu = c\bar{\Delta}_\nu^2(E, P_{z0})/e\hbar H|\bar{v}_x^{(\nu)}\bar{v}_{12}^{(n,\nu)}|\cos\theta.$$

All the quantities on which the breakdown parameter χ_ν depend are taken at the point $\mathbf{p}_\nu$ (see (23)) lying on the M-plane, halfway between the trajectories $\varepsilon_{1,2}(\mathbf{p}) = E$, $p_Z = P_{Z0}$; $\bar{v}_{12}^{(n,\nu)}$ is the off-diagonal matrix element of the n-th component of the velocity operator, and **n** is a unit vector normal to the M-plane. In writing down (26) we used the fact that $\bar{v}_{12}^{(y,\nu)} = \bar{v}^{(n,\nu)}\cos\theta$; the index θ shows that the "joining" of the quasiclassical functions corresponding to different branches of (15a) is effected independently. The matrices $\hat{\tau}$ are unitary, corresponding to conservation of the quantity $\sum_{S=1}^{2} v_X^{(S)}|f_S(P_y)|^2$, which is proportional to the probability flux density in P-space. The quantity ω determines the jump of the phase of the quasiclassical wave function on going through the M-plane ($\omega \to 0$ as $\gamma \to \infty$). The magnetic-breakdown probability (W_ν) is by definition equal to $|\tau_{12}|^2 = |\tau_{21}|^2 = \rho^2$, that is,

$$W_\nu = \exp(-\bar{H}(E, P_{z0})/H), \bar{H}(E, P_{z0}) = c\pi\bar{\Delta}_\nu^2/e\hbar|\bar{v}_x^{(\nu)}\bar{v}_{12}^{(n,\nu)}|\cos\theta. \tag{27}$$

Formula (27) is valid for all H. According to (27) the probability W decreases with increasing angle θ between **H** and the M-plane. When $\theta \to \pi/2$, the parameter $\bar{H} \to \infty$ and $W \to 0$. When **H** is almost parallel to **n**, the trajectories of the first and second bands with equal E and P_{Z0} pass near each other not in a small section but over the entire perimeter. In this case, the method considered above is no longer applicable. From formula (24) it is seen that the interval of values $\Delta\theta \equiv \theta - \pi/2$, where formula (27) remains valid, satisfies the inequality $\Delta\theta \gg \kappa$.[4)]

2) In case (b) the closely-passing trajectories $\varepsilon_{1,2}(p) = E$, $p_Z = E_{Z0}$, shown in Fig. 1, occur when the following condition is satisfied: the difference $\delta P_Z = |P_0 - p_0^{(Z)}(E)| \ll b$ ($p_0^{(Z)}(E)$ is the z-component of the degeneracy point $p_0(E)$; the vector **H** lies outside the solid angle made up by the directions of the normals to the surface of the elliptic cone (13); if **H** lies inside the solid angle, then definite values of E and P_{Z0} correspond to only one classical trajectory, belonging either to the first or to the second zone. For nonzero angles between the z axis ($z \parallel \mathbf{H}$) and the p_0-line, the plane $p_Z = P_{Z0}$ crosses the p_0-line at a certain point $\{p_0^{(X)}(P_{Z0}), p_0^{(Y)}(P_{Z0}), P_{Z0}\}$, which is shifted relative to the symmetry center of the hyperbola (Fig. 1) by an amount $\sim\delta P_Z$. We direct the axes x and y in such a way that (15a) have real solutions $p_X^{(1)}(P_Y)$ and $p_X^{(2)}(P_Y)$ for all values of P_Y lying in the vicinity of $p_0^{(Y)}(P_{Z0})$; within the limits of this limitation, the choice of the axes x and y is arbitrary.

In the case of a spectrum of type (b), the interval of values of P_y where the interband transitions are significant is localized near the point $p_0^{(Y)}(P_{Z0})$. To investigate the dynamics of the electron at small $\delta P_Y = P_Y - p_0^{(Y)}(P_{Z0})$ we introduce, in analogy with the preceding case, the functions $\bar{\chi}_{\mathbf{P}}^{(S)}$, defined by the equation

$$\bar{\chi}_{\mathbf{P}}^{(s)} = \bar{u}_{p_x, p_0^{(y)}, P_{z0}}^{(s)}(\mathbf{r})\exp\{i\mathbf{Pr}/\hbar\}, \quad p_x = P_x + eHy/c, \quad s = 1, 2, \tag{28}$$

where $\bar{u}_{p_X p^{(Y)}(P_{Z0}), P_{Z0}}^{(S)}(\mathbf{r})$ are the eigenfunctions of the operator $\hat{\mathcal{H}}_0(p_X, p_0^{(Y)}, P_{Z0})$, corresponding to the terms $\bar{\varepsilon}_{1,2}(p_X, p_0^{(Y)}(P_{Z0}), P_{Z0})$, which are defined by formulas (10) and (11) and which are analytic in p_X. The smoothness of the variation of $\bar{u}^{(S)}$ with the respect to the argument p_X causes $\bar{\chi}_{\mathbf{P}}^{(S)}$ to satisfy the relations derived from (18)–(20) by the following change of notation: $\varepsilon_S \to \bar{\varepsilon}_S$, $p_Y(P_Z) \to p_0^{(Y)}(P_Z)$ and $\bar{\chi}_{\mathbf{P}}^{(S)} \to \bar{\chi}_{\mathbf{P}}^{(S)}$. With the aid of these relations it is easy to obtain, in the first approximation in κ, the Schrödinger equation which is the analog of (21):

$$\sum_{s'=1}^{2}\left\{\left[\varepsilon_s\left(P_x + i\sigma\frac{\partial}{\partial P_y}, p_0^{(y)}(P_z), P_z\right) - E\right]\delta_{ss'} + \delta P_y v_{ss'}^{(y)}\left(P_x + i\sigma\frac{\partial}{\partial P_y}, p_0^{(y)}(P_z), P_z\right)\right\}\bar{\beta}_{s'}(\mathbf{P}) = 0. \tag{29}$$

Here $\bar{\beta}_S(\mathbf{P})$ are the coefficients of expansion of the stationary function Ψ in terms of the functions $\bar{\chi}_{\mathbf{P}}^{(S)}$. The solution of equation (29) can be represented in the following form:

[4)] Preliminary estimates show that when $\Delta\theta \lesssim \kappa$ the probability W $\sim \exp -(\Delta_M/\hbar\Omega_0)^2$. In practice we always $\Delta_M \gg \hbar\Omega_0$, that is, at sufficiently small $\Delta\theta$ we have $W \ll 1$.

$$\bar{\beta}_s(\mathbf{P}) = \bar{\varphi}_s(P_y)\exp\{iP_y(P_{x0} - p_0^{(x)}(P_{z0}))/\sigma\}\delta(P_x - P_{x0})\delta(P_z - P_{z0}), \tag{30}$$

where $\bar{\varphi}_S(P_y)$ is a function that varies little over distances $\sim\sigma/b$.

Substituting (30) in (29) and taking into account the definition $\bar{\varepsilon}_{1,2}$ and $\bar{\chi}^{(1,2)}$, we get in first approximation in κ:

$$\begin{aligned} i\sigma V_x^{(1)} d\bar{\varphi}_1/dP_y + (\delta P_y V_y^{(1)} + \delta\varepsilon)\bar{\varphi}_1(P_y) + \delta P_y V_y^{(12)}\bar{\varphi}_2(P_y) = 0, \\ i\sigma V_x^{(2)} d\bar{\varphi}_2/dP_y + (\delta P_y V_y^{(2)} + \delta\varepsilon)\bar{\varphi}_2(P_y) + \delta P_y V_y^{(12)}\bar{\varphi}_1(P_y) = 0. \end{aligned} \tag{31}$$

Here $\delta\varepsilon = \varepsilon(p_0(P_{Z0})) - E$; $\varepsilon(p_0(P_{Z0}))$ is the energy of the terms $\bar{\varepsilon}_{1,2}(p_X, p_0^{(y)}, P_{Z0})$ at the point of their intersection: $V_x^{(S)}$, $V_y^{(S)}$, and $V_y^{(12)} = V_y^{(21)}$ are the matrix elements of the operators $\hat{V}_{x,y}$ (see (9)) in the basis $e_x^{(1)}(p_0)$, $e_x^{(2)}(p_0)$, where the operator $\hat{V}_x$ is diagonal. The general solution of the system (31) is given in the Appendix. The basis for "joining" the asymptotic form (A.4) with the functions $f_S^{(\pm)}(P_y)$ (formula (15)) is Eq. (25), in which $\bar{p}_y$ must be replaced by $p_0^{(y)}(P_{Z0})$; the $p_x^{(S)}(P_y)$ dependence in $R_{SS'}$ and $f_S^{(\pm)}(P_y)$ is determined when $|\delta P_y| \ll b$ by the dispersion laws (12). Omitting the rather laborious transformations, we present directly the final expression for the matrices $\hat{\tau}$ (we henceforth omit the index ν):

$$\tau = \begin{pmatrix} \tau e^{i\omega}, & -\rho \\ \rho, & \tau e^{-i\omega} \end{pmatrix}, \qquad \begin{aligned} &\tau^2 + \rho^2 = 1, \quad \rho = \exp(-\pi\gamma/2), \\ &\omega = \frac{\pi}{4} + \frac{\gamma}{2} - \frac{\gamma}{2}\ln\frac{\gamma}{2} + \arg\Gamma\left(\frac{i\gamma}{2}\right), \\ &\gamma = B(\theta,\alpha)\delta P_z^2/\sigma, \quad \delta P_z = P_{z0} - p_0^{(z)}(E), \end{aligned} \tag{32}$$

$$B(\theta,\alpha) = \frac{|A_1A_2A_3|}{8(-A_1A_2\cos^2\theta - A_1A_3\cos^2\alpha\sin^2\theta - A_2A_3\sin^2\alpha\sin^2\theta)^{1/2}}$$
$$W(E,P_{z0}) = \exp\{-c\pi B(\theta,\alpha)\delta P_z^2/e\hbar H\}. \tag{32a}$$

Here $p_0^{(Z)}(E)$ is the z-component of the conical point of equal-energy surface $\varepsilon_S(p) = E$, A_1, A_2, and A_3 are constants in the equation of the elliptic cone (13). θ is the angle between H and the axes of the cone (the axis 3), and is the angle between the axis 1 and the plane passing through H and the cone axis; the constant $B(\theta, \alpha) \sim 1$. Formula (32a) is meaningful only for those orientations of H for which the expression in the brackets in the denominator of $B(\theta, \alpha)$ is positive. (In the opposite case H lies inside the solid-angle indicated above and there is no magnetic breakdown.)

Formulas (32) show that the probability $W \sim 1$ on the interval $\delta P_Z \sim \sqrt{\sigma}$, that is, only a narrow layer of trajectories passing near the degeneracy point at a distance $\delta P_Z \lesssim \sqrt{\sigma} \ll b$ takes part in the magnetic breakdown. This peculiarity of magnetic breakdown in case (b) leads to a number of unique macroscopic effects, which will be considered briefly below (Sec. 4).

4. ELECTRONIC ENERGY SPECTRUM UNDER CONDITIONS OF MAGNETIC BREAKDOWN

The character of the dependence of the energy spectrum on H is determined by the topology of the trajectories that take part in the breakdown, and by the form of the matrices $\hat{\tau}(H)$ defined by formulas (26) and (32) for cases (a) and (b) respectively.

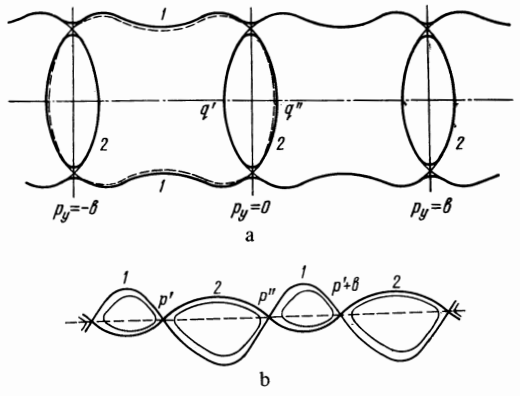

FIG. 2.

1) In case (a) a typical trajectory configuration is the one shown in Fig. 2a: the trajectories of the first zone are open, and the trajectories of the second zone are closed; the direction of the opening and the p_y axis are parallel to one of the vectors (b) of the reciprocal lattice; the solid straight lines represent the trace of the M-plane perpendicular to b and repeating periodically together with the closed trajectories of the second zone. We shall henceforth assume for simplicity that the trajectories are symmetrical about the axis $p_X = 0$ shown in Fig. 2a by the dash-dot line.

In determining the energy spectrum it is necessary to take into account, besides the "joining" conditions (16), also the periodicity condition for the wave function in P, s representation:

$$f_s(P_y) = f_s(P_y + b). \tag{33}$$

The quasiclassical wave function $f_S(P_y)$ is determined by formulas (15) and (15a), where the signs + and − pertain, respectively, to the region $b > P_y > 0$ and $-b < P_y < 0$; the index $\nu = 1, 2$ denotes one of two solutions of (15a): $p_x^{(S,1)}(P_y) = -p^{(S,2)}(P_y)$. In addition, the existence of the turning points $q' + nb$ and $q'' + nb$, which determine the limits of the classical motion in the second zone (see Fig. 2a), gives two more relations between the coefficients $c_{2,\nu}^{(\pm)}$:

$$c_{2,1}^{(-)}\exp\left(\frac{2i}{\sigma}\int_{q'}^{0} p_x^{(2,1)}\,dP_y'\right) = ic_{2,2}^{(-)}, \quad ic_{2,1}^{(+)} = c_{2,2}^{(+)}\exp\left(\frac{2i}{\sigma}\int_{0}^{q''} p_x^{(2,1)}\,dP_y'\right) \tag{34}$$

(The equations in (34) constitute an insignificant modification of well known relations.[13])

With the aid of (16), (33), and (34) we can easily obtain for the eight coefficients $c_{S,\nu}^{(\pm)}$ a system of eight linear homogeneous equations. Equating the determinant of this system to zero and performing a number of algebraic transformations, we obtain

$$\frac{S_2}{2\sigma} - \omega = \pi n - \arccos\frac{\rho^2\sin\Phi_1}{[(2\tau\cos\varphi - (1+\tau^2)\cos\Phi_1)^2 + \rho^4\sin^2\Phi_1]^{1/2}},$$
$$\Phi_1 = \frac{S_1}{2\sigma} + \omega, \qquad \varphi = \frac{P_{x0}b}{\sigma}. \tag{35}$$

Here n is an arbitrary integer, $S_2(E, P_{Z0})$ is the area bounded by the closed trajectory $\varepsilon_2(p) = E$, $p_Z = p_{Z0}$, and $S_1(E, P_{Z0})$ is the area of the figure made up by the straight lines $p_y = 0$, $p_y = b$ (Fig. 2a) and the two open

trajectories of the first zone; the quantities ω, $\rho^2 = W$, and $\tau^2 = 1 - W$ are defined in (26) and (27).[5)]

When n and P_{z0} are fixed, Eq. (25) defines a function $E = E_n(P_{z0}, \varphi)$ which is unique and periodic in φ, that is, the spectrum has a band structure and the integer n is the number of the "magnetic" band. As seen from (35) the characteristic width of the resultant bands is $\delta E \sim (1-W^2)^{1/2}\hbar\Omega_0$, and the characteristic distance between the bands is $\Delta E \sim W\hbar\Omega_0$. The method of band classification becomes clear by analyzing the limiting case of strong breakdown, when the parameter $\gamma \to 0$, $W \to 1$, and $\delta E \to 0$. In this case, Eq. (35) determines (for fixed P_{z0}) the discrete energy levels corresponding to a finite motion of the electron on the closed orbit, made up of sections of classical trajectories of the first and second bands (this orbit is designated by dashed lines in Fig. 2a), that is,

$$S_1(E, P_{z0}) + S_2(E, P_{z0}) = 2\pi\sigma(n + 1/2). \qquad (35a)$$

With increasing γ, the discrete energy levels, determined by (35a), spread out to form a band. In the other limiting case of weak breakdown, the parameter $\gamma \to \infty$, $W \to 0$, and Eq. (35) breaks up into two: $\cos(S_1/2\sigma) = \cos\varphi$ and $S_2(E, P_{z0}) = 2\pi\sigma(l + 1/2)$ (l is an integer); the first equation corresponds to infinite motion along open trajectories of the first band, and the second equation determines the quasiclassical energy levels corresponding to classical motion on closed trajectories of the second band.

In the stationary state characterized by definite P_{z0}, n, and P_{x0}, the average velocity along the x axis ($\bar{v}_{x,n}(P_{z0}, P_{x0})$) differs from zero ($\bar{v}_{y,n} = 0$) and is determined, with quasiclassical degree of accuracy, by the expression

$$\bar{v}_{x,n}(P_{x0}, P_{z0}) = \partial E_n(P_{x0}, P_{z0})/\partial P_{x0} \sim b\delta E/\sigma \sim \sqrt{1-W^2}\, v_0, \qquad (36)$$

where $v_0 \sim \varepsilon_0/b$ is the characteristic value of the velocity. It follows from (36) that the diagonal components σ_{xx} of the electric conductivity tensor in a magnetic field are given in order of magnitude by the formula $\sigma_{xx} \sim \sigma_0\sqrt{1-W}$, where σ_0 is the characteristic value of the electric conductivity at $H = 0$. The latter relation denotes, in particular, that $\sigma_{xx} \to \infty$ if the characteristic relaxation time $t_0 \to \infty$. The indicated estimate for σ_{xx} remains valid so long as the characteristic width of the bands $\delta E \gg \hbar/t_0$. If $\delta E \lesssim \hbar/t_0$, then the relaxation processes lead to a strong smearing of the "magnetic" bands, and formula (36) is no longer valid. Such a situation arises under conditions of very strong breakdown, when $\gamma \to 0$ and $\delta E \to 0$. When $\gamma \lesssim 1$, the inequality $\delta E \gg h/t_0$ is equivalent to the well known criterion $\Omega_0 t_0 \gg 1$ and is well satisfied in fields $H \sim 10^4$ Oe and $t_0 \sim 10^{-9}$ sec. In this case any macroscopic effect must be investigated in terms of the energy band spectrum obtained above (formula (35)).[6)]

In the investigation of a spectrum of type (b), greatest interest is attached to the case of a straight p_0-line, which must be parallel to one of the reciprocal-lattice vectors (b). The surface $\varepsilon_S(p) = E$ is crossed by the p_0-line at two groups of points at $\mathbf{p}_0'(E) + m\mathbf{b}$ and $\mathbf{p}_0''(E) + m\mathbf{b}$ (m—integer, $\mathbf{p}_0' - \mathbf{p}_0'' \parallel \mathbf{b}$) and is made up of periodically alternating cavities corresponding to the first and second zones. According to the analysis carried out in Sec. 2, the neighboring cavities 1 and 2 have a single common point $\mathbf{p}_0' + m\mathbf{b}$ or $\mathbf{p}_0'' + m\mathbf{b}$. When $\mathbf{H} \perp \mathbf{b}$, such an equal-energy surface has only one open trajectory: $\varepsilon_S(\mathbf{p}) = E$, $p_z = p^{(z)}(p_0^{(z)})$ is the z-component of the vectors $\mathbf{p}_0(E)$, which is the same for all E). This self-intersecting trajectory is shown by the heavy line in Fig. 2b, while the thin lines show the trajectories $\varepsilon_S(\mathbf{p}) = E$, $p_z = P_{z0}$, and the straight p_0-line is shown dashed. If $\mathbf{b} \cdot \mathbf{H} \neq 0$, then there are no open trajectories.

We shall consider below the most interesting case $\mathbf{H} \perp \mathbf{b}$. The energy spectrum is obtained in this case as a result of calculations using the "joining" matrix (32) and are completely analogous to those carried out for case (a) above:

$$(S_1 - S_2)/2\sigma = 2\pi n \pm \arccos[\rho^2\cos\varphi - \tau^2\cos(2\omega + (S_1+S_2)/2\sigma)], \quad \varphi = P_{x0}b/\sigma. \qquad (37)$$

Here n is an arbitrary integer; $S_{1,2}(E, P_{z0})$ are the areas contained in the closed trajectories $\varepsilon_{1,2}(p) = E$, $p_z = P_{z0}$; the quantities $\rho^2 = W$ and $\tau^2 = 1 - W$, which are defined by formulas (32) and (32a), depend only on the difference $\delta P_z = |P_{z0} - p_0^{(z)}|$. According to (37), the allowed energy levels are determined by the formula $E = E_n^{(\pm)}(\varphi, P_{z0})$, where n is the number of the magnetic band, $E_n^{(\pm)}(\varphi) = E_n^{(\pm)}(\varphi + 2\pi)$, and the $\pm$ signs correspond to the sign preceding the arccos in (37); the characteristic width of the magnetic band is $\delta E \sim W\hbar\Omega_0$.[7)]

In a stationary state with quantum numbers n, P_{z0}, and P_{x0}, the average velocity in the plane perpendicular to H is determined, in analogy with (36), by the formula

$$\bar{v}_{x,n}^{(\pm)}(P_{x0}, P_{z0}) = \partial E_n^{(\pm)}(P_{x0}, P_{z0})/\partial P_{x0} \sim b\delta E/\sigma \sim W v_0; \quad v_y = 0; \quad \mathbf{b} = \{0, b, 0\}. \qquad (38)$$

As shown by formula (38), magnetic breakdown in case (b) leads to the appearance of stationary quantum states with nonzero transverse current. According to (32a) and (38), the velocity $\bar{v}_{x,n}$ decreases exponentially rapidly with increasing parameter $\gamma = B\delta P_z^2/\sigma$.[8)] Therefore in the macroscopic effect there can appear only those current states which belong to the narrow interval of values $\delta P_z \lesssim \sqrt{\sigma}$. In the diagonal components $\sigma_{xx}(H)$ of the electric conductivity tensor, these quantum states with $\bar{v}_x \sim v_0$ make a contribution $\sigma_{xx}^{(qu)} \sim \sigma_0\sqrt{\kappa}$ (σ_0—characteristic electric conductivity for $H = 0$). On the other hand, the electrons that are located on the closed classical trajectories with $\delta P_z \gg \sqrt{\sigma}$ make, in accordance with the general theory of galvanomagnetic phenomena,[1] a contribution $\sigma_{xx}^{(cl)}$

5)A spectrum of the type (35) was first obtained by Pippard [7] for the particular case of almost-free electrons.

6)These questions will be considered in detail in a separate article.

7)Intraband tunnel transitions can also cause broadening of discrete levels into narrow bands (Zil'berman [18]). However, unlike the case of interband breakdown, this situation has low probability, since its realization requires that the energy E be close to a certain isolated critical value, at which a change takes place in the topology of the equal-energy surfaces.

8)In the limiting case $\gamma \to \infty$, Eqs. (37) go over, as expected, into a system of equations that are independent of φ: $S_{1,2}(E, P_{z0}) = 2\pi\sigma(n + 1/2)$. These relations determine the "ordinary" quantized energy levels of the first and second bands.

$\sim \sigma_0/(\Omega_0 t_0)^2$ to σ_{xx} (t_0--relaxation time). A comparison of $\sigma_{xx}^{(cl)}$ and $\sigma_{xx}^{(qu)}$ shows that at intensities

$$H \gtrsim H_0 = (m_0 c/e) t_0^{-1} (\omega_0 t_0)^{1/4}, \quad \omega_0 = \varepsilon/\hbar, \quad H_0 \sim 10^3 - 10^4 \text{ Oe} \quad (39)$$

(m_0—characteristic value of the effective mass) the "quantum" contribution to σ_{xx} becomes predominant (the magnetic breakdown does not effect the remaining components σ_{ik}.)

The galvanomagnetic characteristics experience appreciable anomalies in fields $H \gtrsim H_0$. To clarify the concrete dependence on H it is necessary to investigate the structure of the current layer $\delta P_z \lesssim \sqrt{\sigma}$ on the Fermi surface $\varepsilon_s(p) = \zeta$. At fixed $E = \zeta$, this current layer consists of values of P_{z0} "allowed" by Eq. (37), which make up a set of bands $P_z^{(n)}(\varphi, \zeta) = P_z^{(n)}(\varphi + 2\pi, \zeta)$. The position of the bands $P_z^{(n)}(\varphi)$ and their width $\Delta P_z^{(n)}$ are determined by the form of the expansion of the functions $S_{1,2}(\zeta, P_{z0})$ with respect to the small δP_z:

$$S_{1,2}(\zeta, P_{z0}) = S_{1,2}^{(0)}(\zeta) + S'_{1,2}\delta P_z + S''_{1,2}\delta P_z^2/2 + O[(\delta P_z/b)^3]. \quad (40)$$

Here $S_{1,2}^{(0)}(\zeta)$ are the areas of the loops of the self-intersecting trajectory on Fig. 2b. Substitution of (30) in (37) shows that it is necessary to separate two qualitatively different cases.

In the first case, at least one of the derivatives $S'_{1,2}$ is not equal to zero and, as follows from (37), the characteristic width $\Delta P_z^{(n)} \sim \sigma/b$. The last relation denotes that the quantity $\sigma_x^{(qu)}$ is not sensitive, accurate to terms $\sim \kappa^{1/2}$, to the detailed structure of the current layer consisting of $N \sim 1/\kappa^{1/2} \gg 1$ bands $P_z^{(n)}(\varphi)$. Thus, when $S'_{1,2} \neq 0$ the states with $\overline{v}_x \sim v_0$ appear as a narrow layer (of width $\sim\sqrt{\sigma}$) of open trajectories, proportional to $\sqrt{H}$. In this case the dependence of the component ρ_{yy} tensor of the magnetoresistance on H has the following character: when $H \ll H_0$ (but $\Omega_0 t_0 \gg 1$), a tendency to saturation, which is usual for closed trajectories, is observed, and when $H > H_0$ the component ρ_{yy} increases like $H^{5/2}$. Such a behavior of the magnetoresistance was observed by Borovik and Volotskaya[15] in aluminum.

A different situation arises if $S'_1 = S'_2 = 0$ (the areas $S_{1,2}$ are extremal). Then the characteristic width $\Delta P \sim (\varphi) \sim \sqrt{\sigma}$ and the current layers consists of only a few bands $P_z^{(n)}(\varphi)$. Since the velocity $\overline{v}_x(P_x)$ changes appreciably over a small interval $\sim\sqrt{\sigma}$, it follows that $\sigma_{xx}^{(qu)}$ now depends strongly on the distance between the bands inside the current layer and on the magnitude of their displacement relative to $p^{(z)}$. Formulas (37) and (40) show that these distances, when $S_1^{(0)} \sim S_2^{(0)}$ are rapidly oscillating aperiodic functions of 1/H, which vary substantially over the interval $\Delta(1/H) \sim e\hbar/c \times (S_1^{(0)} + S_2^{(0)})$. According to the foregoing, the function $\sigma_{xx}^{(qu)}(H)$ has in this case the same oscillating character. When $H \gtrsim H_0$, and $\sigma_{xx}^{(qu)}$, the relative amplitude of the oscillations of σ_{xx} becomes a quantity on the order of unity. "Magnetic breakdown" oscillations of this type were apparently observed by Stark[3] and Gaĭdukov[5] in zinc.

It must be noted that from the point of view of the analysis performed here the term "oscillations of the interband energy gap," introduced by Stark for the interpretation of the effects observed by him, has a physical meaning only with respect to a spectrum of type (b), which has a line of degeneracy points in p-space. In the case of a spectrum of type (a), which is characterized by an M-plane of closest approach of the bands (see Sec. 2), the energy gap on the M-plane and the probability $W(E, P_z)$ determined by it (see (27)) are smooth functions of E and P_{z0} with characteristic variation intervals ε_0 and b respectively. This shows that the occurrence of "magnetic breakdown" oscillations is impossible in case (a).

The author is grateful to I. M. Lifshitz for valuable discussions.

APPENDIX

1. If the crystal lattice of the metal has an inversion center, then $[\hat{I}\hat{\mathcal{H}}_0] = 0$ ($\hat{I} = \hat{I}^*$ is the space inversion operator). Noting further that the velocity operator $v = i[\hat{\mathcal{H}}_0 \hat{r}]/\hbar$ and the operator $\hat{I}$ anticommute, and also using the obvious equations

$$\psi^*_{p,s}(r) = \exp(i\lambda_{s,p})\psi_{-p,s}(r), \quad I\psi_{ps} = \exp(i\gamma_{sp})\psi_{-p,s}(r)$$
$$(\operatorname{Im}\gamma_{s,p} = \operatorname{Im}\lambda_{sp} = 0),$$

we get

$$\langle 1, p|\hat{v}|2, p\rangle^* = \exp\{i(\gamma_1 + \lambda_2 - \lambda_1)\}\langle 1, p|\hat{I}\hat{v}|2, p\rangle$$
$$= \exp\{i(\gamma_1 + \gamma_2 + \lambda_2 - \lambda_1)\}\langle 1, \hat{p}|v|2, p\rangle.$$

The reality of $C(p)$ follows from the fact that the phase factor preceding $|s, p\rangle \equiv \psi_{p,s}(r)$ is arbitrary.

2. Solving the system (31), we introduce in lieu of $\overline{\varphi}_{1,2}(P_y)$ the functions $\Phi_{1,2}(P_y)$, defined by the relations

$$\Phi_s = \exp\left\{i\left[\frac{\alpha\delta P_y^2}{2\sigma} + \frac{\beta\delta P_y}{\sigma}\right]\right\}\sum_{s'=1}^{2} T_{ss'}\sqrt{\overline{V}_x^{(s')}}\,\overline{\varphi}_{s'}(P_y),$$

$$\alpha = -\frac{1}{2}\left(\frac{V_y^{(1)}}{V_x^{(1)}} + \frac{V_y^{(2)}}{V_x^{(2)}}\right), \quad \beta = -\frac{\delta\varepsilon}{2}\frac{V_x^{(1)} + V_x^{(2)}}{V_x^{(1)} V_x^{(2)}}, \quad T_{ss'} = \begin{pmatrix} \cos\lambda, & \sin\lambda \\ -\sin\lambda, & \cos\lambda \end{pmatrix},$$

$$\sin 2\lambda = \xi/\sqrt{\xi^2 + \eta^2} > 0, \quad \xi = |V_y^{(12)}|(V_x^{(1)} V_x^{(2)})^{-1/2},$$
$$\eta = \frac{1}{2}(V_y^{(1)}/V_x^{(1)} - V_y^{(2)}/V_x^{(2)}). \quad (A.1)$$

The product $V_x^{(1)}V_x^{(2)} > 0$; as follows from (12), this is necessary in order for (15a) to have real solutions for all $|\delta P_y| \ll b$. Substituting (A.1) in (31) we obtain the following system of differential equations:

$$\frac{id\Phi_1}{dz} + z\Phi_1 - \sqrt{\gamma}\,\Phi_2 = 0, \quad \frac{id\Phi_2}{dz} - z\Phi_2 - \sqrt{\gamma}\,\Phi_1 = 0;$$

$$z = a\delta P_y/\sqrt{\sigma} + \sqrt{\gamma_1}, \quad a = \sqrt{\xi^2 + \eta^2}, \quad \gamma_1 = \delta_0 \cos 2\lambda / a\sqrt{\sigma}, \quad (A.2)$$
$$\sqrt{\gamma} = \delta_0 \sin 2\lambda/a\sqrt{\sigma}, \quad \delta_0 = \frac{1}{2}|\delta\varepsilon(V_x^{(2)} - V_x^{(1)})|/V_x^{(1)} V_x^{(2)}.$$

Eliminating Φ_2, we get an equation for Φ_1:

$$d^2\Phi_1/dz^2 + (\gamma - i + z^2)\Phi_1 = 0. \quad (A.3)$$

The general solution of (A.3) is represented in the form of an arbitrary superposition of the parabolic-cylinder functions:[16]

$$D_{-i\gamma/2-1}[\pm(1+i)z]. \quad (A.4)$$

The function Φ_2 is expressed in terms of Φ_1 with the aid of the first equation of the system (A.2).

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Translated by J. G. Adashko
86