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Translated by R. T. Beyer
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SOVIET PHYSICS JETP

VOLUME 5, NUMBER 2

SEPTEMBER, 1957

Behavior of an Electron in a Periodic Electric and a Uniform Magnetic Field

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(Submitted to JETP editor November 27, 1955)

J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 296-304 (February, 1957)

The general form of the eigenfunction of an electron in a periodic electric and a uniform magnetic field is derived. The equation of motion and the quasi-classical energy levels are found for an electron with an arbitrary dispersion law in a magnetic field. The broadening of the discrete energy levels of an electron in a crystal in a magnetic field is calculated.

THE magnetic properties of a metal are determined on the basis of the magnetic properties of the electron "gas." The latter is closely connected with the energy spectra of the electrons. To elucidate the magnetic properties of metals, we can go by either of two paths. We can make an assumption on the concrete form of the dispersion law and on the basis of this assumption construct a theory, in the comparison of which with experiment several numerical parameters are determined. The approximations of weakly bound^{1,2} or very strongly bound²⁻⁴ electrons apply to such a type of assumption. The second path consists of a search for the connection of the magnetic properties of the electrons with the law of their dispersion in the general form. In this case the concrete form of the dispersion law which holds in each separate case can be determined from a comparison of theory with experiment (in particular, with experiments on the de Haas-van Alphen effect), although such a comparison is considerably more difficult than is shown above.

Such a course of action was first pointed out by I. Lifshitz and Kosevich,⁵ who determined the energy levels of the electron and the magnetic susceptibility of an electron gas in the quasi-classical approximation.

In this research, a central assumption is that the Hamiltonian of an electron with an arbitrary dispersion law $E(p_x, p_y, p_z)$ in a magnetic field can be determined by replacing p_x, p_y, p_z by the components of the linear momentum operator $\hat{P}_x, \hat{P}_y, \hat{P}_z$.

The present paper is a continuation and development of the work reported in Ref. 5.

The first Section gives the general form of the exact eigenfunction of the electron in a uniform magnetic and a periodic electric field. Later, we give an approximate equation of motion of the electrons, which is shown to be identical to the Hamiltonian constructed by I. Lifshitz and Kosevich.⁵ A quasi-classical solution of this equation and the energy levels of the electron have been found.

In the last Section, we consider the effect of broadening of the discrete energy levels of an electron (in a magnetic field) into narrow bands under the action of the periodic field of the lattice. The author has pointed out this broadening in previous papers.^{1,2} In these researches, a calculation of the broadening of the levels was carried out in the approximations of weakly coupled and strongly coupled electrons. In the present work, this broadening is calculated outside the framework of the approximations pointed out; the results of the researches of Refs. 1 and 2 are entirely substantiated.

2. EIGENFUNCTIONS OF THE ELECTRONS

Let us write out the Schrödinger equation for an electron in a periodic electric potential V_p and a uniform magnetic field $H = H_z$ [the vector potential $A = (-Hy, 0, 0)$]:

$$\hat{H}\psi = -(\hbar^2/2m)\Delta\psi - (i\mu H_y \partial\psi/\partial x) + (e^2 H^2 y^2 / 2mc^2 + V_p)\psi = E\psi. \quad (1)$$

We introduce the translation operator of the electron \hat{T}_m , $m = (m_1 a_1, 0, m_3 a_3)$ is the vector of the lattice,

which lies in the plane x, z . It is evident from the form of the operator \hat{H} that \hat{T}_m and \hat{H} commute:

$$\hat{T}_m \hat{H} = \hat{H} \hat{T}_m, \quad (2)$$

and therefore the eigenfunctions of the operator \hat{H} are also eigenfunctions for the operator \hat{T}_m .

Application of \hat{T}_m to such a function gives $\hat{T}_m \psi = e^{i\mathbf{k}\cdot\mathbf{m}} \psi$. It follows therefore that the eigenfunctions of the operator \hat{H} have the form:

$$\psi = e^{i(h_1 x + h_2 z)} u(x, y, z),$$

where the functions u are periodic with the period of the lattice along the x and z axes, but are non-periodic in y . Equation (7) for the function u shows that the third quantum number ought to be discrete. Thus the function ψ can finally be written in the form

$$\psi_{h_1 n h_2 s} = e^{i(h_1 x + h_2 z)} u_{h_1 n h_2 s}(x, y, z), \quad (3)$$

(s is the number of the band). In the absence of a magnetic field, the solution (Bloch function) can also be represented in the form (3), where, however,

$$u_s = u_{0s} = e^{i h_2 y} v_s(x, y, z), \quad (4)$$

and $v_s(x, y, z)$ are periodic in x, y, z . In the absence of a periodic field,

$$u = \varphi_n \left(\frac{y + \alpha_0^2 k_1}{\alpha_0} \right), \quad (5)$$

where $\varphi_n(x)$ is the Hermite function and

$$\alpha_0 = \sqrt{\hbar c / eH}. \quad (6)$$

2. TRANSFORMATION OF THE EQUATION OF MOTION OF THE ELECTRON

If Eq. (3) is substituted in Eq. (1), then we get for the function u the equation

$$\hat{L}u = -\frac{\hbar^2}{2m} \Delta u \quad (7)$$

$$\begin{aligned} & -i \frac{\hbar^2}{m} \left(k_1 + \frac{y}{\alpha_0^2} \right) \frac{\partial u}{\partial x} - i \frac{\hbar^2}{m} k_3 \frac{\partial u}{\partial z} \\ & + \left[\sum_g V_g e^{2\pi i g r} + \frac{\hbar^2 k_3^2}{2m} \right. \\ & \left. + \frac{\hbar^2}{2m} \left(k_1 + \frac{y}{\alpha_0^2} \right)^2 \right] u - Eu = 0; \end{aligned}$$

at the time when $H = 0$, the equation for the function (4) is

$$-\frac{\hbar^2}{2m} \Delta u_0 - i \frac{\hbar^2}{m} k_1 \frac{\partial u_0}{\partial x} - i \frac{\hbar^2}{m} k_3 \frac{\partial u_0}{\partial z} \quad (8)$$

$$+ \left[\sum_g V_g e^{2\pi i g r} + \frac{\hbar^2 k_3^2}{2m} + \frac{\hbar^2 k_1^2}{2m} \right] u_0$$

$$- E^0(k_1, k_2, k_3) u_0 = 0.$$

Below we shall omit the dependence on the coordinates and write the solution of this equation in the form

$$u_0 = u_0(k_1, k_2, k_3). \quad (9)$$

We shall consider further the limiting case of a weak magnetic field. As a criterion of weakness of the field we use the relation

$$\varepsilon = a / \alpha_0 \ll 1, \quad (10)$$

where a is the lattice constant. Conditions (10) are satisfied in practice down to fields of $H \sim 10^5 - 10^6$ Oe (for $H = 10^4$ Oe and $a = 2.5 \times 10^{-8}$ cm, $\epsilon = 10^{-2}$).

In Eq. (9), we make the formal substitution

$$k_1 \rightarrow k_1 + y / \alpha_0^2$$

and seek a solution of Eq. (7) in the form

$$u = \sum_s \int g_s(k_1, k_2, k_3) \quad (11)$$

$$\times u_{0s}(k_1 + y / \alpha_0^2, k_2, k_3) dk_2.$$

Substituting (11) in (7), we multiply by

$$u_{0r}^*(k_1 + y / \alpha_0^2, k_2', k_3)$$

and integrate over all space. Equation (7) has the following form (see Appendix A1).

$$\begin{aligned} & \sum_s \int g_s(k_1, k_2', k_3) \quad (12) \\ & \times \left[\int (E_s^0(k_1 + y / \alpha_0^2, k_2', k_3) - E) u_{0r}^*(k_2) u_{0s}(k_2') d\tau \right. \\ & \left. - \frac{\hbar^2}{m \alpha_0^2} \int u_{0r}^*(k_2) \frac{\partial^2}{\partial k_1 \partial y} u_{0s}(k_2') d\tau \right] dk_2' = 0. \end{aligned}$$

Here

$$E_s^0(k_1, k_2, k_3) \quad (13)$$

$$= \sum_n A_{ns} \exp(ik_1 n_1) \exp(ik_2 n_2) \exp(ik_3 n_3).$$

Equation (12) was obtained by neglecting terms of order $\epsilon^4 = (a/\alpha_0)^4$ [see Appendix, Eq. (A-1)].

Below we shall neglect such terms everywhere. The distance between levels is (in corresponding dimensionless units) a quantity of order ϵ^2 ; therefore, neglect of quantities of higher order of magnitude is legitimate (in our case, such a neglect does not change the character of the equation).

As shown in the Appendix, Eqs. (A2), (A3), transitions between bands in (12) give terms of order not greater than ϵ^3 ; generally speaking, they will be of order ϵ^4 . With accuracy up to terms of such an order of smallness, Eq. (12) can be written in the form

$$\sum_n A_{nr} \exp\{ikn - in_1 n_2 / 2\alpha_0^2\} \quad (14)$$

$$\times g_2(k_1, k_2 - n_1 / \alpha_0^2, k_3) = E_r g_r(k_1, k_2, k_3).$$

Introducing the operator

$$\hat{Q}_{n_1} = \exp in_1 (k_1 - (1/i\alpha_0^2) \partial / \partial k_2), \quad (15)$$

we can write (14) also in the form

$$E_r^0(k_1 - (1/i\alpha_0^2) \partial / \partial k_2, k_2, k_3) \quad (16)$$

$$\times g_r(k_1, k_2, k_3) = E_r g_r(k_1, k_2, k_3).$$

Here, by the product of the operators \hat{Q}_n and $\exp(ik_2 n_2)$ [see Eq. (13)], one understands the symmetrized expression

$$1/2 [\hat{Q}_{n_1} e^{ik_2 n_2} + e^{ik_2 n_2} \hat{Q}_{n_1}].$$

Thus, the equation of motion of the electron in the magnetic field is obtained by substitution in Eq. (13) (which is for the energy of the electron in the absence of a magnetic field) of the quantum number k_1 for the operator $k_1 - (1/i\alpha_0^2) \partial / \partial k_2$ (under conditions of application of the order of operation pointed out for non-commutative multipliers).

3. SOLUTION OF THE EQUATION OF MOTION OF THE ELECTRON

Let us transform Eq. (14) to the form (17), omitting

the band index:

$$\sum_n A_n \exp\{ikn - in_1 n_2 / 2\alpha_0^2\} \quad (17)$$

$$\times g(k_1, k_2 - n_1 / \alpha_0^2, k_3) = E g(k_1, k_2, k_3).$$

The solution of this equation will be sought in the form

$$g(k_1, k_2, k_3) \quad (18)$$

$$= \exp\{i\alpha_0^2 k_1 k_2 - i\psi(k_1, k_2, k_3)\}.$$

The function ψ has a real and an imaginary part

$$\psi = \varphi + i\varphi_1.$$

Here the imaginary part is small (of the order ϵ^2) in comparison with the real. Considering the function ψ to be slowly changing in a change of k_2 by a/α_0^2 , we expand $\psi(k_2 - n_1/\alpha_0^2)$ in a series and, neglecting terms of order $(a/\alpha_0)^4$, we get, after substitution of Eq. (18) in Eq. (17):

$$E^0\left(\frac{\varphi'(k_2)}{\alpha_0^2}, k_2, k_3\right) + i \frac{\varphi_1'(k_2)}{\alpha_0^2} \frac{\partial E^0}{\partial \kappa_1} \quad (19)$$

$$+ \frac{i}{2\alpha_0^2} \left(\frac{\partial^2 E^0}{\partial \kappa_1 \partial k_2} + \frac{\partial^2 E^0}{\partial k_1^2} \frac{\partial \kappa_1}{\partial k_2} \right) = E.$$

Here the prime denotes differentiation with respect to k_2 , $\kappa_1 = \varphi'(k_2)/\alpha_0^2$.

We so choose the function φ_1 that the terms in Eq. (19) which are of order $(a/\alpha_0)^2$ (the second and third terms on the left) cancel each other. This gives for the function φ_1

$$\varphi_1 = -1/2 \ln |\partial E^0 / \partial \kappa_1|. \quad (20)$$

For the function φ we get a differential equation of first order:

$$E^0(\kappa_1, k_2, k_3) = E. \quad (21)$$

Solving this equation for κ_1 , we get (because of its parity) two* roots: $\pm |\kappa_1|$ and therefore,

*We consider only the case in which the simply connected curve $\kappa_1 = \kappa_1(k_2)$ is double-valued.

$$\varphi(k_2) = \pm \alpha_0^2 \int x_1 dk_2. \quad (22)$$

Consequently, we can write the total eigenfunction $g(k_1, k_2, k_3)$

in the form of a linear combination

$$\begin{aligned} g(k_1, k_2, k_3) &= |\partial E^0 / \partial x_1|^{-1/2} e^{i\alpha_0^2 k_1 k_2} \left(A \exp \left\{ i\alpha_0^2 \int x_1 dk_2 \right\} \right. \\ &\quad \left. + B \exp \left\{ -i\alpha_0^2 \int x_1 dk_2 \right\} \right) \end{aligned}$$

or in the form

$$\begin{aligned} g(k_1, k_2, k_3) &= |\partial E^0 / \partial x_1|^{-1/2} e^{i\alpha_0^2 k_1 k_2} \sin \left(\alpha_0^2 \int x_1 dk_2 + \gamma \right). \end{aligned} \quad (23)$$

The function (23) differs from the usual quasi-classical function of one-dimensional motion (the coordinate in the given case is k_2) only by the factor

$$\exp(i\alpha_0^2 k_1 k_2).$$

The quantity $\alpha_0^2 x_1$ plays the role of the momentum as was noted by I. Lifshitz and Kosevich.⁵

The turning points of the classical motion are those points of the phase plane (x_1, k_2) in which the derivative $\partial E^0 / \partial x_1 = 0$. In particular, such points are always points for which $x_1 = 0$ or

$$\pm \pi / a_1 \quad (\text{for } x_1 = 0, \pm \pi / a_1,$$

the derivative $\partial E^0 / \partial x_1$ is necessarily equal to zero).

Let us consider the case in which the curve $x_1 = x_1(k_2)$ is closed and double-valued, and lies wholly inside a single cell of the reciprocal lattice, while at the turning point, $x_1 = 0$. In order to find the phase γ of the wave function (23), we expand E^0 about the turning point in a series in powers of $x_1 - x_1^0$ and $k_2 - k_2^0$.

Since

$$\partial E^0 / \partial x_1 = 0 \quad \text{and} \quad \partial^2 E^0 / \partial x_1 \partial k_2 = 0$$

at $x_1 = 0$, Eq. (21) in the vicinity of the turning point will be

$$E^0(x_1, k_2, k_3) = E_0^0 \quad (24)$$

$$+ \frac{\partial E_0^0}{\partial k_2} (k_2 - k_2^0) + \frac{1}{2} \frac{\partial^2 E_0^0}{\partial x_1^2} x_1^2 = E.$$

Hence

$$(25)$$

$$x_1 = \pm \left[-(\partial E_0^0 / \partial k_2) (k_2 - k_2^0) / \frac{1}{2} (\partial^2 E_0^0 / \partial x_1^2) \right]^{1/2},$$

which must be substituted in Eq. (23),

The exact equation [by exact is meant Eq. (17) or Eq. (16)] near the turning point has, as is easy to show, the solution

$$e^{i\alpha_0^2 k_1 k_2} \sin \left[\alpha_0^2 \int x_1 dk_2 + \pi / 4 \right], \quad (26)$$

where by x_1 is meant Eq. (25).

Thus if the curve $x_1 = x_1(k_2)$ is closed, double-valued, and located in a single cell of the reciprocal lattice, then $\gamma = \pi / 4$.

The rules of quasi-classical quantization are based on the coincidence of the wave functions (23), written in such form which guarantees the correct value of the phase at the turning point. The factor

$$\exp(i\alpha_0^2 k_1 k_2)$$

here falls out from the condition of quasi-classical quantization and has the usual form

$$\alpha_0^2 \int_a^b x_1 dk_2 = \pi \left(n + \frac{2}{\pi} \gamma \right). \quad (27)$$

The quantity

$$2\hbar^2 \int_a^b x_1 dk_2$$

for the case of a closed, double-valued curve in a single cell represents the area of the intersection of the surface of constant energy (in the momentum space $(\hbar x_1, \hbar k_2, \hbar k_3)$), with the plane

$k_3 = \text{const}$; therefore, Eq. (27) can be written in the form

$$cS(E, k_3) / \hbar |e| H = n + 2\gamma / \pi, \quad (28)$$

which was obtained earlier by I. Lifshitz and Kosevich.⁵ This condition also determines in implicit form the energy levels of the electron $E = E(n, k_3)$.

We note that upon the introduction of the phase

γ , in addition to the double-valuedness of the curve

$$\kappa_1 = \kappa_1(k_2),$$

we have implicitly assumed the fulfillment of the following inequalities (in the neighborhood of the turning point b):

$$\alpha_0^2 \kappa_1 (b - k_2) \gg 1 \quad (29)$$

[which is necessary for writing out the Airy function in asymptotic form],

$$d\kappa_1 / dk_2 \ll \alpha_0^2 \kappa_1 / a \quad (30)$$

(quasi-classical condition), which has, in the neighborhood of the turning point, the form

$$b - k_2 \gg a / \alpha_0^2 \quad (30')$$

and, finally,

$$\frac{\partial E_0^0}{\partial k_2} (b - k_2) \gg \frac{1}{2} \frac{\partial^2 E_0^0}{\partial k_2^2} (b - k_2)^2 \quad (31)$$

which was used in the expansion of Eq. (24).

The first and second inequalities do not contradict each other. However, (29) and (30) or (31) are contradictory if $\partial E_0^0 / \partial k_2$ is small. For strongly coupled electrons, for example, it takes place within 1/3 of the zone. The inequalities that have been shown are also contradictory for the lower levels of the zone.

The function (23) takes place in the limits of the region of classical motion. Outside of the limits of this region, the eigenfunctions decay exponentially and have the form

$$g(k_1 k_2 k_3) = e^{i\alpha_0^2 k_1 k_2} f(k_2) \quad (32)$$

$$= e^{i\alpha_0^2 k_1 k_2} \frac{1}{2} \left| \frac{\partial E_0^0}{\partial \kappa_1} \right|^{-1/2} \exp \left\{ -\alpha_0^2 \int |\kappa_1| dk_2 \right\}.$$

The functions are discussed by us in a subsequent section.

For sufficiently large filling of the band, curves of constant energy have the form of closed trajectories surrounding the points $\pm \pi / a_1$ and $\pm \pi / a_2$.

In this case we can also obtain the energy levels from Eq. (28), if we make the transformation

$$\kappa_1 = \kappa'_1 \pm \pi / a_1; \quad k_2 = k'_2 \pm \pi / a_2,$$

in (6) and then write

$$E^0(\kappa'_1 \pm \pi / a_1, k'_2 \pm \pi / a_2, k_3) = E^{0'}(\kappa'_2, k'_2, k_3).$$

If the curve in the new coordinates lies in a single cell of the reciprocal lattice, then the equation of I. Lifshitz and Kosevich (28) is valid. In that equation we must understand by $S(E, k_3)$

the cross section of the plane $k_2 = \text{const}$, not with the surface $E^0 = E$, but with the surface $E^{0'} = E$ (the dispersion law

$$E^{0'}(\kappa'_1, k'_2, k'_3)$$

differs from the dispersion $E^0(\kappa_1, k_2, k_3)$ by

the fact that the coefficients A_{n_1, n_2, n_3} in Eq. (13) are substituted for the coefficients $(-1)^{n_1 + n_2} A_{n_1, n_2, n_3}$.

If the curve $\kappa_1 = \kappa_1(k_2)$ is multiply connected and consists of closed contours which have the κ_1 and k_2 axes as axes of symmetry [where the individual contours do not abut on one another, but intersect, and the function $\kappa_1(k_2)$ is doubly valued in the limits of each contour], then, shifting the origin to the center of each curve (κ_1^0, k_2^0) we get the quantization condition in the form (28), in which S denotes the cross section of the surface

$$E^0(\kappa_1^0 + \kappa_1, k_2^0 + k_2, k_3) = E^0(\kappa_1^0, k_2^0, k_3) = E$$

with the plane $k_3 = \text{constant}$.

4. DISTRIBUTION OF THE ENERGY LEVELS OF THE ELECTRON

In the preceding Sections, it was shown that the eigenfunction of the electron in k space, $g(k_1, k_2, k_3)$, is determined by the equation $\hat{E}^0 g = E g$ [Eq. (17)]. The energy E was shown to be dependent on the two quantum numbers n and k_3 . It had been shown earlier² that the electron's energy should depend on all three quantum numbers k_1, n, k_3 , where the dependence on k_1 leads to a broadening of the discrete energy levels of the electron in a narrow band. This broadening has, generally speaking, the order of magnitude ϵ^4 . However, there are special cases when the broadening becomes appreciable. This takes place when the energy surfaces in neighboring cells of the reciprocal lattice are almost in contact, and also for

open trajectories (which will be considered in later research). A penetration is then possible from one region of quasi-classical motion* into another through the "potential barrier," by virtue of which the discrete energy levels merge into narrow bands.

The eigenfunction of the electron in periodically arranged regions can be written in the form

$$\begin{aligned} \psi_{k_1} &= \sum_m \exp \left\{ i \alpha_0^2 k_1 \left(k_2 - \frac{2\pi}{a_2} m \right) \right\} f \left(k_2 - \frac{2\pi}{a_2} m \right) \\ &= \sum_m g \left(k_1, k_2 - \frac{2\pi}{a_2} m, k_3 \right). \end{aligned} \quad (33)$$

Substituting (33) in Eq. (17), multiplying by

$$g^*(k_1, k_2, k_3)$$

and integrating over k_2 , we get an expression for the energy levels of the electron with their broadening taken into account:

$$E_{k_1 k_3} = E_{n k_3} + E''_{n k_3} J_{n k_3} \cos \frac{2\pi \alpha_0^2 k_1}{a_2}. \quad (34)$$

Here $E_{n k_3}$ are the levels obtained from Eq. (28),

$$E''_{n k_3} = \partial^2 E_{n k_3} / \partial k_2^2$$

is the second derivative at the point $k_2 = \pi / a_2$,

and

$$J_{n k_3} = \int f_{n k_3}(k_2) f_{n k_3} \left(k_2 - \frac{2\pi}{a_2} \right) \quad (35)$$

$$\times \left(k_2 - \frac{2\pi}{a_2} \right)^2 dk_2.$$

Here $f_{n k_3}(k_2)$ is defined by Eq. (32).

Let us carry out an estimate of this integral. We can write down the following expansion about the turning point k_{20} :

$$k_2 = k_{20} + \frac{1}{2} \frac{\partial^2 k_{20}}{\partial \alpha_1^2} \alpha_1^2 = k_{20} - \frac{a_2}{2R} \alpha_1^2, \quad (36)$$

where R is a dimensionless radius of curvature of the curve $\alpha_1 = \alpha_1(k_2)$ at the point $(0, k_{20})$.

We also introduce the small parameter α_0 as the distance between neighboring trajectories (in units of $1/a$).

Making use of the Eq. (32), we get

*If such regions have such cells, then everything pointed out below refers in equal measure to them.

$$J \sim \exp \left\{ -4 \sqrt{2R} x_0^{3/2} / 3\epsilon^2 \right\} a_2^{-2} x_0^2 \sqrt{x_0/R} \quad (37)$$

For a fixed energy level, determined by the parameters R and x_0 at $\epsilon \rightarrow 0$, $J \rightarrow 0$. However, for

each ϵ there are other values of the small parameters x_0 and R for which $J \sim x_0^2$. Usually, as $x_0 \rightarrow 0$, R also $\rightarrow 0$. If $R \sim x_0$, then $J \sim x_0^2$ means $x_0 \approx \epsilon$ (just as the quasi-classical approximation is invalid only in the region $\sim \epsilon^2$ around the turning point, so our calculation is valid).

The author expresses his sincere gratitude to I. M. Lifshitz for his interest in the present work and for discussions.

APPENDIX

1. Application of the operator \hat{L} of Eq. (7) to the function $u_{0s}(k_1 + y/\alpha_0^2, k_2, k_3)$ gives

$$\begin{aligned} \hat{L}u_{0s} &= \left(E_s^0 \left(k_1 + \frac{y}{\alpha_0^2}, k_2, k_3 \right) - E \right) u_{0s} \\ &\quad - \frac{\hbar^2}{2m\alpha_0^4} \frac{\partial^2 u_{0s}}{\partial k_1^2} - \frac{\hbar^2}{m\alpha_0^2} \frac{\partial^2 u_{0s}}{\partial y \partial k_1}. \end{aligned} \quad (A-1)$$

We discard the second term since its value

$$\sim \hbar^2 a^2 / 2m\alpha_0^4.$$

The last term $\sim \hbar^2 / m\alpha_0^2$, and we take it into account.

2. The function (9), as is well known, can be written in the form

$$u_{0s}(k_1, k_2, k_3) \quad (A-2)$$

$$= e^{ik_2 y} \sum_{\mathbf{h}} e^{2\pi i \mathbf{h} \cdot \mathbf{r}} b_{\mathbf{h}s}(k_1, k_2, k_3).$$

The properties of (9) of interest to us, according to which the expansion (11) is carried out, are based on the following properties of the coefficients

$$b_{\mathbf{h}s}(k_1, k_2, k_3)$$

(these properties do not change under the substitution $k_1 \rightarrow k_1 + y/\alpha_0^2$):

a) $b_{\mathbf{h}s}(k_1 k_2 k_3)$ are real and even functions of the arguments $k_i + 2\pi h_i$; ;

b) for identical \mathbf{k} , the coefficients $b_{\mathbf{h}s}$ are orthogonal. We shall consider them to be normalized:

$$\sum_{\mathbf{h}} b_{\mathbf{h}s}(k_1 k_2 k_3) b_{\mathbf{h}r}(k_1 k_2 k_3) = \delta_{rs}; \quad (A-3)$$

c) Proceeding directly from the equation which is satisfied by the coefficients $b_{\mathbf{h}s}$,

$$b_{\mathbf{h}s} \left[\frac{\hbar^2}{2m} (\mathbf{k} + 2\pi\mathbf{h})^2 - E_s^0 \right] + \sum_{\mathbf{g}} V_{\mathbf{g}} b_{\mathbf{h}-\mathbf{g},s} = 0 \quad (\text{A-4})$$

we can obtain the well known connection between the current and the energy:

$$\sum_{\mathbf{h}} (k_2 + 2\pi h_2) b_{\mathbf{h}s}^2(k_1 k_2 k_2) = \frac{m}{\hbar^2} \partial E_s^0 / \partial k_2; \quad (\text{A-5})$$

e) from this same equation for $b_{\mathbf{h}s}$ we can obtain a much more general relation

$$(2m/\hbar^2) [E_r^0(k_2') - E_s^0(k_2)] \sum_{\mathbf{h}} b_{\mathbf{h}s}(k_2) b_{\mathbf{h}r}(k_2') + \sum_{\mathbf{h}} b_{\mathbf{h}s}(k_2) b_{\mathbf{h}r}(k_2') [(k_2 + 2\pi h_2)^2 - (k_2' + 2\pi h_2)^2] = 0,$$

from which it follows, in particular, that for $k_2 = k_2'$

$$(E_r^0 - E_s^0) \sum_{\mathbf{h}} b_{\mathbf{h}s} \frac{\partial b_{\mathbf{h}r}}{\partial k_2} = -\frac{\hbar^2}{m} \sum_{\mathbf{h}} b_{\mathbf{h}s} b_{\mathbf{h}r} (k_2 + 2\pi h_2); \quad (\text{A-7})$$

$$\sum_{\mathbf{h}} \frac{\partial b_{\mathbf{h}s}}{\partial k_1} b_{\mathbf{h}r} (k_2 + 2\pi h_2) = -\frac{m}{\hbar^2} \frac{\partial E_s^0}{\partial k_1} \sum_{\mathbf{h}} b_{\mathbf{h}s} \frac{\partial b_{\mathbf{h}r}}{\partial k_2}. \quad (\text{A-8})$$

To obtain Eq. (14) and what follows it, use is made of the properties that have been pointed out, and of the expansion

$$\sum_{\mathbf{h}} b_{\mathbf{h}s}(k_2') b_{\mathbf{h}r}(k_2) = \delta_{rs} + (k_2' - k_2) \sum_{\mathbf{h}} \frac{\partial b_{\mathbf{h}s}}{\partial k_2} b_{\mathbf{h}r} + \dots \quad (\text{A-9})$$

3. Making use of the properties of the coefficients $b_{\mathbf{h}s}$, we can compute the integrals in (12). Neglecting quantities of order ϵ^4 , we obtain the following equation:

$$\sum_{\mathbf{n}} A_{\mathbf{n}r} \exp \{ i\mathbf{k}\mathbf{n} - in_1 n_2 / 2\alpha_0^2 \} \times g_r(k_1, k_2 - n_1/\alpha_0^2, k_3) - E_r g_r(k_1, k_2, k_3) + \sum_{s \neq r} (E_s - E_r) \times \int g_s(k_2') (k_2' - k_2) F_{sr}(\alpha_0^2 (k_2' - k_2)) d(k_2 a_2) = 0, \quad (\text{A-10})$$

where g_r, g_s, E_r, E_s refer to different bands but to one and the same quantum number, and

$$F_{sr}(\alpha_0^2 (k_2' - k_2)) = e^{-i(k_2' - k_2) k_1 \alpha_0^2} \times \int e^{i(k_2' - k_2) \alpha_0^2 \xi / a_1} \sum_{\mathbf{h}} \frac{\partial b_{\mathbf{h}s}}{\partial k_2} b_{\mathbf{h}r} d\xi, \quad (\text{A-11})$$

$$\xi = a_1 (k_1 + y/\alpha_0^2).$$

In Eq. (A-10), there are small non-diagonal terms in addition to the diagonal terms. Since the sum in the integrand is periodic in ξ (with period 2π), we can write:

$$\sum_{\mathbf{h}} b_{\mathbf{h}r} \partial b_{\mathbf{h}s} / \partial k_2 = \sum_m B_m e^{-im\xi}. \quad (\text{A-12})$$

Then F_{sr} will be the sum of δ -functions:

$$F_{sr} = \sum_m B_m e^{-i(k_2' - k_2) k_1 \alpha_0^2} \delta \left(\frac{\alpha_0^2}{a_1} (k_2' - k_2) - m \right), \quad (\text{A-13})$$

and the non-diagonal terms in (A-10) are written as

$$\sum_m \sum_{s \neq r} (E_s - E_r) m B_m \frac{a_1}{\alpha_0^2} e^{-ik_1 a_1 m} g_s \left(k_2 + \frac{ma_1}{\alpha_0^2} \right). \quad (\text{A-14})$$

In view of the smallness of these terms, we can regard them as a perturbation. Inasmuch as this perturbation is of order ϵ^2 , it is necessary to compute only the diagonal matrix element

$$\sum_m \sum_{s \neq r} (E_s - E_r) \frac{a_1}{\alpha_0^2} m B_m e^{-ik_1 a_1 m} \times \int g_s \left(k_2 + \frac{ma_1}{\alpha_0^2} \right) g_r^*(k_2) dk_2. \quad (\text{A-15})$$

Employing (18), we write the integral in the form

$$\int \exp \{ -i\varphi_s(k_2 + ma_1/\alpha_0^2) + i\varphi_r(k_2) + \varphi_{1s}(k_2 + ma_1/\alpha_0^2) + \varphi_{1r}(k_2) \} dk_2 \quad (A-16)$$

Since [see Eq. (22)]

$$\varphi_r(k_2) = \alpha_0^2 \int_c^{k_2} \kappa_{1r} dk_2,$$

$$\varphi_s \left(k_2 + \frac{ma_1}{\alpha_0^2} \right) = \alpha_0^2 \int_c^{k_2 + ma_1/\alpha_0^2} \kappa_{1s} dk_2,$$

then the imaginary part of the exponent is very large ($\alpha_0 \rightarrow \infty$) and the integral can be solved by the method steepest descents. A saddle point will exist if there is a point of the plane (κ_1, k_2) in which $\kappa_{1r}(k_2) = \kappa_{1s}(k_2 + ma_1/\alpha_0^2)$. Since $a_1/\alpha_0^2 \ll \pi/a_2$, then the conditions given above will be satisfied only if the curves $\kappa_{1r}(k_2)$ and $\kappa_{1s}(k_2)$ intersect (more precisely, if they

come very close to one another, or intersect). In this case we can employ the method of steepest descents. It is easy to convince oneself of the fact that the integral in this case will be of order ϵ while the entire matrix elements will be of order ϵ^3 .

If κ_{12} and κ_{12} (which refer to states with identical n and k_3 in the bands r and s) do not intersect, the saddle points will not exist and the integral will be of order ϵ^2 , while the matrix element will be of order ϵ^4 .

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Translated by R. T. Beyer
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The Acceleration of a Plasma by a Magnetic Field

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(Submitted to JETP editor November 28, 1955)

J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 305-310 (February, 1957)

Acceleration of a current-conducting plasma jet by a magnetic field is considered. The nature of the processes is preliminarily elucidated by examining the case of motion of conductors possessing some resistance and inductance. Furthermore, the motion of ions and electrons is studied under conditions where collisions, magnetic interaction of the particles and excitation of waves are negligible. The existence of a critical charge density in accelerators has been established for this case. Peculiarities of acceleration of very dense jets are also considered.

IF a current is flowing in a plasma jet situated in a magnetic field, there will be a force of the volume density $f = [jH]/c$ acting upon the jet and imparting to it an acceleration. As an example, we might consider the case of the motion of an electric arc, burning between two electrodes connected to a current source, in a magnetic field. Such a process was experimentally studied by Bron^{1,2} at atmospheric pressure. In his experiments, the velocity of the arc attained several hundred meters per second despite air resistance.

It is of interest to consider the motion of the arc in the absence of the resistance of the surrounding

medium, i.e., in a vacuum. In that case, the process of divergence of the jet can be prevented by several means. In particular, we shall assume that the time during which the jet is accelerated is sufficiently small, or that the jet is contracted by its proper magnetic field. We shall not consider the processes of jet formation (consult, for instance, Ref. 3)

1. ON THE MOTION OF CONDUCTORS

We can obtain a rudimentary picture of the motion of a current-conducting plasma jet in a magnetic