equilibrium solution, existing in the absence of external forces of the type considered above, is the simultaneous fulfillment of the following equations

$$\frac{\partial \varphi_s}{\partial y_i} \frac{\alpha}{m} = \varphi_s y_i; \quad \frac{\partial \varphi_s}{\partial y_i} F_i + \frac{\partial F_i}{\partial y_i} \varphi_s = 0 \qquad (35)$$

and, consequently, the forces F_i must satisfy the condition

$$(m/\alpha)(y_i F_i) + \partial F_i / \partial y_i = 0. \qquad (36)$$

In particular it follows from (36) that gyroscopic forces will not disturb the equilibrium condition of the system. In an analogous way one can treat the more general conditions mentioned in Ref. 2.

I take this occasion to express my gratitude to N. N. Bogoliubov for proposing the problem, and also to M. A. Leontovich and Ia. B. Lopatinskii for discussion of questions connected with the work.

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Electron Energy Spectrum in a Crystal Located in a Magnetic Field

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It is shown that the discrete energy levels of an electron in a crystal are widened into narrow bands in strong magnetic fields. The structure of the energy zone in a crystal located in a magnetic field is studied. The possible influence of the broadening on the de Haas-van Alphen effect is discussed.

A FREE electron in a uniform magnetic field performs a finite motion[1] which corresponds to a classical revolution (at least in the direction perpendicular to the magnetic field H). The minimum quantum-mechanical "radius" of this revolution is

$$\alpha_0 = \sqrt{\hbar c / eH}. \qquad (1)$$

In addition to the magnetic field the electron is acted upon in the crystal by a periodic electric field (the lattice constant will be designated by a), and for all real fields H.

$$\varepsilon = a / \alpha_0 \ll 1 \qquad (2)$$

(thus, for example, with $H \sim 10^4$ oersteds and $a = 2.5 \times 10^{-8}$ cm we have $\epsilon = 10^{-2}$).

In the theory of electron motion in a crystal placed in a magnetic field the only terms that are retained (except in Ref. 2) are those which remain finite when $\epsilon \to 0$. As a result, the energy levels of the electron in a magnetic field are degenerate and depend, just as in the case of free electrons, on only two quantum numbers (see, for example, Refs. 3 and 4). If terms that vanish together with ϵ are retained the degeneracy is removed and the character of the spectrum is changed.

1. In the absence of the periodic field the energy levels of the motion of a free electron in the plane $\perp H$ are expressed by the equation $E_n = \mu H (n + 1/2)$ and the eigenfunctions are

$$\psi_{k, n} = e^{i k_1 x} \varphi_n \left(\frac{y + \alpha_0^2 k_1}{\alpha_0} \right),$$

where the φ_n are Chebyshev-Hermite functions. The energy is independent of the quantum number k_1 which determines the position of the "center of oscillation" of the electrons $y_0 = -\alpha_0^2 k_1$, since all y_0 are equivalent in free space. In a periodic field this equivalence disappears and the degeneracy is removed. In the approximation of weakly bound electrons (when the periodic field

can be considered a small perturbation) the following dispersion law holds for small n (at the bottom of the energy zone):

$$E_{k,n} = \mu^* H \left(n + \frac{1}{2} \right) \tag{3}$$

$$+ \sum_{p=1}^{\infty} A_p (n, H) \cos \left(\frac{4\pi p \alpha_0^2 k_1}{a} \right),$$

where $A_1 (n, H) = (-1)^n n (\mu H)^2 V^2 E_0^{-3} \pi^{-4}$; $E^0 = \hbar^2/ma^2$ and V is a quantity of the order of the first Fourier coefficients of the potential.

For large n (close to the middle of the energy zone) the ordinary perturbation theory of a degenerate state can be used, resulting in the dispersion law

$$E_{k,n} = \mu H (n + \frac{1}{2}) \tag{4}$$

$$+ V J_{nn} \left(\frac{2\pi}{\varepsilon} \right) \left(\cos \frac{2\pi y_0}{a} + \cos \frac{\pi}{p+1} m \right),$$

$$J_{nm} \left(\frac{2\pi}{\varepsilon} \right) = \int_{-\infty}^{+\infty} \varphi_n (x) \varphi_m (x) e^{2\pi i x/\varepsilon} dx.$$

in (4) p designates the rank of the secular determinant and m is any integer $m \le p$. As $p \to \infty$ the argument $\pi m/(p + 1)$ changes continuously from 0 to π. The integral $J_{nn} (2\pi/\varepsilon)$ is always small for small n ($N \equiv \sqrt{2n + 1} \ll \pi/\varepsilon$). Therefore, for small n a second-order correction of the energy must be made (which is given by (3)]. For $N > \pi/\varepsilon$ ($\varepsilon N - \pi \equiv \varepsilon N_1 \ll \pi$),

$$J_{nn} (2\pi/\varepsilon) = (-1)^{n+1} \varepsilon 2^{-1/4} \pi^{-5/4} (\varepsilon N_1)^{-1/4}$$

$$\times \sin [2\pi \varepsilon^{-2} (\varepsilon N_1)^{3/2} - 3/4 \pi]$$

and thus $J_{nn} \sim \varepsilon$.

It can be seen from (3) and (4) that to each n there corresponds not a level but a narrow zone or band, whereas for free electrons the levels are very sharp.

The relative level width (the width compared with the distance μH between levels) is for small n:

$$\delta (n, H) = \varepsilon^2 n 2 \pi^{-4} V^2 E_0^{-2}, \tag{5}$$

and for large n:

$$\delta (n, H) = 8 V J_{nn} (2\pi/\varepsilon) (\mu H)^{-1}. \tag{6}$$

The level width vanishes when $a \to 0$ or $V \to 0$.

From (5) and (6) it can be seen that in the approximation of weakly bound electrons the relative level width at the bottom of the zone is $\sim \epsilon^2$ and close to the middle of the zone it is $\sim \epsilon$. The levels broaden towards the middle of the zone.

2. The broadening of discrete levels into narrow bands also occurs in the approximation of strongly bound electrons. In this approximation and in the absence of a magnetic field the electron energy spectrum is known to be composed of allowed and forbidden zones. We shall examine the structure of an allowed energy zone in a magnetic field (the edges of the zone are almost unshifted).

The problem consists of the approximate solution of the equation

$$\frac{1}{2m} \left(\hat{\mathbf{p}} - \frac{e}{c} \mathbf{A} \right)^2 \psi + V_p \psi = E \psi, \tag{7}$$

$$(A_x = -Hy, \quad A_y = A_z = 0).$$

For our approximation we represent ψ by the series

$$\psi = \sum_n a_n \exp (-i n_2 x / \alpha_0^2) \varphi_0 (\mathbf{r} - \mathbf{n}), \tag{8}$$

where $\mathbf{n}$ is the radius-vector of a lattice site, the functions in the sum satisfy the equation

$$\frac{1}{2m} \left(\hat{p} - \frac{e}{c} A \right)^2 \psi + V (\mathbf{r} - \mathbf{n}) \psi = E_0 \psi, \tag{9}$$

and $V (\mathbf{r})$ is the potential function in an atom at the point $\mathbf{n} = 0$.

A difference equation is obtained for the coefficients a_n. Separating the variables which refer to motion along the magnetic field, we obtain for the motion in a plane perpendicular to $\mathbf{H}$

$$\lambda_\perp a (n_1, n_2) = a (n_1 + 1, n_2) \tag{10}$$

$$+ a (n_1 - 1, n_2) + a (n_1, n_2 + 1) e^{-i \varepsilon^2 n_1}$$

$$+ a (n_1, n_2 - 1) e^{i \varepsilon^2 n_1},$$

where $\lambda_\perp$ is the energy of motion in this plane. This equation also follows from the polar model of a metal[5], where it determines the energy of motion of a quasi-particle (an excitation of the crystal, bearing an electric charge). In this paper it is shown that from (10) under the most general assumptions, there follows the functional equation

$$(\pm \lambda_\perp - 2 \cos \varepsilon x) \varphi (x) \tag{11}$$

$$= \varphi (x + \varepsilon) + \varphi (x - \varepsilon).$$

The signs + and − correspond to the lower and upper halves of the energy zone, while $\lambda_{\perp} = 0$ corresponds to the middle of the zone (± will be omitted hereafter).

Introducing the operator $\hat{K} = i\partial/\partial x$ we can write (11) as

$$(2\cos\varepsilon\hat{K} + 2\cos\varepsilon x)\,\varphi(x) = \lambda_{\perp}\,\varphi(x).$$

Since the operator in the left-hand side of the equation is invariant with respect to the substitution $\varepsilon x \to \varepsilon x + 2\pi$, the solution of this equation by the Flock-Bloch theorem is

$$\varphi(x) = e^{ik\varepsilon x}\,U_k(x)$$

and can be written as

$$\varphi(x) = \sum_{m=-\infty}^{+\infty} C(m\varepsilon + k\varepsilon)\,e^{i(m\varepsilon + k\varepsilon)x}. \tag{12}$$

We expand the coefficients C in a series of Chebyshev-Hermite functions:

$$C(m\varepsilon + k\varepsilon) = \sum_{r=0}^{\infty} b_r\,\varphi_r(m\varepsilon + k\varepsilon).$$

Substituting this in (12) and, furthermore, employing Poisson's sum formula and a Fourier integral for the Chebyshev-Hermite functions:

$$\varphi_r(x) = \frac{1}{\sqrt{2\pi\,i^r}} \int_{-\infty}^{+\infty} \varphi_r(t)\,e^{itx}\,dx,$$

we write the solution as

$$\varphi(x) = \sum_{p=-\infty}^{+\infty} e^{-2\pi iph} \sum_{r=\infty}^{\infty} i^r b_r \varphi_r\left(x + \frac{2\pi p}{\varepsilon}\right). \tag{13}$$

Substituting (13) in (11) and multiplying by $\varphi_n(x + 2\pi q/\epsilon)$, we integrate along the entire axis Ox and, using the relationships which exist for the functions $\varphi_n{}^2$:

$$\Phi_{mn}(\alpha) \equiv \int_{-\infty}^{+\infty} e^{i\alpha x}\,\varphi_n(x)\,\varphi_m(x)\,dx$$

$$= e^{i(n-m)\pi/2} \int_{-\infty}^{+\infty} \varphi_m(x-\alpha)\,\varphi_n(x)\,dx$$

$$= e^{i(m-n)\pi/2} \int_{-\infty}^{+\infty} \varphi_m(x+\alpha)\,\varphi_n(x)\,dx,$$

we obtain

$$b_n\lambda - 4\sum_q b_{n+4q}\,\Phi_{n,n+4q}(\varepsilon) \tag{14}$$

$$+ \sum_{r=0}^{\infty} i^{r-n} b_r\,[e^{2\pi ik} + (-1)^{r-n}\,e^{-2\pi ik}]$$

$$\times \left\{ \lambda\Phi_{rn}\left(\frac{2\pi}{\varepsilon}\right) - \int_{-\infty}^{+\infty} 2\cos\varepsilon x\;\varphi_r\left(x - \frac{2\pi}{\varepsilon}\right)\varphi_n(x)\,dx \right.$$

$$- \int_{-\infty}^{+\infty} \varphi_r\left(x - \frac{2\pi}{\varepsilon} + \varepsilon\right)\varphi_n(x)\,dx$$

$$\left. - \int_{-\infty}^{+\infty} \varphi_r\left(x - \frac{2\pi}{\varepsilon} - \varepsilon\right)\varphi_n(x)\,dx \right\} = 0.$$

Here we have dropped terms containing $\Phi_{rn}(4\pi/\epsilon)$, etc., which are of an order degree of exponential smallness than those which have been retained in (14).

In order to solve (14) in first approximation we also neglect these terms (i.e., the second summation). The coefficients $\Phi_{n,n+4q}(\epsilon)$ diminish rapidly with increasing q (as $1/(4q)!$]. It can be assumed that the coefficients b_{n+4q} change much more slowly (as will be confirmed later). Then we obtain

$$\lambda_{\perp} = 4\sum_q \Phi_{n,n+4q}(\varepsilon), \tag{15}$$

where the summation actually extends only to $|q| \sim 2-3$. This assumption can be checked by setting $b_{n+2q} \approx b_n(-1)^q$ in a definite small interval of change of q and writing (13) with these b_{n+2q}.

The function which results agrees with the fundamental Eq. (11), where $\lambda_{\perp}$ agrees with (15). For small n, Eq. (15) or (16) gives $\lambda_{\perp} = 4 - \epsilon^2 N^2$, ($N^2 \equiv 2n + 1$), which is a solution that was obtained earlier[5].

The integrals $\Phi_{n,n+4q}(\epsilon)$ are expressed in terms of the Chebyshev-Laguerre polynomials $L_n^{(4q)}(\epsilon^2/2)$. By using the asymptotic expression for these polynomials in terms of Bessel functions[6], we obtain $\Phi_{n,n+4q}(\epsilon) \approx J_{4q}(N\epsilon)$. From the theory of Bessel functions it is known that

$$2J_0(x) + 4\sum_{q=1}^{\infty} J_{4q}(x) = 1 + \cos x,$$

whence we obtain for $\lambda_{\perp}$

$$\lambda_\perp = \pm 2(1 + \cos \varepsilon N). \qquad (16)$$

This equation determines the energy levels of the particle as a function of the level number n. The width of the zone is 8 as in the absence of a magnetic field when $\lambda_\perp$ is expressed by $\lambda_\perp = 2 \times (\cos k_1 a + \cos k_2 a)$.

In second approximation we take the neglected terms into consideration, using for b_r the values obtained in first approximation [for the integrals $\Phi_{n,n+p}(2\pi/\varepsilon)$, $q \ll n$ it is possible to use other asymptotic representations of the Chebyshev-Laguerre polynomials which fit the case $N < \pi/\varepsilon$]. We then obtain instead of (16)

$$\lambda_\perp \qquad\qquad\qquad\qquad (17)$$

$$= \pm 2(1 + \cos \varepsilon N)/[1 + J_n(2\pi/\varepsilon)\cos 2\pi k],$$

where

$$J_n\left(\frac{2\pi}{\varepsilon}\right) = {}^1\!/_2 (-1)^n \sqrt{\varepsilon N}\left[\left(\frac{\pi}{\varepsilon N}\right)^2 - 1\right]^{-1/4} N^{-1/3} \quad (18)$$

$$\times \exp\left\{-\frac{4}{3} N^2 \left(\frac{\pi}{\varepsilon N} - 1\right)^{3/2}\right\}$$

[(17) is valid when $J_n(2\pi/\varepsilon) \ll 1$].

Thus even in the approximation of strongly bound electrons each n corresponds to a narrow band rather than to a single level. The width of this band, as can be seen from (18), depends strongly on n in the present approximation. Below and above the zone (for $\varepsilon N \ll 1$) the levels are actually quite sharp; in the middle of the zone ($\varepsilon N \lesssim \pi$) the levels broaden to distinct even though narrow bands.

Since $J_n(2\pi/\varepsilon)$ is small, (17) can be written as

$$\lambda_\perp = \pm 2(1 + \cos \varepsilon N) \qquad (19)$$

$$\times [1 - J_n(2\pi/\varepsilon)\cos 2\pi k].$$

Band widths in the approximation of weakly bound electrons are greater than in the strong binding approximation, but the general characteristics of the bands are identical. Thus, in both approximations if εN (i.e., the energy) is fixed and ε is decreased the width of the bands is diminished. If ε is fixed and N is increased (i.e., for levels closer to the middle of a zone) the band width increases.

It is seen from (16) that the structure of a zone is preserved in a magnetic field and that its edge is not shifted. For $H \to 0$, $\varepsilon \to 0$ the number of

levels within a zone increases and the width of each zone approaches the vanishing point. In the limit all levels fuse into a continuous zone.

3. If the broadening of levels is sufficiently large it must influence the de Haas-van Alphen effect. That is, the oscillations of magnetic susceptibility and of other physical quantities can in some cases possess the character of more or less strongly marked beats. In order to prove this let us assume that

$$E_{nk_3}(k_1) = f(n, k_3) + \Delta(k_1, n, k_3)$$

[k_1 is understood to stand for two continuously changing quantum numbers in (4)]. The number of electron states

$$Z(E, H) \sim \int dk_1 \sum_n k_3(n, E)$$

$$= \int dk_1 \sum_{p=-\infty}^{+\infty} \int e^{2\pi i p n} k_3(n, E)\, dn.$$

The integrals in the summation can be calculated by the method of steepest descents, after which for the oscillating terms that enter into the thermodynamical potential Ω we obtain the following expression:

$$\cos\left(\frac{2\pi pc}{h|e|H} S_{\max} - \gamma\right) \int dk_1 \qquad (20)$$

$$\times \exp\left\{2\pi i p \frac{c}{h|e|H}\frac{\partial S_{\max}}{\partial \zeta}\Delta_{\max}(k_1, \zeta)\right\}$$

instead of the cosine which is obtained when the broadening is neglected. Here $S_{\max}$ is the extremal area of the section of the surface $E=$const cut off by the plane perpendicular to H [3], and ζ is the Fermi energy.

The effect of the additional factor in (20) can be studied by using the example of almost-free electrons, for which the integral in (20) is calculated as

$$J_0^2(2\pi p \Delta_{\max}/\mu H),$$

(J_0 is the zero-order Bessel function). Here the quantity $\Delta_{\max}/\mu H = \delta_{\max}$ in (6) oscillates as H changes [with considerably lower frequency than the cosine in (20)]. This leads to small fluctuations of J_0 without a change of sign (when the width of the levels is not large). Such modulated oscillations (beats) of magnetic susceptibility have actually been observed[7] in some metals. From the form of the argument of J_0 it can be seen

that beats in small fields must be clearer than in larger fields, as is fully confirmed for beryllium[7], in which the beats were investigated in the range $3 \times 10^3 - 2 \times 10^4$ oersteds.

We note in conclusion that the broadening of the levels is strongly dependent on the approximation that is assumed and the the broadening must therefore be calculated outside the framework of the approximations for weakly or strongly bound electrons. It is easily shown that broadening occurs in the general case. In any periodic field V_p the state of an electron is described by the same quantum numbers k_1, n, k_3 by which we describe a free electron in a magnetic field. In fact, if in the Schrödinger equation[7] we put $A_x = -Hy$, $A_y = A_z = 0$, then because of the symmetry of the Hamiltonian (which remains periodic in the Ox and Oz directions) the general solution must be of the form

$$\psi_{k_1 n k_3} = e^{i(k_1 x + k_3 z)} u_{k_1 n k_3}(x, y, z), \qquad (21)$$

where the functions $u_{k_1 n k_3}(x, y, z)$ is periodic with the period of the lattice along Ox and Oz and decreases as $\exp(-y^2 / 2\alpha_0^2)$ at infinity. We see from the equation for $u_{k_1 n k_3}$ that the energy of the electron $E_{n k_3}(k_1)$ is a periodic function of k_1 with the period a/α_0^2.

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Note added in proof: Attention has recently[8] been called to the broadening of levels and, in part, to the influence which this broadening has on the de Haas-van Alphen effect. The author is apparently unfamiliar with Ref. 2, which was published in 1952.

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