SOME PROBLEMS OF THE ELECTRON THEORY OF METALS I. CLASSICAL AND QUANTUM MECHANICS OF ELECTRONS IN METALS

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1. INTRODUCTION

ALL the concepts of the electron theory of metals and all its successes are closely related to ideas of quantum mechanics. Fundamental to the theory was the concept of free electrons -- the carriers of the conduction in metals. Even the most primitive pictures of free electrons in a metal, forming an ideal, highly degenerate Fermi gas, proved to be very fruitful in explaining (at least qualitatively) a variety of experimentally observed regularities (the linear variation of the electronic specific heat, the temperature behavior of electric and thermal conductivity, etc.)

It was possible to go much further with the theory after the fundamental work of Bloch and Peierls, in which the concept of free electrons was developed significantly. In Bloch's theory the interaction of the conduction electron with the crystalline medium was described by introducing an effective electric field with a periodic potential, to take account of the symmetry of the lattice. The study of the motion of particles in a periodic field led to the explanation of the following facts. The energy spectrum of the electron has a zone structure, i. e., it consists of a series of bands (zones), separated by forbidden energy regions. These bands may overlap partially, but their individuality is nevertheless preserved and manifests itself primarily in a different dependence of the particle

energy ϵ on its quasimomentum p, i. e., in a different dispersion law for the electrons. This more complicated dispersion law replaces the formula $\epsilon = p^2/2m$, which holds for free electrons.

One of the most important consequences of the band theory was the conclusion that it was possible to divide all crystals into metals and dielectrics, using as criterion the filling of the zones in the ground state (i. e., the state of lowest energy): in accordance with the Pauli principle, the electrons can be accelerated only when the neighboring energy levels are unoccupied, i. e., a material is a metal if there is a zone which is only partially filled with electrons.

The Bloch model is not entirely satisfactory because it is formulated as a one-electron problem; it is not clear whether or not a consistent inclusion of electron interactions will cause fundamental changes in the concepts of the band theory. For this reason many attempts were made to use other models, in which one or another aspect of the interaction between electrons was taken into account, and in which the problem was formulated as a many-electron problem. However most of these formulations are extremely artificial and unconvincing, and most importantly, cannot be carried through to reach specific results.

A new approach to the problem of the electron theory of metals is associated with the attempt to avoid the difficulties which arise in choosing models for determining the electron spectrum in a metal. This approach is based on general notions of possible types of energy spectra of quantized systems, and on the idea of quasiparticles which have this spectrum.

The concept of quasiparticles is related to the treatment of the low levels of excitation of macroscopic bodies: the energy levels of such bodies are described as the sum of the energies of individual elementary excitations, each of which has its own momentum (or quasimomentum, in a crystal). The simplest examples of such elementary excitations or quasiparticles are the phonons in crystals, spin waves in ferromagnets, excitons in semiconductors and dielectrics, etc. Depending on the statistics of the particles which produce the energy spectrum of

the system, we say that the spectrum is a Bose or a Fermi spectrum.

A macroscopic system can have an energy spectrum with several branches, some of which are Fermi and others Bose. We shall start from the hypothesis that the spectrum of the carriers of the conduction in a metal is a Fermi spectrum. This means that the transfer of charge is accomplished by quasiparticles obeying Fermi statistics. Thus the set of valence electrons interacting with one another and with the crystalline field can, so far as their kinetic and statistical-thermodynamic properties are concerned, be replaced by an ideal gas of charged Fermi quasiparticles. From now on we shall call these quasiparticles conduction electrons or, simply, electrons. The assumption of the Fermi character of the energy spectrum of the carriers of the conductivity clearly does not exclude the possibility that there are other branches of the spectrum which are associated with excitations of Bose type. If we consider the metal as a whole, such excitations surely exist. However, on the basis of the whole body of experimental data now available, it is extremely improbable that in the nonsuperconducting state there is a Bose branch of the spectrum which is associated with the transfer of charge.

As for the energy spectrum of the individual quasiparticle (i. e., its dispersion law $\epsilon = \epsilon$ (p)), because of the crystal symmetry ϵ (p) must be a periodic function of the quasimomentum with the period of the reciprocal lattice (multiplied by Planck's constant $2\pi\hbar$). In the general case this function is multivalued, corresponding to the different energy zones for the electron. Thus this aspect of the band theory is not related to the one-electron model of Bloch, and has a much more general character.

The assumption that the gas of quasiparticles is ideal is, of course, a first approximation appropriate to low excitations (low temperatures). In kinetic problems it is necessary to take account of interactions both within a branch and between branches of excitation (for example, between electrons and phonons). In the simplest case, this interaction corresponds to a collision of the quasiparticles. However, it is possible that such a treatment of the interaction is not good enough and that it is necessary to consider the change in the dispersion law for an individual particle as a function of the number of excitations, in a way similar to that used in the quantum theory of the Fermi liquid which was developed by L. D. Landau.

For a semiphenomenological approach to the development of an electron theory of metals, one must make a careful and deep study of all those properties of the electrons which do not depend on the genesis of the electron energy spectrum, and are determined solely by the dispersion law $\epsilon = \epsilon$ (p). Usually in developing the electron theory of metals emphasis is put on the similarity of an electron in a metal and a free electron, and there is no careful description of the peculiarities in the behavior of the electron, which are related to the complicated nature of its dispersion law. As investigations carried out in recent years have shown, many important properties of metals can be explained only by starting from the assumption that the electron energy spectrum of metals is complicated and is essentially different from the energy spectrum of free electrons. For this reason the development of the electron theory of metals should start from the study of the mechanics (classical and quantum) of an electron with a complicated dispersion law. It then becomes clear that the mechanics of a conduction electron has several important special features, which manifest themselves in a large variety of macroscopic properties of the metal.

The above describes the essential idea, which is to study the consequences of the assumption that the energy spectrum of the conduction electrons in a metal is of Fermi type, disregarding the question of the genesis of such a spectrum and not giving any specific model which leads to such quasiparticles. It turns out that most of the kinetic and statistical-thermodynamic properties of a metal (including its magnetic properties) can be expressed in terms of the parameters characterizing the quasiparticles (their number, dispersion law, etc.). We can therefore also formulate and solve the inverse problem -- to determine the energy spectrum of the quasiparticles (electrons) from the experimental data concerning various macroscopic characteristics of the metal. The most sensitive tools for such a determination of the energy spectrum are the various properties of a metal in a magnetic field, when the radius of curvature of the electron trajectory is much smaller than its mean free path and where the electron can, between collisions, make its dynamical properties apparent (e. g., the low-temperature oscillations of the susceptibility, galvanomagnetic phenomena in strong fields, high-frequency properties of metals, and resonance effects).

As a consequence of the Fermi statistics, in the ground state (i. e., at absolute zero) all the energy levels of the electrons up to the limiting value ϵ_0 are filled. Therefore for temperatures $T \ll \epsilon_0 /k$, in all effects, only those particles play an essential part which have energies close to ϵ_0 (i. e., which lie in a band of width $\delta\epsilon \sim kT$). In most cases the

degeneration temperature $T_0 = \epsilon_0 /k$ is extremely high ($T_0 \sim 10^4$ degrees), and the inequality holds practically always. This means that mainly only those aspects of the dispersion law for electrons manifest themselves which are related to the behavior of the function ϵ (p) near the constant energy surface ϵ (p) = ϵ_0 in momentum space. This surface is called the Fermi surface, and its characteristics determine the properties of the electrons. In addition to the shape of the Fermi surface, a second quantity characteristic for the energy spectrum is $v = \partial\epsilon/\partial p$, which has the significance of a velocity of the electrons. Thus in the sequel, when we talk of determining the energy spectrum, we shall mean only the determination of these two most important characteristics of it.

This summary is divided into three closely related parts. The first part contains the mechanics (classical and quantum) of the conduction electron. In the second part we develop the statistical thermodynamics of the electron gas, i. e., we explain the thermal and magnetic properties of metals under equilibrium conditions. Finally, the third part is devoted to the investigation of kinetic phenomena, in particular the study of galvanomagnetic and resonance effects.

A large part of the results presented are based on the work of the Khar'kov theoretical group. Some of the results are published here for the first time. It was not the purpose of the authors to cover all the papers on the theory of metals which have appeared in recent years, so that the literature cited is not a bibliography of the subject. Attention was mainly given to those effects which can serve as a clue to the electronic energy spectra of metals.

2. GEOMETRY OF CONSTANT-ENERGY SURFACES FOR ELECTRONS.

As we have already said, the dispersion law for a conduction electron is essentially different from that for a free electron.

In particular, the periodicity of the crystal lattice leads to a periodic dependence of the energy on the quasimomentum, with the period of the reciprocal lattice multiplied by $2 \pi\hbar$ ($2 \pi\hbar = h$ is Planck's constant). In general the symmetry elements of the crystal impose conditions on the symmetry of the function $\epsilon = \epsilon$ (p). In addition, because of the invariance of the equations of quantum mechanics under time reversal, we always have ϵ (-p) = ϵ (p).

Since several values of the energy ϵ correspond to a single value of the quasimomentum, ϵ (p) is a

multiple valued function. It would therefore be more accurate to write $\epsilon = \epsilon_s$ (p), where s denotes a set of discrete quantum numbers which determine the "number" of the energy band (zone). These energy bands (or zones) may overlap partially (i. e., min $\epsilon_s <$ max $\epsilon_s <$ max $\epsilon_{s'}$), but, naturally, their individuality is preserved since each zone has its own dispersion law. In all cases where it would not lead to a misunderstanding, we shall omit the index s.

Within each zone, for definite values of the quasimomentum, the energy attains its minimum and maximum values.

In the neighborhood of the points of minimum (or maximum) energy, we can expand in powers of the deviation from the momentum value for which the energy takes on its minimum (maximum) value. If we disregard cases of degeneracy, the expansion has the following form*:

$$\varepsilon (p) = \varepsilon (p_0) + \frac{1}{2} \left(\frac{\partial^2 \varepsilon}{\partial p_i \partial p_k} \right)_{p=p_0} (p_i - p_{i_0}) (p_k - p_{k_0}), \quad (2.1)$$

$\left(\frac{\partial^2 \varepsilon}{\partial p_i \partial p_k} \right)_{p=p_0}$ — is a symmetric tensor of rank two; if

p_0 corresponds to an energy minimum, the principal values of the tensor are positive, whereas they are negative for a maximum. The components of the tensor have the dimensions of reciprocal mass (gm^{-1}). For this reason the tensor is called the reciprocal effective mass tensor, and is denoted by m^{-1}_{ik} .

Thus

$$\varepsilon (p) = \varepsilon (p_0) + \frac{1}{2} m^{-1}_{ik} (p_i - p_{i_0}) (p_k - p_{k_0}). \quad (2.1a)$$

In the neighborhood of the extremal points, the constant energy surfaces in quasimomentum space are closed, and as we see from the expansions (2.1) or (2.1a) they are ellipsoids in the immediate neighborhood of these points.

It should be remembered that any closed energy surface near a minimum point encloses a region in momentum space in which the energy is less than

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*Degeneracy near a zone boundary, i.e. near a minimum or maximum, is not a rare occurrence. It is frequently a consequence of the crystal symmetry. We then still have a quadratic dependence on the modulus of the momentum in the neighborhood of the minimum (or maximum), but the angular dependence is more complicated. Thus the energy spectrum of "holes" in G_e and S_1 crystals has the form[1]

$$\varepsilon = A p^2 \pm \sqrt{B^2 p^4 + C^2 (p_x^2 p_y^2 + p_x^2 p_z^2 + p_y^2 p_z^2)},$$

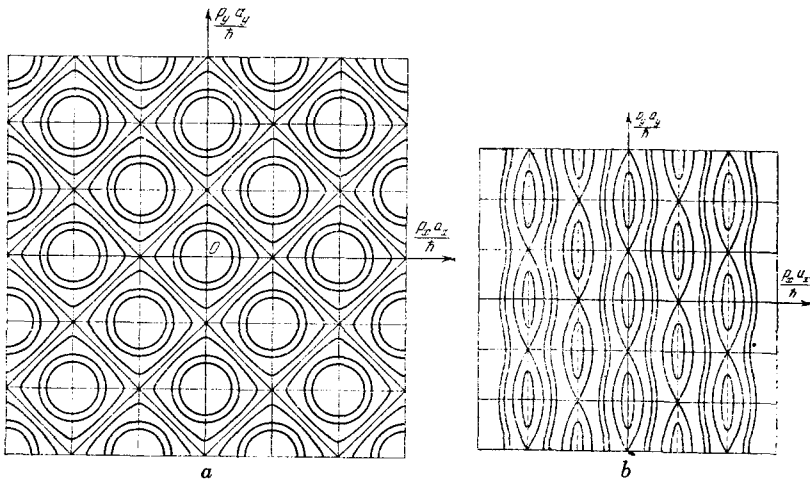where A, B, C are constants, and $p_0 = 0$.

FIG. 1. Lines of equal energy. Dispersion law:

$$\varepsilon = A_1 \cos \frac{p_x a_x}{h} + A_2 \ \cos \frac{p_y a_y}{h}$$

a) $A_1 = A_2$; the lines at 45° are the "open surfaces"; b) $A_1 = A_2$; between the ellipses is a layer of "open surfaces".

its value on the surface, while near a maximum point any closed surface encloses a region in which the energy is greater than its value on the surface. This means that in the first case (near a minimum) the vector $\mathbf{v} = \frac{\partial \varepsilon}{\partial \mathbf{p}}$ is directed along the external normal to the surface of constant energy, while in the second case (near a maximum) it points toward the interior.

Since ε (p) is a periodic function, the surfaces described above are repeated periodically over the whole reciprocal lattice. Despite this periodic repetition, we shall say that they are closed.

It is obvious that between these surfaces which are topologically simple there must be more complicated surfaces -- self-intersecting and open surfaces (i. e., surfaces which extend throughout the whole reciprocal lattice), for otherwise it would be impossible to have a continuous transition from the surfaces which surround minimum points to those which surround maximum points.

As an example we show in Fig. 1 the constant energy "surfaces" (curves) in the two-dimensional case

$$\varepsilon = A_1 \cos \frac{p_x a_x}{h} + A_2 \cos \frac{p_y a_y}{h}$$

It is clear that if $A_1 = A_2$ there is one open "surface" (the system of straight lines shown in Fig. 1a); but if $A_1 \neq A_2$, there is a whole layer of such surfaces (cf. Fig. 1b).

We note that in the three-dimensional case open surfaces must occur very frequently. For example, such a "simple" dispersion law as

$$\varepsilon = \varepsilon_0 \left\{ 1 - \frac{1}{3} \left(\cos \frac{p_x a_x}{h} + \cos \frac{p_y a_y}{h} + \cos \frac{p_z a_z}{h} \right) \right\}, \quad (2.2)$$

leads to layers of open surfaces which fill approximately 1/3 of the volume of the entire reciprocal lattice (cf. Fig. 2).

The dispersion law (2. 2) can be regarded as representing the first terms in the Fourier expansion of the dispersion law $\varepsilon = \varepsilon$ (p). In Bloch's theory this law corresponds to the inclusion of interaction of the electrons with the neighboring atoms in a simple cubic lattice.

As was shown in references 2 and 3, the inclusion of further terms in the expansion (which would correspond in the Bloch theory to taking account of the interaction of the electrons not only with nearest-neighbor atoms but also with more distant atoms) makes the constant energy surfaces considerably more complicated. In particular, there are frequent cases where the connectivity of the energy surfaces is complicated (Fig. 3).
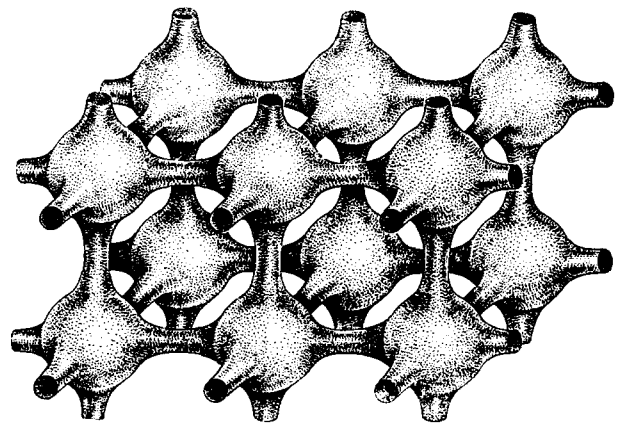

FIG. 2. Typical open surface of constant energy (space grid). The dependence of energy on quasimomentum is given by Eq. (2.2).
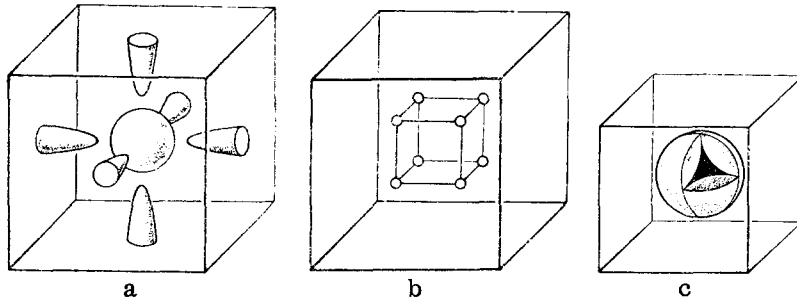
FIG. 3. Energy surfaces for the dispersion law

$$\varepsilon = A_0 + A_1 \left(\cos \frac{p_x a}{h} + \cos \frac{p_y a}{h} + \cos \frac{p_z a}{h} \right) + A_2 \left(\cos \frac{p_x + p_y}{h} a + \cos \frac{p_x + p_z}{h} a + \right.$$

$$\left. + \cos \frac{p_y + p_z}{h} a \right) + A_3 \left(\cos \frac{p_x + p_y + p_z}{h} a + \cos \frac{p_x + p_y - p_z}{h} a + \cos \frac{p_x - p_y + p_z}{h} a + \right.$$

$$\left. + \cos \frac{p_x - p_y - p_z}{h} a \right) + A_4 \left(\cos \frac{2 p_x}{h} a + \cos \frac{2 p_y}{h} a + \cos \frac{2 p_z}{h} a \right)$$

for various values of the parameters A_j and the energy
ϵ. FIG. 3c shows a case where one part of the surface
of constant energy is contained in another part. A por-
tion of the outer surface has been cut away.

The open surfaces can be of all types -- simply
connected or multiply connected (some examples of
open surfaces are shown in Figs. 2 and 4).

The topology of the constant energy surfaces
and, in some cases, the nature of the curves of
intersection of these surfaces with a plane deter-
mine the dynamics of the electron in electric and
magnetic fields. It is therefore convenient to
classify the surfaces as follows:

I. Closed surfaces. These naturally do not
contain any open plane curves.

II. Open surfaces:

a) Open curves occur only for fixed directions
of the normal to the intersecting plane, or not at
all (an example is Fig. 4b).

b) There is a one-dimensional manifold
(dihedral angle) of directions of the normal to the
intersecting plane which give open curves (exam-
ples are Fig. 4a -- the "crimped" cylinder; the
dihedral angle is equal to 2 π).

c) There is a two-dimensional manifold (solid
angle) of normal directions giving open curves
(examples are Fig. 4d -- the "embossed" plane,
with solid angle equal to 4π, and Fig. 2 -- the
"space grid" with solid angle less than 4π).

In the case of complicated energy surfaces, the
directions of the normals to planes which give open
sections are conveniently shown in stereographic
projection (Fig. 5).

Since the energy ϵ is a periodic function of the
quasimomentum p, the whole p-space can be
divided, according to the symmetry class of the

particular crystal, into regions in which the energy
takes on the same set of values. Such regions
were introduced by Brillouin in studying the energy
spectrum of electrons in a weak periodic field, and
are called Brillouin zones.

The location of the zone boundaries, i. e., the
planes which separate one Brillouin zone from
another, is very important for the explanation of
the symmetry of the surfaces of constant energy.
Often, however, by using the periodicity of the
energy ϵ (p), all the zones are "contracted" into one
(the first) zone, so that the quasimomentum p is
treated as a quantity defined within the first Bril-
louin zone, thus emphasizing the distinction
between the quasimomentum and the true momen-
tum. However it is then very difficult to treat the
motion of the electron in electric and magnetic
fields, in which case the quasimomentum is not
conserved. In fact one is immediately faced with
the question of what happens to an electron when it
reaches the boundary of a Brillouin zone.

It is more convenient to assume that the quasi-
momentum of the electron is defined over the whole
reciprocal lattice space, and that its energy and
velocity are periodic functions of p.

3. CLASSICAL MECHANICS OF A PARTICLE
WITH AN ARBITRARY DISPERSION LAW.

An electron in a metal is unquestionably a
quantum mechanical object, i. e., its laws of
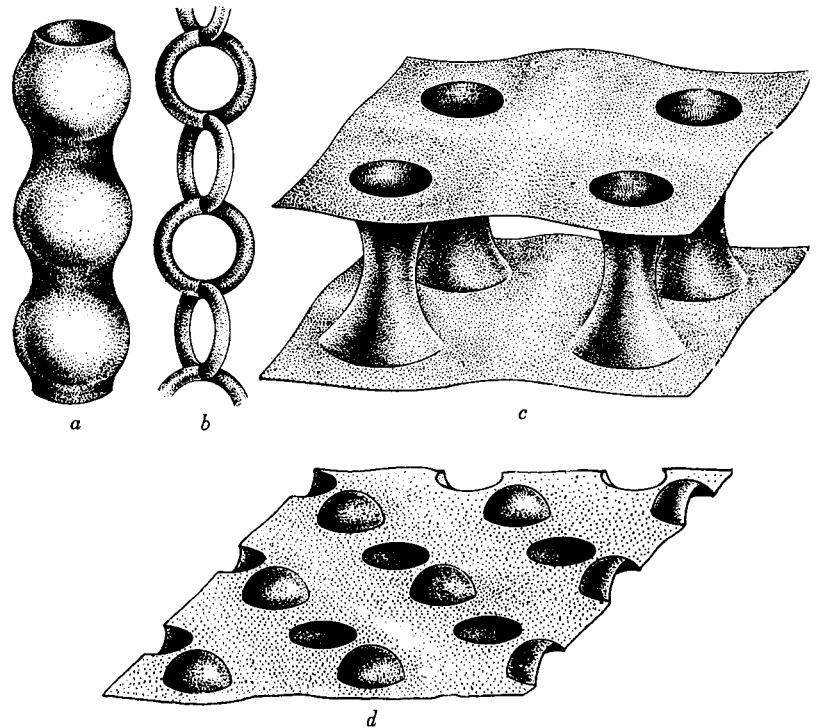motion can be found only on the basis of a quantum

FIG. 4. Possible types of surfaces of constant energy.

mechanical treatment. In particular, only quantum mechanics could explain the "freedom" of the electron in a metal -- its ability to move through an ideal lattice without resistance. Only quantum mechanics allows us to formulate such concepts as quasiparticle, dispersion law, etc. However, since these concepts are already formulated and we can now regard the electron in a metal as a particle with a complicated dispersion law, it becomes possible to treat a variety of problems purely classically. For such a treatment it is necessary that the following conditions be fulfilled:
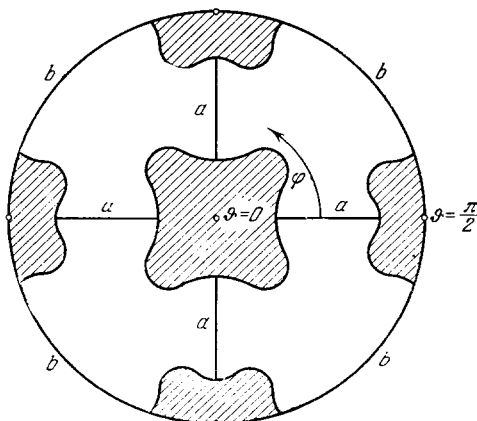

FIG. 5. Stereographic projection of directions of normals to the intersecting plane for which there are open sections, for the energy surface shown in FIG. 2. The directions are those in the shaded regions and the lines a and b.

a) The de-Broglie wavelength of the electron must be much less than the characteristic length associated with the electron trajectory; this is the usual requirement for a classical motion, which in general allows us to speak of a definite trajectory of the particle.

b) The length characterizing the trajectory of the particle must be much greater than the lattice constant a, in order that the state of the electron can be described by using the quasimomentum.

c) The distance between quantum energy levels must be much less than the energy of the electron.

The most important cases of quantization of the energy of an electron are the motion of an electron in a constant magnetic field and the motion in a potential field (thin film).

First let us estimate the limits which the conditions given above impose on the magnetic field. We shall later examine the motion of an electron with a complicated dispersion law in a magnetic field. Here (for an estimate) we shall assume that we have a quadratic, isotropic dispersion law. Then the radius of the electron orbit (a helix) is r = cp/eH, where H is the magnetic field strength, and conditions a), b), and c) can be expressed as the inequalities

$$\text{a) } \frac{cp}{eH} \gg \frac{\hbar}{p}; \quad \text{b) } \frac{cp}{eH} \gg a; \quad \text{c) } \hbar\omega \ll \varepsilon, \ \omega = \frac{eH}{mc}. \quad (3.1)$$

We know that the most interesting case is that of electrons with energy close to the Fermi energy

$\epsilon_0 = p^2 / 2m$, $p_0 = 2 \pi \hbar (3n/8\pi)^{1/3}$, where n is the electron density. Since usually $n \sim 1/a^3$, $p_0 \sim \hbar/a$. Making use of this it is easy to see that all three inequalities (3.1) coincide, and that they impose only a very weak restriction on the value of the magnetic field:

$$H \ll \frac{ch}{ea^2} \sim 10^8 - 10^9 \text{ oersted.} \qquad (3.2)$$

As we see, the effective mass does not appear in this inequality. Later we shall see that this result is more generally valid (for electrons with an arbitrary dispersion law).

In similar fashion it is easy to show that the motion of an electron in a film can be treated classically if the film thickness is much greater than the interatomic distance (d >> a).*

In this section we shall assume that condition (3.1) is satisfied, so that we can use a classical treatment for an electron with an arbitrary dispersion law. It is then natural not to distinguish between quasimomentum and momentum. This is justified if we do not include the specifically quantum-mechanical effect of transitions between energy zones.

If a metal is put into an electric or magnetic field, the state of the electron with a definite momentum is not stationary -- its momentum changes with time. Our problem is to find the equations which describe this change. It is most convenient to start from a Hamiltonian formalism. If the electric and magnetic fields are described by a vector and a scalar potential, A and $\mathcal{Y}$, the Hamiltonian of the electron can be written as follows:

$$H = \varepsilon \left(\mathbf{P} - \frac{e}{c} \mathbf{A} \right) + e\varphi. \qquad (3.3)$$

Here $\mathbf{P} = \mathbf{p} + \frac{e}{c}\mathbf{A}$ is the generalized momentum of the electron (where $\mathbf{p}$ is its kinematic momentum). The equations of motion have the usual form:

$$\mathbf{P} = -\frac{\partial H}{\partial \mathbf{r}}; \quad \mathbf{r} = \frac{\partial H}{\partial \mathbf{P}}. \qquad (3.4)$$

*We should make one remark. Quantum-mechanical effects associated with the discreteness of the energy levels may occur not only in the motion of a single electron but also in the behavior of a gas or an aggregate of electrons. If we are interested in the macroscopic properties of such a gas, the conditions for classical behavior are much stricter than those given above. In order to neglect quantum effects it is necessary in this case that the separations of energy levels be much less than kT, i.e., it is necessary that the magnetic field be much less than $kT/\mu \sim 10^4$ oersted (for $T = 1°$ K and μ equal to a Bohr magneton), and that the film thickness be much less than $a(\epsilon_0/kT)$.

Since $\dot{\mathbf{r}}$ is the electron velocity $\mathbf{v}$, and since only the potentials depend on the coordinates, we find from (3.4), using

$$\mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla\varphi; \quad \mathbf{H} = \text{curl } \mathbf{A}$$

the equation

$$\frac{d\mathbf{p}}{dt} = e \left\{ \mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{H} \right\}; \quad \mathbf{v} = \frac{\partial \varepsilon}{\partial \mathbf{p}} \qquad (3.5)$$

which is a generalization of the Lorentz equation. It differs from the ordinary Lorentz equation because the electron velocity $\mathbf{v}$ is here a complicated periodic function of the kinematic momentum $\mathbf{p}$. As we shall see later, this causes the motion of electrons in a metal to have many peculiarities.

Let us first consider the motion in a constant, uniform electric field.

Since the magnetic field is zero,

$$\frac{d\mathbf{p}}{dt} = e\mathbf{E}.$$

If the electric field strength $\mathbf{E}$ is independent of the coordinates, the electron will move with a constant "velocity"

$$\mathbf{p} = \mathbf{p}_0 + e\mathbf{E}t.$$

in momentum space. It is interesting to note that the motion of a conduction electron in a constant and uniform electric field is finite along the direction of the field. In fact, it follows from the conservation of energy that

$$\varepsilon - e\mathbf{E}\mathbf{r} = \text{const.}$$

Since ε is a bounded function of $\mathbf{p}$, it is then clear that the electron will carry out a finite motion

$$(\mathbf{r} - \mathbf{r}_0)\mathbf{E} = \varepsilon(\mathbf{p}_0 + e\mathbf{E}t) - \varepsilon(\mathbf{p}_0).$$

along the direction of the field. If the field is along one of the crystallographic directions, the electron carries out oscillations with a frequency $\omega_E = \frac{2eE}{\Delta p_E}$, where Δp_E is the period of the function $\varepsilon(\mathbf{p})$ along the direction of the electric field. Since $\Delta p_E \sim 2\pi\hbar/a$ (where a is the lattice parameter), $\omega_E \sim eEa/\hbar$ The oscillation amplitude is then $\Delta\varepsilon/eE$ where $\Delta\varepsilon$ is the width of the energy band. In the general case, when the field direction is not along one of the crystallographic directions, the motion of the electron is close to periodic. For reasonable values of the field, the amplitude of oscillation of the electron in an electric field is extremely large, millions of times greater than the mean free path ($\Delta\varepsilon/eE \sim 10^6$ cm for E 10^{-8} cgs units*; while $\Delta\varepsilon \sim 10^{-12}$ ergs). Therefore in computing the resistance of a metal and in other analogous cases, we can disregard the periodic character of the

*$E = 10^{-8}$ cgs units corresponds to a current density in the metal of $j = 10^2$ amp/cm^2 for a specific resistivity of $\delta = 10^{-8}$ $ohm\text{-}cm$.

electron motion. Over short sections of its path the electron moves uniformly.

One can pose the question: how is the limiting transition made from the electron in a metal (for simplicity, let us say in the periodic field V(r) of a crystal lattice) to the free electron, as the periodic potential tends toward zero? How does the motion change from a finite periodic motion to an infinite motion? To answer this question we must remember that under the influence of the electric field transitions can occur from one zone to another[4], while for V → 0 the gaps between zones tend to zero and the transition probability tends toward unity.

We note, finally, that the anisotropic nature of the dispersion law leads to the result that, in the plane perpendicular to the applied field, the electron does not move freely: its velocity in this plane changes when the projection of its momentum on the field direction changes. This is one of the elementary reasons for the anisotropy of resistance, thermal conductivity and other kinetic coefficients.

Now let us study the motion in a constant, uniform magnetic field (E = 0, H ≠ 0).

In this case the Lorentz equation has the following form:

$$\frac{d\mathbf{p}}{dt} = \frac{e}{c}\ \mathbf{v} \times \mathbf{H}\ .\qquad(3.6)$$

Taking the scalar product first with v, then with H, we conclude that, as for the case of a free electron, when the conduction electron moves in a magnetic field the electron energy ϵ is conserved ($d\epsilon = \mathbf{v}\cdot d\mathbf{p}$) and the component of the momentum p along the field direction is conserved. If we take the z axis along the magnetic field, we find

$$\epsilon = const, \qquad p = const. \qquad(3.7)$$

Equations (3.7) describe the electron trajectory in momentum space. Depending on the topology of the energy surfaces, the trajectory may be closed (i. e., it may break up into closed curves, each of which is within a single cell of the reciprocal lattice*), or it may be open (i. e., extending continuously through the whole reciprocal lattice). The classification of the various curves was given in Section 2.

In this paragraph we shall not include quantum transitions, which accompany any abrupt change of

*We may mention that in those cases where the (x, y) plane does not coincide with one of the crystallographic planes, the curves located in different cells of the reciprocal lattice are not identical. This obviously does not contradict the periodicity of the function $\epsilon = \epsilon(\mathbf{p})$.

quasimomentum. We may therefore assume that the electron moves along one of the closed curves described by (3.7). If the curve (3.7) does not break up into closed curves, but extends continuously throughout the whole reciprocal lattice, the electron will of course carry out an infinite motion in the reciprocal lattice.

The location of the electron on the trajectory (3.7) in momentum space is conveniently defined by giving the time of arrival computed from any point on the trajectory.

Projecting (3.6) on the (x, y) plane, we find

$$\frac{dl}{dt} = -\frac{eH}{c}v_{\perp}.\qquad(3.8)$$

Here dl is the element of arc of the curve (3.7), while $v_{\perp} = \sqrt{v_x^2 + v_y^2}$. We recall that the z axis is along the magnetic field. The minus appears because the electron charge is taken to be negative: -e > 0.

Integration of (3.8) gives

$$t = -\frac{c}{eH}\int \frac{dl}{v_{\perp}}\ .\qquad(3.9)$$

If the curve (3.7) is closed, the electron in the magnetic field will obviously carry out a periodic motion with period

$$T_H = -\frac{c}{eH}\oint \frac{dl}{v_{\perp}}\ .\qquad(3.10)$$

This expression can be transformed by using the fact that $v_{\perp}$ (the vector with components v_x and v_y) is normal to the plane of the curve (3.7). We denote by $S(\epsilon, p_z)$ the area bounded by one of the curves (3.7) (i. e., by one of the closed, nonintersecting curves).

Since

$$S(\epsilon, p_z) = \int\int dp_x\ dp_y = \int d\epsilon\ \oint \frac{dl}{v_{\perp}}\ ,$$

$$\oint \frac{dl}{v_{\perp}} = \frac{\partial S}{\partial \epsilon}\ ,\qquad(3.11)$$

and we find[5,6]

$$T_H = -\frac{c}{cH}\frac{\partial S}{\partial \epsilon}\ .\qquad(3.12)$$

It is natural to call the quantity $\frac{1}{2\pi}\frac{\partial S}{\partial \epsilon} = m^*$ the effective mass of the electron in the magnetic field; m^* is a function of the quantities ϵ and p_z, which are conserved in the magnetic field. This makes its use more convenient than the usual reciprocal effective mass tensor (cf. Sec. 1), which in general depends on all the components of the vector p.

The period and frequency of rotation have the same form as for a free electron:

$$T_H = -\frac{2\pi m^* c}{eH}, \qquad \omega_H = -\frac{eH}{m^* c}\ .\qquad(3.12')$$

From this it is clear that for a free electron
$m^* = m$. In fact, if $\epsilon = p^2/2m$, the curve (3.7) is
a circle; it bounds a circular area equal to $S = \pi$
$(2m\epsilon - p_z^2)$. Then $\frac{\partial S}{\partial \epsilon} = 2\pi m$.

Since the effective mass m^* depends on ϵ and
p_z, it naturally differs for different electrons in the
metal. Therefore, unlike a gas of free electrons,
the conduction electrons do not rotate in the mag-
netic field with a common frequency for all elec-
trons. Different electrons carry out different
periodic motions. Those electrons which move
along open trajectories in the planes perpendicular
to the magnetic field (in momentum space) carry
out an infinite motion.

So far we have not considered the direction of
motion of the electron, which obviously is deter-
mined by the relative orientation of the vectors $\mathbf{v}_\perp$
and $\mathbf{p}_\perp$. From Eq. (3.6) it is easy to show that the
direction of motion is related to the sign of the
effective mass: if $m^* > 0$, the electron moves
along a left helix (like a free electron), but if $m^* <$
0 it moves along a right helix like a positively
charged particle. The effective mass has the sign
of the derivative $\frac{\partial S}{\partial \epsilon}$, which obviously depends on
whether the energy in the interior of the surface
$\epsilon(\mathbf{p}) = \epsilon$ is less than or greater than ϵ. In the first
case, the derivative $\frac{\partial S}{\partial \epsilon} > 0$, which means that the
effective mass m^* is also positive, while in the
second case it is negative. *

It should still be emphasized that one cannot
introduce in a natural way the concept of an effect-
ive mass in the magnetic field (which is related to
the period of revolution in the orbit) for open
trajectories. We can however establish a rule for
determining the direction of motion of the electron,
which is valid both for closed and open trajectories:
the electron moves so that at every point of the
trajectory, if we look to the right of the direction
of motion of the electron, we see a region of lower
energy.

So far we have talked of the motion of the elec-
tron in momentum space. From the Lorentz
equation it is clear that the electron trajectory in
momentum space is closely related to the projec-
tion of the electron trajectory in ordinary space
onto a plane perpendicular to the magnetic field.
In face, we see from Eq. (3.6) that the velocity of
the electron in the magnetic field is perpendicular
to its "velocity" in momentum space:

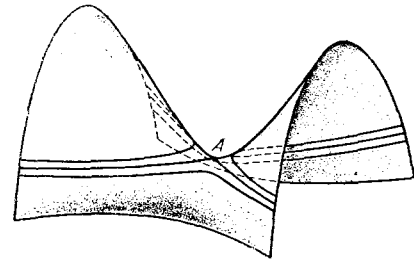$$\frac{d\mathbf{p}}{dt} = \frac{e}{c} \frac{d\mathbf{r}}{dt} \times \mathbf{H} \ .$$

FIG. 6. Trajectory of an electron in a magnetic field
near a saddle point on the energy surface. Point A is the
saddle point.

But this means that the actual trajectory of the
electron is obtained from its trajectory in momen-
tum space by a rotation through angle $\pi/2$ and a
change of scale (multiplication by c/eH). In par-
ticular this means that the period and frequency of
motion of the electron in ordinary space are equal
to T_H and ω_H .

The motion of a conduction electron in a mag-
netic field has all sorts of interesting features if
the energy surface is open. So for example, its
trajectory in momentum space may be open, but
this means that in ordinary space the electron, in
the plane perpendicular to the magnetic field goes
through an infinite motion, and goes off to infinity.
One can also have the case where, at the same
time, the electron carries out a finite motion along
the magnetic field direction (or where the electron
is at rest).

Open trajectories (or open sections) are of
course possible only for electrons which are on
open energy surfaces. In these cases, however, as
we have already stated, the sections may be either
open or closed, depending on the direction of the
field and the magnitude of p_z.

We now explain how the period of motion of the
electron along its trajectory becomes infinite as the
parameters of the motion are changed (i. e., as we
change the direction of the field or the value of p_z).
In doing this we must remember that the period
becomes infinite in two different cases. The first
case occurs when a change of one of the parameters
(ϵ, p_z, magnetic field direction) brings the elec-
tron trajectory toward a saddle point (point A in
Fig. 6). The other case occurs when the electron
is on an energy surface like the "crimped" cylin-
der, and the transition to an infinite motion occurs
because the angle between the axis of the "cylinder"
and the field direction approaches 90° (Fig. 8). *
We begin with the first case.

At the saddle point (point A in Fig. 6), the electron velocity $\mathbf{v} = \partial \epsilon / \partial \mathbf{p}$ is zero. So as the electron moves along a trajectory which passes through the saddle point, it approaches it asymptotically. An electron which is at the saddle point does not move at all. From this it is clear that electrons which move along trajectories which pass close to the saddle point (Figs. 6, 7) spend a large part of the time near the saddle point. This means that their period is determined mainly by the nature of the electron motion near the singularity. For a suitable choice of axes, the equation of the electron trajectory (in momentum space) in a magnetic field, near the saddle point has the form

$$\epsilon - \epsilon_0 (p_z) = \frac{1}{2} \left(\frac{p_1^2}{m_1} - \frac{p_2^2}{m_2} \right). \qquad (3.13)$$

Here ϵ_0 (p_z) is the value of the energy at the saddle point; the directions of the axes 1 and 2 are shown in Fig. 7 and the z axis, as usual, is along the magnetic field; $1/m_1$ and $1/m_2$ are the values of the respective second derivatives of ϵ with respect to $\mathbf{p}$ at the saddle point (m_1, $m_2 > 0$). According to (3.10) the period of the electron motion is

$$T_H = \frac{c}{|e|H} \oint \frac{dl}{v_\perp}$$

Since over most of the trajectory the motion proceeds with finite velocity, whereas it is infinitesimal near A,

$$T_H \cong \frac{c}{|e|H} \int_{-p_0}^{p_0} \sqrt{\frac{1 + \left(\frac{dp_1}{dp_2} \right)^2}{v_1^2 + v_2^2}} \, dp_2$$

$$\cong \frac{2c}{|e|H} \sqrt{\frac{m_1 + m_2}{m_2}} \int_0^{p_0} \frac{dp_2}{\sqrt{\frac{p_1^2}{m_1^2} + \frac{p_2^2}{m_2^2}}} \qquad (3.14)$$
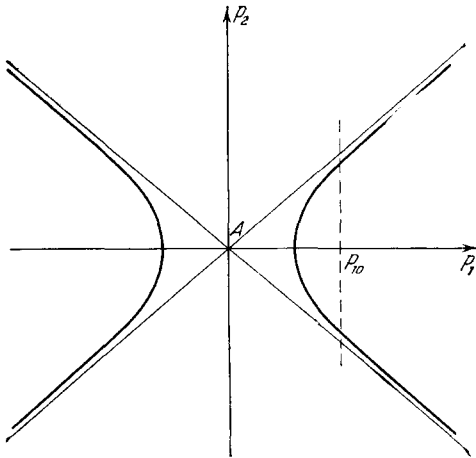

FIG. 7. Electron trajectory near a saddle point. At the saddle point A the velocity is zero.
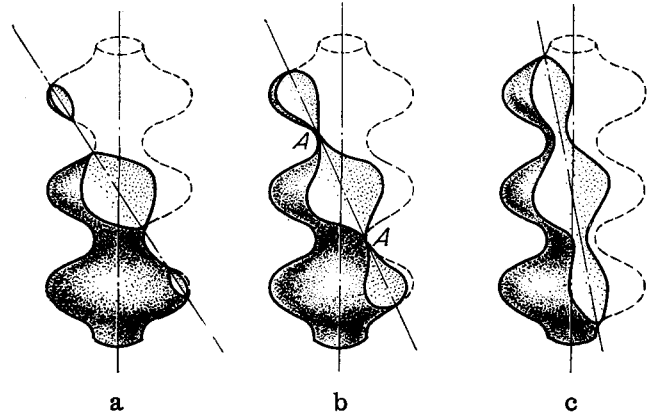

FIG. 8. Change in the character of the electron trajectory as a function of the angle between the magnetic field and the axis of the crimped cylinder. The points A are the saddle points.

$(p_0$ is a value of p_z for which the trajectory has essentially gotten away from the saddle point, Figs. 6 and 7). From (3.13)

$$\frac{p_1^2}{m_1} = 2\Delta\epsilon + \frac{p_2^2}{m_2},$$

$$\Delta\epsilon = \epsilon - \epsilon_0 (p_z).$$

From this and (3.14) we have

$$T_H \cong \frac{2c}{|e|H} \sqrt{m_1 m_2} \left| \ln \frac{\Delta\epsilon}{\epsilon} \right|. \qquad (3.15)$$

Thus as the trajectory approaches a saddle point the period increases logarithmically. From the derivation of formula (3.15) it is clear that the approach to the singularity can occur both because of a change of the energy (the case considered here) or because of a change of p_z or of the field direction.

Now let us consider the case of the "crimped" cylinder. For a right cylinder ("uncrimped"), as the angle $\phi = \pi/2 - \theta$ (where θ is the angle between the cylinder axis and the magnetic field) is decreased, the period would increase inversely as $\sin\phi \sim \phi$. However, the crimping makes an essential change. It is easy to see that as the angle θ between the axis of the cylinder and the magnetic field approaches 90°, the trajectory must pass through saddle points (Fig. 8). As we approach the saddle point, the period becomes logarithmically infinite. Because of this, the angular dependence of the period becomes very complicated: the logarithmic dependence is superposed on the $1/\phi$ dependence, as shown in Fig. 9. The points at which the period becomes infinite correspond to those angles for which the trajectory passes through saddle points.

Now we consider the motion of the conduction electron in crossed electric and magnetic fields, which for simplicity we assume to be perpendicular
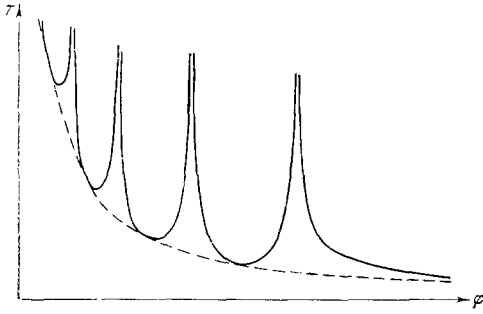
FIG. 9. Dependence of period of revolution of electron on angle between cylinder axis and magnetic field (compare with FIG. 8). The dashed line gives the dependence for an uncrimped cylinder.

to one another. We know that a free electron, placed in crossed fields, drifts in a direction which is perpendicular to the electric and magnetic fields. The drift velocity, i. e., the average velocity of the electron, is *

$$v_0 = \frac{c}{H^2}\, E \times H .\qquad (3.16)$$

Let us see what the situation is for an electron with an arbitrary dispersion law. Using (3.16), Eq. (3.5) can be written as follows:

$$\frac{dp}{dt} = \frac{e}{c}\,[v - v_0] \times H.\qquad (3.17)$$

Taking the time average of this equation, we see that in those cases where the trajectory in momentum space is closed, $\frac{d\overline{p}}{dt} = 0$ and the average velocity in the plane perpendicular to the magnetic field is identical with v_0, as for a free electron, i. e.,

$$\overline{v} = v_0 + v_{\parallel}, \quad v_{\parallel} = \frac{H(vH)}{H^2} .$$

$$\frac{d\overline{p}}{dt} \neq 0 \text{ and } v_\perp \neq v_0.$$

However, in those cases where the trajectory is open, $\frac{d\overline{p}}{dt} \neq 0$ and $v_\perp \neq v_0$. We should emphasize that we are not talking about trajectories in a magnetic field, but rather of trajectories in crossed fields.

We see from Eq. (3.17) that the motion in crossed fields of a particle with the dispersion law $\epsilon = \epsilon\,(p)$ can be regarded as the motion in a magnetic field alone of a particle with the dispersion law

$$\epsilon^*(p) = \epsilon\,(p) - v_0 p.\qquad (3.18)$$

In this case the equations of the trajectory in momentum space have the form

$$\epsilon\,(p) - v_0 p = \text{const}, \quad p_z = \text{const}.\qquad (3.19)$$

It is easy to see that, even when the trajectory in a magnetic field is closed, the trajectory (3.19) in crossed fields may be open.* Knowing the trajectory in momentum space, we can easily construct the trajectory of the conduction electron in coordinate space, by noting that it follows from the law of conservation of energy,

$$\frac{d\epsilon}{dt} = v\,\frac{dp}{dt} = evE$$

that the velocity v is always perpendicular to the vector

$$\frac{dp^*}{dt}\, , \text{ where } p^* = p - eEt.$$

In those cases where the electron trajectory in momentum space is a closed curve, it is easy to determine the period T_{EH} of rotation of the electron. From (3.17) it is clear that, just as in the absence of an electric field,

$$T_{EH} = -\frac{c}{eH}\,\frac{\partial S^*}{\partial \epsilon^*} ;$$

where S* is the area bounded by the curve defined by Eq. (3.19). $\frac{\partial S^*}{\partial \epsilon^*}$ depends in general on the electric field. It is interesting to note that this dependence disappears for a quadratic dispersion law. The electric field is practically always small compared with the magnetic field ($E/H \ll 1$). Using this fact, we can determine the explicit dependence of the rotation period on the electric field:

$$T_{EH} \approx T_H \left\{ 1 - \frac{v_0}{eHT_H} \oint \frac{dl}{v_\perp^2}\left(n + \frac{p}{R} \right) \right\}; \quad n = \frac{v_\perp}{v_\perp}.$$

Here R is the radius of curvature of the trajectory in the magnetic field; the integral is taken along the trajectory in the magnetic field.

In concluding this paragraph we mention that in computing the electrical conductivity of a metal in a magnetic field, we can treat the electric field as perturbation. The properties of a metal in crossed fields are therefore determined by the dynamics of the electron in the magnetic field alone.

4. COLLISION OF QUASIPARTICLES. SCATTERING.

In the preceding paragraph we treated the classical motion of a conduction electron in electric

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*The momentum of the electron (and its velocity) along the magnetic field direction is conserved. Therefore the true average velocity is directed at an angle to the magnetic field.

*It is only the presence of open trajectories that enables us to explain the fact that the total current of a completely filled energy band is equal to zero in crossed fields.
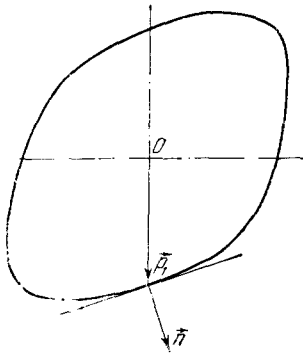
FIG. 10a. Determination of the momentum of an electron scattered in the direction n. The point p_1 is the point where a plane perpendicular to n is tangent to the energy surface $\epsilon = \epsilon(p)$.

FIG. 10b. Determination of the momentum of electrons scattered in the directions n and n_1. We see that a complicated geometry of the energy surfaces causes the appearance, for certain directions, of several values of p corresponding to a given direction of scattering.

and magnetic fields. The fields were assumed to be such that the characteristic dimensions of the trajectories of the quasiparticles were much greater than atomic dimensions: this permitted us to speak of a definite trajectory of the conduction electron. But such motions do not exhaust all the possible changes which the conduction electron undergoes. Because of its interaction with some sort of inhomogeneity of the crystal, having dimensions of the order of the cell length a, the electron changes its state suddenly (over distances of order a): both its momentum and its energy change. In such cases we say that the electron suffers a collision with a local disturbance in the periodicity of the crystal.

Some important conclusions concerning the scattering of the electron can be drawn using only the conservation laws, though the problem of the scattering cross section cannot be solved in the general case: the cross section depends essentially on the structure of the local inhomogeneity, i. e., on the shape of the potential energy of the electron in the neighborhood of the inhomogeneity.

We may mention that, even in the mechanics of a classical particle, the scattering cross section can be calculated completely only in the simplest case of central symmetry. In our case the anisotropy of the crystal makes this problem much more complicated. *

As a rule the local inhomogeneities in a crystal consist of impurity atoms (in particular, isotropic impurities), or defects like vacancies or dislocations. Their mobility is much less than the mobility of the electrons, since they are heavy. Therefore the scattering by such inhomogeneities should be treated as the scattering by a force center.

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*The quantum mechanical problem of the scattering of particles with an arbitrary dispersion law is treated in Sec. 7.
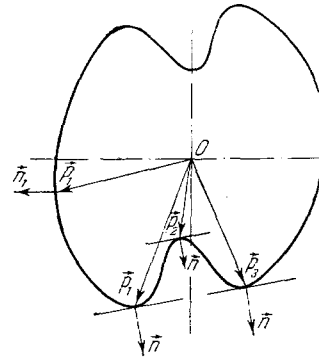
Then if the collision is elastic (and we shall treat only such collisions), the quasimomentum of the electron changes, but its energy is conserved. The complicated dispersion law has a peculiar effect: the scattering angle is determined by the direction of the electron velocity (and not by the momentum direction) after collision. Then if the energy surface in momentum space is convex, there is a single value of the momentum (its location is apparent from Fig. 10a) which corresponds to each value of the velocity. But if the geometry of the energy surface is more complicated, there necessarily exist directions for which the scattering differs from the usual scattering of free particles by the fact that there are several values of the momentum of the scattered particle for the same angle of scattering (cf. Fig. 10b). Within the limits of classical theory, nothing can be stated as to the momentum of the scattered electron. In a quantum mechanical treatment we can calculate the probability of scattering into a given direction with a given value of the quasimomentum (Sec. 7).

In addition to collisions with local inhomogeneities, the conduction electrons in a metal can also "collide" with other quasiparticles (with other electrons, with phonons, with spin waves, etc.). In such collisions we must of course satisfy the laws of conservation of quasimomentum and energy:

$$\mathbf{p}_i = \mathbf{p}_e + 2\pi\hbar\mathbf{b}, \quad \varepsilon_i = \varepsilon_e;$$

where b is a vector of the reciprocal lattice, $\mathbf{p}_i$ and $\mathbf{p}_e$ are the sums of the quasimomenta of the particles before and after the collision; for example, in the collision of two electrons, $\mathbf{p}_i = \mathbf{p}_{1i} + \mathbf{p}_{2i}, \ldots$ and ϵ_i, ϵ_e are the energies of the particles before and after the collision.

It should be remembered that the number of bosons before and after "collision" can be different: creation and annihilation of phonons, spin waves and other quasiparticles can occur. The number of electrons is conserved in such interactions if there are no fermions of the opposite sign (holes*) in the metal, which act as antiparticles for the electrons.

If holes are present or can be produced in the metal, the electrons and holes can be annihilated or created in pairs, so that the difference between the numbers of electrons and holes remains constant.

5. QUASICLASSICAL ENERGY LEVELS.

The quantum mechanics of the conduction electron will be developed in later sections. Here we shall limit ourselves to the calculation of the quasiclassical energy levels in several fundamental cases.

It is obvious that quantization of the energy will occur whenever the electron carries out a finite motion in any one of its degrees of freedom.

The most important case of finite motion is undoubtedly the motion in a magnetic field.

In connection with the study of the diamagnetism of the electron gas and of the de Haas -- van Alphen effect, a large number of papers were written on the theoretical treatment of the behavior of electrons in a magnetic field, culminating in the work of L. D. Landau in 1930. In this paper it was shown that the energy levels of a free electron in a magnetic field H which is directed along the z axis have the form

$$\varepsilon_{n,\,p_z} = \left(n + \frac{1}{2} \right) \hbar \omega_H + \frac{p_z^2}{2m} \, . \tag{5.1}$$

Here

$$\omega_H = \frac{eH}{mc} \, , \qquad n = 0,\ 1,\ 2,\ \ldots \tag{5.2}$$

The appearance of discrete energy levels for a fixed value of p_z is obviously related to the fact that the electron carries out a finite periodic motion in the (x, y) plane perpendicular to the magnetic field. But as we made clear in Sec. 3, this property is retained for an electron with a complicated dispersion law, if its trajectory in momentum space is a closed curve.

To compute the quasiclassical energy levels, we may use the Bohr quantum conditions

$$\oint P_i \, dQ_i = n_i h, \tag{5.3}$$

where Q_i and P_i are conjugate coordinates and momenta of the electron, and the n_i are integers. At this point, as before, we shall make no distinction between quasimomentum and momentum. The limits of validity of our results will be stated later.

Let us then determine the energy levels of an electron with the dispersion law $\epsilon = \epsilon$ (p) in a magnetic field H parallel to the z axis. If we choose the vector potential in the form

$$A_x = -Hy, \quad A_y = A_z = 0,$$

the projection P_x of the momentum is conserved, while condition (5.3) can be written as follows for the motion along the y axis:

$$\oint P_y \, dy = nh. \tag{5.4}$$

The integral is taken along the classical trajectory of the particle, i. e., the dependence of P_y on y should be calculated for definite values of the momentum projection p_z and the particle energy ϵ.

If we treat (5.4) as an equation in which the energy is unknown, and solve it, we can determine the energy levels of the electron in the magnetic field. However it is convenient to transform Eq. (5.4) somewhat, by writing it in a more symmetric form. To do this we transform from integration over y to an integration over the kinetic momentum p:

$$p_x = P_x + \frac{e}{c} Hy. \tag{5.5}$$

Since $dy = \frac{c}{eH} \, dp_x$, and $P_y = p_y$, we have from (5.4),

$$\oint p_y \, dp_x = \frac{eH}{c} nh,$$

where the integral is taken along the electron trajectory in momentum space. The integral in the last equation determines the area $S(\epsilon, p_z)$ of the section of the energy surface by a plane perpendicular to the magnetic field, so that the condition for determination of the quasiclassical energy levels of a conduction electron can be written as follows:[7, 8, 9]

$$S(\varepsilon, p_z) = \frac{eHh}{c} n. \tag{5.6}$$

Naturally, the energy levels ϵ_{n, p_z} do not depend on the form chosen for the vector potential A. This is clear from the invariant form of (5.6) in which the x and y axes are not distinguished.

If $\varepsilon (\mathbf{p}) = \frac{p^2}{2m^*} \, .$

then $S(\varepsilon, p_z) = \pi (2m^* \varepsilon - p_z^2).$

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*The concept of "holes" will be introduced rigorously in the second part of this survey.

and we arrive at formula (5.1) (aside from a factor 1/2 in the first term*:

Formula (5.7) remains valid if the dispersion law is quadratic but anisotropic. But then the effective mass should be taken as a quantity depending on the angles between the magnetic field and the axes of the effective mass tensor:

$$m^* = \left(\frac{\alpha_1^2}{m_2 m_3} + \frac{\alpha_2^2}{m_1 m_3} + \frac{\alpha_3^2}{m_1 m_2} \right)^{-\frac{1}{2}}, \qquad (5.8)$$

(m_j are the principal values of the effective mass tensor, and α are the direction cosines of the magnetic field $\left(\sum_{j=1}^{3} \alpha_j^2 = 1 \right)$.

Using (5.6) for determining the level energies, we calculate the spacing $\Delta\epsilon$ between energy levels. Since only levels of high energy can be treated quasiclassically, $n \gg 1$, and so $\Delta\epsilon \ll \epsilon$. We therefore have from (5.6):

$$\Delta\varepsilon = \frac{2\pi |e| \hbar H}{c \left(\frac{\partial S}{\partial \varepsilon} \right)}. \qquad (5.9)$$

Using the definition of the effective mass

$$m^* = \frac{1}{2\pi} \frac{\partial S}{\partial \varepsilon}, \qquad (5.10)$$

we get

$$\Delta\varepsilon = \frac{|e| \hbar H}{m^* c} = \hbar\omega_H, \qquad (5.11)$$

where ω_H is the frequency of revolution of the electron in the magnetic field (3.12'). The last equality is entirely reasonable -- it is a special case of the general correspondence principle: in the quasiclassical approximation the spacing of energy levels is identical with the classical frequency of the periodic motion. We note that, unlike the energy levels of a free electron, the energy levels of a conduction electron in a magnetic field are not equidistant: the effective mass m^*, and consequently the frequency ω_H, depends on the energy ϵ and on p_z. The difference between a free electron and a conduction electron is made particularly clear by the existence of open surfaces and open sections -- the motion is not quantized for

all electrons in the metal, but only for those which have $\frac{\partial S}{\partial \epsilon} \neq \infty$.

The occurrence or absence of discrete energy levels is determined not only by the energy surface on which the electron is located, but also by the direction of the magnetic field and, for fixed field, by the value of p_z. The transition from closed to open trajectories was treated in detail in Sec. 3.

The formulas found here for the energy of an electron in a magnetic field show that the infinite degeneracy which occurs for the free electron case -- the fact that the energy is independent of the conserved momentum component P_x -- is also true in the quasiclassical approximation for the case of an electron with an arbitrary dispersion law. However, as we shall see later, this degeneracy is lifted when we take account of the difference between momentum and quasimomentum. In other words, there is a slight smearing out of the energy levels (5.6) because of the dependence of ϵ on P_x. Physically this dependence is related to the fact that P_x determines the location of the electron trajectory in space (in the case of a free electron, cP_x/eH is the center of the orbit in the (x, y) plane in which the electron revolves). Whereas in free space (for a free electron) all the points of the space are equivalent (since the magnetic field is taken to be homogeneous), in a periodic structure, such as a crystal, this homogeneity does not exist.[22]

In those cases where the electron trajectory in momentum space in a magnetic field is open, the quasiclassical treatment does not lead to a quantization of the energy. However, as will be clear from the sequel, a more rigorous treatment shows that, because of the periodicity of the dependence of energy on quasimomentum, characteristic breaks occur in the continuous spectrum of the electron.

It may be possible, by using different expressions for the dispersion law, to determine the explicit dependence of the electron energy on the magnetic field and the quantum numbers p_z and n. But this is unnecessary, since all the macroscopic characteristics of the metal can be expressed in terms of S and $\frac{\partial S}{\partial \epsilon}$. Besides, we may mention that a knowledge of the quasiclassical energy levels is sufficient for determining many of the macroscopic properties of the metal.

It was shown in Sec. 3 that the motion in crossed electric and magnetic fields can be regarded as the motion of a particle with the dispersion law

$$\varepsilon^*(\mathbf{p}) = \varepsilon(\mathbf{p}) - \mathbf{v}_0\mathbf{p} \qquad (5.12)$$

---

*The quasiclassical energy levels coincide with the true levels for large n ($n \gg 1$). We can get more exact energy values if we use instead of formula (5.3) the more exact quantization conditions

$$\oint P_i \, dQ_i = (n+\gamma) h, \qquad (5.3')$$

where $0 < \gamma < 1$. However the value of γ can be found only by choosing a specific dispersion law and studying the character of the electron motion near the turning point. For a quadratic dispersion law, $\gamma = \frac{1}{2}$, and we can, starting from (5.3''), obtain the exact energy levels in this special case.

in a magnetic field alone. Furthermore, if the trajectory in momentum space is closed, the particle carries out a finite motion along the y axis (the z axis was taken along the magnetic field, the x axis along the electric field). This enables us to take over our previous results to the case of motion of a particle in crossed fields. In fact, proceeding exactly as before, we get the quantization conditions in the form

$$S^*(\varepsilon, \ p_z) = \frac{|e|H\hbar}{c} n, \qquad (5.13)$$

where S* is the area of the section of the surface $\varepsilon^*(p) = $ const by the plane $p_z = $ const. It is immediately evident that the spacing $\Delta\varepsilon$ of the energy levels is equal to the frequency w_{EH} multiplied by Planck's constant, i. e.,

$$\Delta\varepsilon = \hbar\omega_{EH} = \frac{2\pi|e|\hbar H}{c\left(\dfrac{\partial S^*}{\partial\varepsilon}\right)}. \qquad (5.14)$$

We recall that the frequency ω_{EH} for the case of an arbitrary dispersion law depends on the value of the applied electric field, and that this dependence disappears for a quadratic dispersion law. Consequently the spacing between the discrete energy levels of an electron in crossed fields also must depend on the value of the electric field.

If we do not take account of transitions between bands, the conduction electron in a uniform electric field carries out a finite motion (Sec. 3). To this finite motion there should correspond a quantization of the energy levels, whose spacing is easily found by using the correspondence principle,

$$\Delta\epsilon = \hbar\omega_E.$$

It appears to be impossible to observe effects which might occur as a result of this quantization. Even if we assume that transitions between zones are extremely improbable, the electron cannot carry out a full oscillation because of collisions with irregularities of the lattice.

The crystalline lattice in which the electron moves is always limited by the dimensions of the sample. However the dimensions are usually so large that they can be assumed to be infinite. All the same, cases may occur where it is necessary to take account of the finite dimensions of the metal (for example, in treating the properties of thin films). The surface of the metal is always somewhat deformed, i. e., in the neighborhood of the surface there are necessarily defects in the periodicity of the structure. The study of the behavior of an electron near the surface is a complicated problem, which is often not even formulated clearly. On the other hand, if the electron spends most of its time in the bulk of the metal,

the irregularity of the structure over distances of the order of the lattice dimensions need not be taken into account, and we can assume that the boundary of the metal is a potential barrier, or in other words we can treat the electron in a metal as a particle in a potential well. If the electron energy is much less than the height of the barrier, we can assume the barrier to be infinite. Then the momentum components can, of course, take on only discrete values, which are easy to determine if we assume that the sample is a rectangular parallelepiped:

$$p_{ju} = \frac{\pi n_j \hbar}{d_j};$$

d_j are the lengths of the edges of the parallelepiped, along which we put the coordinates, and the n_j are integers. The quantization of the momentum leads to a quantization of the energy:

$$\varepsilon_{n_x, n_y, n_z} = \varepsilon\left(\frac{\pi n_x \hbar}{d_x}, \ \frac{\pi n_y \hbar}{d_y}, \ \frac{\pi n_z \hbar}{d_z}\right). \qquad (5.15)$$

Relatively simple and compact formulas can also be obtained for the case where the electron is in a constant magnetic field H $(H_x = H_y = 0; H_z = H)$ and a potential field U(y). If we again choose the vector potential in the form $A = A_x = -$ Hy, it is easy to see that the x coordinate is a cyclic variable, i. e., the component P_x of the momentum is conserved. This means that, proceeding as before, we can find:[10]

$$S(\varepsilon, \ p_z, \ P_x) = \frac{2\pi\hbar|e|H}{c} n. \qquad (5.16)$$

Here $S(\varepsilon, p_z, P_x)$ is the area bounded by the electron trajectory (a plane curve) in the space of kinetic momenta. The equation of the trajectory is determined by the integrals of the motion:

$$\varepsilon(p_x, \ p_y, \ p_z) + U\left[\frac{c}{eH}(p_x - P_x)\right] = \text{const}$$

$$p_z = P_z = \text{const}, \quad P_x = \text{const} \qquad (5.17)$$

Equations (5.16) and (5.17) determine the dependence of the level energy on the quantum number n, the momentum components $P_z = p_z$ and P_x, and on the value of the magnetic field:

$$\varepsilon = \varepsilon(p_z, \ P_x, \ n). \qquad (5.18)$$

We call attention to the fact that in this case there is no degeneracy in P : because of the presence of the field U, different trajectories corresponding to the same energy ε and p_z are not equivalent.

The formulas obtained here can be used to explain the dependence of the energy levels of an

electron in a magnetic field on the dimensions of
the film. Let us therefore take U(y) to be an
infinitely deep potential well

$$U(y) = \begin{cases} 0, & |y| < d, \\ \infty, & |x| > d, \end{cases} \qquad (5.19)$$

where d is the halfwidth of the film (the potential
well).

For this case the region (5.17) is given by the
conditions

$$\varepsilon(p_x, p_y, p_z) = \varepsilon: \quad |p_x - P_x| < \frac{|e|Hd}{c};$$

$$P_x = \text{const}; \quad p_z = P_z = \text{const}. \qquad (5.20)$$

We denote by $R_1(\varepsilon, p_z)$ and $R_2(\varepsilon, p_z)$ the left and
right limits of the p_x coordinates of the closed curve

$$\varepsilon(p_x, p_y, p_z) = \varepsilon: \quad p_z = \text{const}. \qquad (5.21)$$

If

$$R_1(\varepsilon, p_z) > P_x - \frac{|e|Hd}{c},$$

$$R_2(\varepsilon, p_z) < P_x + \frac{|e|Hd}{c} \qquad (5.22)$$

(cf. Fig. 11), the curve (5.21) is located between
the lines $P_x = p_x \pm |e|Hd/c$, i. e., the electron
trajectory (in coordinate space) is entirely within
the film and does not "feel" it at all. The energy
levels of electrons with values of ε, P_x and p_z
which satisfy the conditions (5.22) coincide with
those found earlier in (5.16). If the electron
trajectory is not all within the film, the area which
enters into Eq. (5.16) is the area within the curve
(5.21) which is bounded by one or both of the
straight lines $P_x = p_x \pm |e|Hd/c$.

For electrons moving along closed trajectories
in momentum space, in a sufficiently large mag-
netic field most of the trajectories will lie entirely
within the film, i. e., these electrons will not be
"aware" at all of the boundary of the film. The
situation is different for electrons which move
along open trajectories: no matter how large the
field, they will carry out an infinite motion in the
plane perpendicular to the field and will therefore
collide with the wall.

The experimental study of the de Haas -- van
Alphen effect requires the use of a pulse technique
for obtaining high magnetic fields. But then,
because of the skin effect, the electrons are in an
inhomogeneous magnetic field. Let us consider the
case[11] where the magnetic field, which is along the
z axis, is inhomogeneous in the y direction: H_z =
H(y). Again the x component of the generalized
momentum is conserved, so that we can, in the
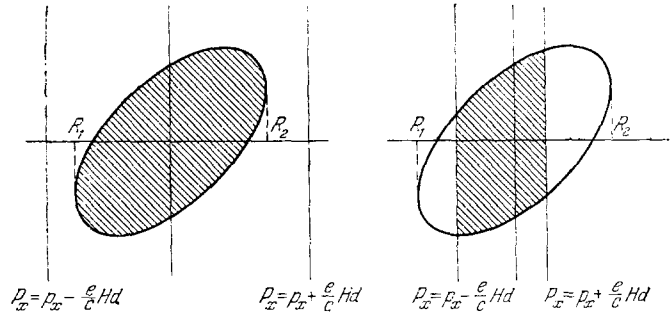Bohr quantum condition

$$\oint P_y\, dy = nh$$

FIG. 11. Trajectory of electron in a film. The shaded
area enters in the quantum condition (5.16).

carry out an integration over the kinetic momentum
p_x:

$$\oint \frac{p_y\, dp_x}{H(y)} = \frac{e}{c} nh. \qquad (5.23)$$

The integral is taken along the trajectory in
momentum space

$$\varepsilon(p_x, p_y, p_z) = \text{const}; \quad p_z = P_z = \text{const}, \qquad (5.24)$$

where y is the root of the equation

$$A(y) = \frac{c}{e}(P_x - p_x); \quad P_x = \text{const}. \qquad (5.25)$$

All the cases of quantization considered here
are special cases of a very general method of
quasiclassical quantization which consists in find-
ing action variables I_j corresponding to a finite
motion, and equating them to $n_j h$ (where the n_j are
integers). Then the energy levels (the energy can
be expressed in terms of the action variables) is
given by:[12]

$$\varepsilon_{n_1, n_2, n_3} = \varepsilon(n_1 h; n_2 h; n_3 h).$$

This expression is valid if the motion is finite for
all three degrees of freedom. If the motion is
infinite for one or two of the degrees of freedom,
the energy depends only on the two or one corre-
sponding discrete quantum numbers.

The quantization of the electron energy leads to
interesting features of the behavior of an electron
gas. Very detailed studies have been made exper-
imentally and theoretically, of the properties of an
electron gas (i. e., of a metal) at low temperature
(de Haas -- van Alphen effect, Shubnikov -- de
Haas effect, cyclotron resonance, etc.). All of
these effects can be divided into oscillatory effects,
i. e., phenomena in which one observes a nonmono-
tonic dependence of a physical characteristic of the
metal on the magnetic field, and resonance effects,
i. e., phenomena in which one observes transitions
of the electrons from one stationary state to
another, where these transitions are accompanied

by the absorption of energy quanta from an external field. The detailed theory of these phenomena, starting from the description of electrons as quasi-particles with a complex dispersion law, will be presented in the second and third parts of the present summary.

However, some important features of the phenomena can be explained using just the formulas for quantization. Thus, for example, the oscillatory dependence on the magnetic field of a large number of physical characteristics of a metal (magnetic susceptibility, resistance, etc.) is related to the fact that the number of occupied levels (with a fixed value of P_z), i. e., of levels with energy less than the limiting Fermi energy ϵ_0, changes by unity when the reciprocal of the magnetic field strength changes by an amount $\Delta 1/H$ equal to $\frac{|e|h}{cS(\epsilon_0, p_z)}$ (cf. 5.6). The dependence of the period on p_z smears out somewhat the sharp dependence on the magnetic field. Therefore those electrons are most important for the oscillatory effects which have values of p_z for which $S(\epsilon_0, p_z)$ is an extremal (Fig. 12), since the period has a relatively weak dependence on p_z near these values. Thus the period of oscillation in the phenomena of de Haas – van Alphen, Shubnikov – de Haas etc. is determined by the extremal cross sections of the Fermi surface:[9, 13, 14]

$$\Delta \frac{1}{H} = \frac{|e|h}{cS_{extr}(\epsilon_0)} .$$ (5.26)

According to reference 15, the dependence of the period of oscillation on the direction of the magnetic field makes it possible to establish the shape of the Fermi surface for those groups of electrons which are responsible for the oscillatory effects.*

The Fermi surfaces for aluminum[16], zinc, and lead[17] were determined in this way.

While the oscillatory effects give a convenient means for studying the extremal areas of sections of the Fermi surface, these effects are extremely unsuited for the determination of the effective mass of the electrons, $m^* = \frac{1}{2\pi} \frac{\partial S}{\partial \epsilon}$, which is related to the velocity distribution on the Fermi surface. (The effective mass enters in a factor depending on the temperature, which is very sensitive to the state of the sample and in particular to its purity.) For the experimental determination of effective masses it is natural to use the resonance effects.

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*The point is that the most important oscillations occur in those cases where the metal contains small electron groups. Thus, for example, in zinc the fundamental harmonic (the one with the longest period) in the oscillations of the magnetic moment corresponds to an electron group having $\sim 10^{-6}$ electrons per atom.
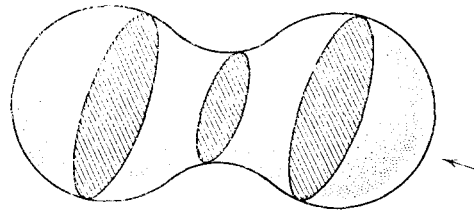

FIG. 12. Example of extremal cross sections of the Fermi surface. The direction of the magnetic field is indicated by the arrow.

It can be shown that, because of the dependence of the Larmor frequency ω_h for an electron with a complex dispersion law on energy ϵ and on p_z, there is no resonance absorption in metals. However a rigorous treatment shows that, although the smearing out of the resonance frequencies somewhat reduces the sharpness of the resonance, in many cases it does not destroy it completely. Then, naturally the true resonance frequencies are those corresponding to extremal values of the effective mass:[18]

$$\omega_{res} = (\omega_H)_{extr} = \frac{eH}{cm^*_{extr}} .$$ (5.27)

The observation of resonance effects in a metal is complicated by the skin effect, and can therefore only be done when the constant magnetic field is strictly parallel to the surface of the sample (cyclotron resonance).

It seems that there should be an interesting peculiarity of diamagnetic resonance for those semiconductors in which the dependence of the energy of the current carriers on quasimomentum is markedly different from quadratic (for example, hole-type germanium). We have already remarked on the fact that for such "electrons" the frequency of the finite motion in crossed fields depends on the strength of the electric current. But this means that, in principle, we should observe a dependence of the resonance frequency of diamagnetic resonance on the current passing through the sample. The observation of such a phenomenon in metals is in all probability impossible, since, because of the large electrical conductivity, we cannot produce any significant electric field inside the metal.

In describing the oscillatory and resonance effects we have used the quasiclassical formulas (5.6), (5.9) and (5.14). This is entirely justified, since the most important electrons for such effects (especially at low temperatures) are those having energies near to the limiting Fermi energy ϵ_0, and we practically always have $\epsilon_0 \gg \hbar\omega_H$. Thus we are dealing with large values of the quantum number n.

6. QUANTUM MECHANICS OF AN ELECTRON WITH AN ARBITRARY DISPERSION LAW.

It is usually convenient to write the Schrödinger equation in the coordinate representation. The reason for this is that the kinetic energy operator is easily expressed as a differentiation operator. Because of this the Schrödinger equation is a linear partial differential equation. The theory of such equations has been developed in detail.

For an electron in a metal it is more natural to use the quasimomentum representation, in which the state of the electron is completely specified by giving the quasimomentum and the band number s. The kinetic energy ϵ_s (p) is assumed to be a known function of its arguments s and p. In this representation (the s, p representation), the coordinate operator has the form

$$r_{ss} = -\frac{\hbar}{i}\,\delta_{ss'}\frac{\partial}{\partial p} + \Omega_{ss'}(p). \tag{6.1}$$

The second term $\Omega_{ss'}$ occurs because the coordinate is a quantity which is canonically conjugate to the quasimomentum and satisfies the commutation relation

$$\{p_i, x_k\} = \frac{\hbar}{i}\,\delta_{ik}, \tag{6.2}$$

and does not commute with the zone number operator $\hat{s}$, i. e., with the operator whose eigenvalues are the quantum numbers which determine the zone number.

Knowing the coordinate operator (6.1) enables us to construct the Hamiltonian for the conduction electron moving in external fields and thus, in principle, to solve any problem of the quantum mechanics of an electron with a complex dispersion law. Naturally, when we do this, the results will be expressed in terms of various characteristics of the electron which are related to its dispersion law, and also in terms of the matrix elements of the operator $\hat{\Omega}$. However the more usual situation is one where we do not know the operator $\hat{\Omega}$, but do know the wave functions $\psi_{sp}(r)$ of the conduction electron, since, from considerations of crystal symmetry*, they have the following form:

$$\psi_{sp}(r) = e^{\frac{ipr}{\hbar}} u_{sp}(r), \tag{6.3}$$

where u_{sp} (r), as a function of the radius vector, is periodic with the period of the direct lattice,

$$u_{sp}(r + a) = u_{sp}(r). \tag{6.4}$$

In addition, the functions u_{sp} (r) are assumed to be orthonormal, i. e.,

$$\int u_{sp}^*(r)\, u_{s'p}(r)\, dv = \delta_{ss'}. \tag{6.5}$$

The integration extends over a single cell of the crystal.

The whole wave function ψ_{sp} (r), as a function of the quasimomentum p, is periodic with the period of the reciprocal lattice, multiplied by $2\pi\hbar$:

$$\psi_{s,\, p+2\pi\hbar b}(r) = \psi_{sp}(r), \tag{6.6}$$

since states with quasimomenta differing by $2\pi\hbar$ b are equivalent. ψ_{sp} (r) is the wave function of the conduction electron in the coordinate representation. The coefficients in the expansion of the wave function $\psi(r)$ an arbitrary state in terms of the wave functions ψ_{sp} (r) gives the wave function in the (s, p) representation. Thus the wave function in the (s, p) representation for an electron having a definite quasimomentum $p = p_0$, and a definite zone number $s = s_0$, is

$$g_s(p) = A\delta_{ss_0}\,\delta\,(p - p_0); \tag{6.7}$$

where A is a normalization factor.

Using the form of the wave functions ψ_{sp} (r), one can show that

$$\Omega_{ss'}(p) = i\hbar \int u_{sp}^*(r)\frac{\partial}{\partial p} u_{s'p}(r)\, dv, \tag{6.8}$$

where the integration extends over a unit cell.

Because of the periodic dependence of the functions ψ_{sp} (r) on quasimomentum, and of the functions u_{sp} (r) on the coordinates, it follows that

$$\psi_{sp}(r) = \sum_b A_s\,(p + 2\pi\hbar b)\, e^{\frac{i\,(p + 2\pi\hbar b,\ r)}{\hbar}}, \tag{6.9}$$

where b is an arbitrary vector in the reciprocal lattice.* From the expansion (6.9) and formula

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*The functions ψ_{sp} (r) are chosen so that they transform according to an irreducible representation of the symmetry group of the crystal.

*The representation of the function ψ_s (r) in the form (6.9) follows from the following chain of equations:

$$\psi_{sp}(r) = e^{\frac{ipr}{\hbar}} u_{sp}(r) = \sum_{b'} A_{sb'}(p)\, e^{\frac{i\,(p + 2\,\tau b'\hbar)r}{\hbar}}$$

$$= \sum_{b'} A_{sb}\,(p + 2\pi\hbar b)\, e^{\frac{i\,(p + 2\pi\hbar b + 2\pi\hbar b')\, r}{\hbar}}$$

$$= \sum_{b'} A_{s,\, b'-b}\,(p + 2\pi\hbar b)\, e^{\frac{i\,(p + 2\pi\hbar b')\, r}{\hbar}}$$

Then $\qquad A_{s,\, b'}(p) = A_{s,\, b'-b}\,(p + 2\pi\hbar b),$

or $\qquad A_{s,\, b}(p) = A_{s,\, 0}\,(p + 2\pi\hbar b) = A_s\,(p + 2\pi\hbar b).$

(6.3) it follows that

$$A_s(\mathbf{p}) = \frac{1}{v_0} \int u_{s\mathbf{p}}(\mathbf{r})\,dv;$$ (6.10)

v_0 is the volume of the unit cell.

Thus, in order to give the wave functions for the conduction electron, it is sufficient to assign the quantities A_s (p), i. e., the average values of the modulating functions $u_{s\mathbf{p}}(\mathbf{r})$ for all values of p.

The matrix elements of the operator $\hat{\Omega}$ can be expressed in terms of the quantities A_s (p). In fact, from (6.8), (6.3) and (6.9) we have

$$\Omega_{ss'} = ihv_0 \sum_{\mathbf{b}} A_s^*(\mathbf{p} + 2\pi h\mathbf{b}) \frac{\partial}{\partial \mathbf{p}} A_{s'}(\mathbf{p} + 2\pi h\mathbf{b}).$$ (6.11)

In estimating the magnitude of the matrix elements $\Omega_{ss'}$ it is convenient to use a model. If we use the model of tightly bound electrons (Bloch[20]), we find in the one-dimensional case (which we choose for simplicity),

$$\Omega_{ss'} = i \int_{-\infty}^{\infty} \varphi_s(x)\, x\varphi_{s'}(x)\,dx$$
$$+ i \sum_{l \neq 0} e^{-\frac{2\pi i l p a}{h}} \int_{-\infty}^{\infty} \varphi_s(x - la)\, x\varphi_{s'}(x)\,dx.$$

Here the $\phi_s(x)$ are atomic functions. From this formula it is evident that the matrix elements of the operator $\hat{\Omega}$ are of the order of the lattice constant a. We note that in the limit of infinitely tight binding, i. e., for cases where the overlap of the wave functions of neighboring atoms can be neglected, $\Omega_{ss'} \neq 0$, since transitions to an excited state can occur without a transition to a neighboring cell of the lattice. At the same time the effective mass of the electron tends to infinity while the mobility approaches zero.

For the case where the periodic field V(r) is treated as a perturbation (Brillouin[21]), the $\Omega_{ss'}$ are proportional to the Fourier components of the periodic function V(x) for $|s - s'| \neq 1$; for $|s - s'| = 1$, they are inversely proportional. Again (for simplicity) we have used the one-dimensional case. When V(x) tends to zero, the matrix elements $\Omega_{ss'}$ $|s - s'| = 1$) tend toward δ functions:

$$\Omega_{s,s+1} = 2 \sum_{m=-\infty}^{\infty} \delta\left(\frac{s+1}{2}b + mb\right),$$

$$\Omega_{s,s-1} = -2 \sum_{m=-\infty}^{\infty} \delta\left(\frac{sb}{2} + mb\right), \quad b = \frac{2\pi}{a}.$$

Now we calculate the electron velocity operator. Since

$$\hat{v} = \frac{d\hat{r}}{dt} = \frac{i}{h}\{\varepsilon_s(\mathbf{p})\,\hat{r} - \hat{r}\,\varepsilon_s(\mathbf{p})\}.$$

we have from (6.1)

$$\hat{v} = \frac{\partial \varepsilon_s(\mathbf{p})}{\partial \mathbf{p}} + \hat{\Omega}.$$ (6.12)

The matrix elements of $\hat{\Omega}$ are related to the matrix elements of $\hat{\Omega}$ by the relation

$$\dot{\Omega}_{ss'}(\mathbf{p}) = \frac{i}{h}\{\varepsilon_s(\mathbf{p}) - \varepsilon_{s'}(\mathbf{p})\}\,\Omega_{ss'}(\mathbf{p}).$$

From this formula we see that $\dot{\Omega}_{ss'} = 0$ for s = s', i. e., $\hat{\Omega}$ has no diagonal elements.

The (quantum mechanical) average value of the velocity is equal to the diagonal matrix element of the operator (6.12). From what we have said, it is simply

$$\bar{\mathbf{v}} = \frac{\partial \varepsilon_s(\mathbf{p})}{\partial \mathbf{p}}.$$ (6.13)

Thus the average velocity is obtained by differentiating the energy with respect to the quasimomentum -- in complete analogy to the classical relation between energy, momentum and velocity. We have used expression (6.13) repeatedly in the earlier paragraphs.

Let us assume that the metal is put in a uniform electric field E, in which a force eE acts on the electron. Then the quasimomentum of the electron and the zone number will not be conserved. We now determine their time derivatives. The homogeneous field adds a term $-e\mathbf{E}\cdot\mathbf{r}$ to the Hamiltonian, i. e.,

$$\hat{H} = \varepsilon_s(\mathbf{p}) - e\mathbf{E}\mathbf{r}.$$ (6.14)

Commuting p and s with the Hamiltonian, we find, using (6.1), that

$$\dot{\mathbf{p}} = e\mathbf{E}, \quad (\dot{s})_{ss'} = \frac{ie}{h}(s - s')(\mathbf{E}\Omega_{ss'}).$$ (6.15)

The operator for the time derivative of the quasimomentum is equal to the force exerted on the electron by the uniform field, precisely as is the case for the true momentum of a free electron.

The operator for the derivative of the zone number is naturally related to the operator $\hat{\Omega}$. The operator $\dot{s}$ has no diagonal elements.

The situation is more complicated when the conduction electron moves in a magnetic field.

The components of the kinetic momentum operator $\hat{\mathbf{p}} = \hat{\mathbf{P}} - e\mathbf{A}$ do not commute with one another, and also do not commute with the zone number operator $\hat{s}$, since the vector potential A depends on r, and P and r are connected by the commutation relations (6.2).* From (6.1) and (6.2) we can

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*In expression (6.1) we must now replace p by P, the generalized quasimomentum of the electron.

easily establish the usual commutation relations between the components of the kinetic momentum operator:

$$\{\hat{p}_i, \hat{p}_k\} = \frac{e\hbar}{ic} \varepsilon_{ikl} H_l \qquad (6.16)$$

(ε_{ikl} is the unit antisymmetric tensor of the third rank), as well as the commutation relation between the zone number operator and the kinetic momentum operator

$$\{\hat{s}, \hat{p}\}_{ss'} = -\frac{e}{2c} (s - s') H \times \Omega_{ss'}(p). \qquad (6.17)$$

The last relation is easily derived, using a vector potential taken in the form A = ½ H × r.

Because of the periodicity of the dispersion law in P-space, we can expand ε_s (p) in a Fourier series

$$\varepsilon_s(p) = \sum_a A_a^{(s)} e^{\frac{iap}{\hbar}}, \qquad (6.18)$$

where the summation extends over all the periods **a** of the crystal lattice.

The transition from the classical expression (6.18) for the energy to the Hamiltonian is made by replacing the quantities p and s by operators with the commutation rules (6.16) and (6.17).

Since the components of the kinetic momentum do not commute with one another or with the zone number operator, the expression (6.18) requires further definition -- we must state what we mean by the function ε_s (p) of the noncommuting variables $\hat{s}$, $\hat{p}_x, \hat{p}_y, \hat{p}_z$. It seems that this question cannot be solved in general; it is related to the genesis of the Fermi branch of the energy spectrum. However if we neglect transitions between zones, i.e., if we treat the operator $\hat{s}$ as a c-number, we can determine the proper symmetrization of the function ε_s (p) from quite general considerations. Suppose the magnetic field is along the z axis. Then $\hat{p}_z$ commutes with $\hat{p}_x$ and $\hat{p}_y$, while $\hat{p}_x$ and $\hat{p}_y$ do not commute with one another:

$$\{\hat{p}_x, \hat{p}_y\} = \frac{e\hbar}{ic} H. \qquad (6.19)$$

When we go over to a Hamiltonian operator, i. e., when we replace the components of the kinetic momentum by operators with the commutation rules (6.19), it is natural to start from the expansion (6.18) in which each term is treated as an exponential function of a single operator a·$\hat{p}$. In other words, if we neglect transitions between zones,

$$\varepsilon_s(\hat{p}) = \sum_a A_a^s e^{\frac{ia\hat{p}}{\hbar}}. \qquad (6.20)$$

This conclusion is based on the fact that, in the plane perpendicular to the magnetic field, the x and y axes are not fixed, so that we can choose as canonically conjugate variables* any linear combination of the quantities p_x and p_y. The expression (6.20) corresponds to a "complete symmetrization" of the Hamiltonian in the components of the kinetic momentum.

This conclusion that complete symmetrization of the Hamiltonian is necessary is confirmed by an investigation of G. E. Zil'berman[22], based on the model of an electron in a periodic field.

We now calculate the time derivative of the kinetic momentum. (Again we neglect transitions between zones.)

Commuting $\hat{p}$ with the Hamiltonian $\hat{H} = \varepsilon(\hat{p})$, using (6.19), we find

$$\frac{d\hat{p}}{dt} = \frac{e}{c} \frac{\partial\hat{\varepsilon}}{\partial\hat{p}} \times H, \qquad (6.21)$$

where the derivative of the Hamiltonian operator is to be understood as follows:

$$\frac{\partial\hat{\varepsilon}}{\partial\hat{p}} = \frac{i}{\hbar} \sum_a a A_a e^{\frac{ia\hat{p}}{\hbar}}. \qquad (6.22)$$

$\frac{\partial\hat{\varepsilon}}{\partial\hat{p}}$ is obviously the operator for the electron velocity $\frac{d\hat{r}}{dt} \equiv v = \frac{\partial\varepsilon}{\partial\hat{p}}$ If electric and magnetic fields act on the conduction electron,

$$\frac{d\hat{p}}{dt} = e\{E + \frac{1}{c} v \times H\}. \qquad (6.23)$$

According to (6.23), the average value of the time derivative of the quasimomentum operator is equal to the generalized Lorentz force:

$$\frac{d\hat{p}}{dt} = e\{E + \frac{1}{c} \hat{v} \times H\}.$$

In quantum mechanics, problems can be formulated in two different ways: we can consider the change of the state (wave function) with time, or we can look for stationary solutions, i. e., determine the energy levels of the particles. Let us consider two very simple examples.

We start with a problem of the first type. Let us find the time dependence of the wave function of an electron when it is acted on by a constant homogeneous force eE (where E is the electric field intensity). In the spirit of the preceding treatment, we shall solve the problem in the quasimomentum representation. In accordance with (6.4) and (6.1),

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*To within a constant factor, the components of the kinetic momentum are canonically conjugate to one another.

in this representation the Schrödinger equation for the wave function $g_s(\mathbf{p}, t)$ has the form

$$-\frac{\hbar}{i}\frac{\partial g_s}{\partial t} = \varepsilon_s g_s + \frac{e\hbar}{i}\,\mathbf{E}\,\frac{\partial g_s}{\partial \mathbf{p}} - \sum_{s'} e\mathbf{E}\mathbf{\Omega}_{ss'}g_{s'}. \qquad (6.24)$$

In many cases this equation can be solved by the method of successive approximations, treating the last term on the right as a small perturbation. This is justified to a certain extent by the fact that the applied field is small, while the dimensionless small parameter is the quantity $eaB/(\epsilon_s - \epsilon_s)$. (We remind the reader that the matrix elements of the operator $\hat{\Omega}$ are of the order of the lattice constant a.) Before we use the method of successive approximations, we first transform (6.24) somewhat, by introducing in place of the time t a new variable

$\pi = p_x - eEt$ (the x axis is along the electric field, and we shall write p_x simply as p from now on):

$$-\frac{\hbar}{i}eE\left(\frac{\partial g_s}{\partial p}\right)_\pi = \varepsilon_s g_s - eE\sum_{s'}\Omega^x_{ss'}g_{s'}; \qquad (6.25)$$

p and p enter as parameters in the last equation.

We now introduce a new function $\phi_s(\mathbf{p},)$ equal

to $e^{\displaystyle\int\frac{\varepsilon_s\,dp}{\hbar Ee}}g_s(p, \pi)$. . The equation for ϕ_s is particularly simple:

$$\left(\frac{\partial \varphi_s}{\partial p}\right)_\pi = \sum_{s'} q_{ss'}\varphi_{s'}(p,\pi), \qquad (6.26)$$

where

$$q_{ss'} = \frac{i}{\hbar}e^{i\int\frac{\varepsilon_s\,dp}{\hbar eE}}\Omega_{ss'}e^{-i\int\frac{\varepsilon_{s'}dp}{\hbar eE}}. \qquad (6.27)$$

We now use successive approximations. In the zeroth approximation, which corresponds to neglecting transitions between zones,

$$\left(\frac{\partial \varphi_s^{(0)}}{\partial p}\right)_\pi = 0, \qquad (6.28)$$

i.e.,

$$\varphi_s^{(0)} = \varphi_s^{(0)}(\pi) = \varphi_s^{(0)}(p - eEt). \qquad (6.29)$$

Now we satisfy the initial conditions. If at t = 0, $g_s(\mathbf{p}, 0) = g_s(\mathbf{p})$, then according to (6.29)

$$g_s^{(0)}(p, t) = g_s(p - eEt)e^{\frac{i}{eE\hbar}\int_p^{p-eEt}\varepsilon_s\,dp}. \qquad (6.30)$$

The quantity $|g_s(p)|^2$ gives the probability that an electron in the s'th zone has a momentum in the interval (p, p + dp). The last equation shows that in the zero'th approximation (when we neglect transitions between zones) the probability distribution moves as a whole in momentum space with the constant "velocity" $\frac{d\mathbf{p}}{dt} = e\mathbf{E}$. In particular this applies to a δ-function probability distribution: if

the particle initially has a definite value of its quasimomentum, then at any time t it will have a definite quasimomentum which can be determined from the classical equation of motion

$$\frac{d\mathbf{p}}{dt} = e\mathbf{E}.$$

Now we find the first approximation for the function $\phi_s(\mathbf{p}, t)$. From Eq. (6.26) we have

$$\left(\frac{\partial \varphi_s^{(1)}}{\partial p}\right)_\pi = \sum_{s'} q_{ss'}\varphi_{s'}^{(0)}(\pi).$$

Since $\phi_s^{(1)} = 0$ at the initial time,

$$\varphi_s^{(1)}(p, \pi) = \sum_{s'} Q_{ss'}(p, \pi)\varphi_{s'}^{(0)}(\pi), \qquad (6.31)$$

$$Q_{ss'}(p, \pi) = \int_\pi^p q_{ss'}(p)\,dp.$$

If at the initial time the electron had a definite value of s, equal to s_0, then according to formulas (6.30) and (6.31), at any time t, the function ϕ_s has the form

$$\varphi_s(p, \pi) = \varphi_{s_0}(\pi)\{\delta_{ss_0} + Q_{ss_0}\}.$$

to within terms linear in $\Omega_{ss'}$. Going over from the functions ϕ_s to electron wave functions $g_s(\mathbf{p}, t)$, it is easy to show that the probabilities W_{ss_0} for transition of the electron from one zone to another are given by the squares of the matrix elements Q_{ss_0}:

$$W_{ss_0}(t) = A\,|Q_{ss_0}|^2, \qquad (6.32)$$

where A is a normalization factor.

We shall use the example of an electron in a magnetic field to show how one determines the quantum energy levels for an electron with a complex dispersion law.

The Schrödinger equation in this case obviously has the following form:

$$\varepsilon_s(\hat{\mathbf{p}})g_s(\mathbf{P}) = \varepsilon g_s(\mathbf{P}), \qquad (6.33)$$

where

$$\varepsilon_s(\hat{\mathbf{p}}) \equiv \varepsilon_s(\hat{p}_x, \hat{p}_y, \hat{p}_z) = \varepsilon_s\left(P_x - \frac{e\hbar H}{ic}\frac{\partial}{\partial P_y}, P_y, P_z\right) \qquad (6.34)$$

where the Hamiltonian has been completely symmetrized (cf. above). The components P_x and P_z enter as parameters in (6.33).

It is of course impossible to solve (6.33) in general form. However, from (6.34) we see that Planck's constant $\hbar$ appears in the equation in combination with the magnetic field H, and the appropriate dimensionless constant can be seen from (6.34) and (6.20) to be the quantity $a^2eH/\hbar$,

where a is the lattice constant. In other words, Eq. (6.33) can be written as follows:

$$\varepsilon_s \left(u_x + i\delta \frac{\partial}{\partial u_y}, \, u_y, \, u_z \right) g_s(\mathbf{u}) = \varepsilon g_s(\mathbf{u}), \qquad (6.35)$$

where

$$\mathbf{u} = \frac{a\mathbf{P}}{\hbar} \qquad (6.36)$$

is the dimensionless momentum, and

$$\delta = \frac{a^2 e H}{\hbar c}. \qquad (6.37)$$

The parameter δ has a simple physical significance. As we see from (4.6), $a^2 eH/\hbar c$ is the ratio of the area of a unit cell of the lattice to the minimum area which the electron traces out in the magnetic field H. We recall that the trajectory of the electron in coordinate space is obtained from its trajectory in momentum space by rotating through angle $\pi/2$ and changing the scale (multiplying by c/eH), i.e., the area in coordinate space is equal to the area in momentum space multiplied by c^2/e^2H^2. For all actual fields, $\delta \ll 1$ (cf. Eq. 1.2). Therefore we can look for a solution of (6.35) in the form of an expansion in powers of δ. Such a method corresponds to the quasiclassical approximation. It may seem that it is the "reverse" of the usual quasiclassical approximation, since Planck's constant appears in the denominator of (6.36). Actually, of course, this is the "usual" quasiclassical approximation. The apparent difference is related to the fact that Eqs. (6.33) -- (6.35) are written in the momentum representation. The expression for the parameter δ can be rewritten as

$$\delta = \frac{e\hbar H}{cp^2} \qquad (6.38)$$

(where $p = \hbar/a$ is the period in quasimomentum space). It is then perfectly clear that we are expanding with respect to Planck's constant. Without going through the derivations, we now present the results of the quasiclassical treatment (G. E. Zil'berman[22, 23]).

In the second approximation, the quasiclassical solution of Eq. (6.35) has the form

$$g_s(\mathbf{P}) = e^{\frac{icP_x P_y}{e\hbar H}} \frac{1}{\sqrt{\left| \frac{\partial \varepsilon_s}{\partial p_x} \right|}} e^{\pm i \frac{c}{e\hbar H} \int^{P_y} P_x(\varepsilon, P_y, P_z) \, dP_y}, \qquad (6.39)$$

where $P_x = P_x(\varepsilon, P_y, P_z)$ is the equation of the trajectory in momentum space, i.e., an actual solution of the equation

$$\varepsilon(p_x, p_y, p_z) = \varepsilon.$$

In the region between closed trajectories, the wave function is exponentially damped:

$$g_s(\mathbf{P}) = e^{\frac{icP_x P_y}{e\hbar H}} \frac{1}{\sqrt{\left| \frac{\partial \varepsilon_s}{\partial p_x} \right|}} e^{\pm \frac{c}{e\hbar H} \int^{P_y} |P_x| \, dP_y}. \qquad (6.40)$$

The energy levels $\varepsilon_s(p_z, n)$ of the electron are given by the Bohr quantum conditions (cf. § 4):

$$S = \oint P_x \, dP_y = \frac{2\pi \hbar e H}{c}(n + \gamma), \qquad (6.41)$$

where $\gamma = 1/2$ if the component P_x approaches zero like $\sqrt{P_y - P_y^{(0)}}$ at the turning point $P_y = P_y^{(0)}$.

As we have already stated, degeneracy of the energy levels of an electron in a magnetic field occurs approximately also for an electron with an arbitrary dispersion law. The investigation of Eq. (6.35) shows that the degeneracy is lifted if we retain terms of order δ^2. This means that (for fixed p_z), to each value of the quantum number n there corresponds not a single level but rather a zone whose width is of order $\hbar \omega \delta^2$, if the neighboring electron trajectories are far from one another. If the neighboring trajectories are close to one another, there is an additional broadening associated with the transition of the electron from one trajectory to another through the "potential barrier." The width of the smeared out region is then

of order $\hbar \omega_H e^{-\frac{\pi}{\delta} x_0^2} \sqrt{\frac{R}{x_0}}$, where x_0 is the halfwidth of the "barrier," R is the radius of curvature at the point of closest approach of the trajectories, and the quantities x_0 and R are in dimensionless units (cf. Fig. 13). Usually the broadening because of transitions of the electron from trajectory to trajectory is unimportant. It begins to be significant only for anomalously small separations between trajectories $(x_0 \sim \delta$, since for small x_0, $R \sim x_0$). However when we go over from closed to open sections, the effect of broadening because of transitions is extremely important. Because of this, the region of smearing broadens more and more and the spectrum goes over from a discrete to a continuous spectrum. It is true that, because of the periodic nature of the electron trajectory,
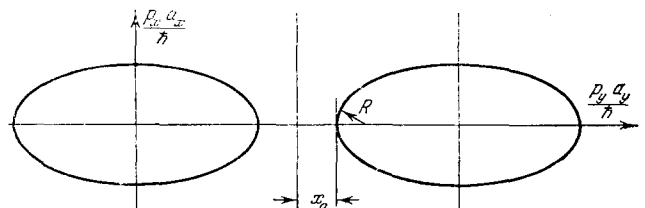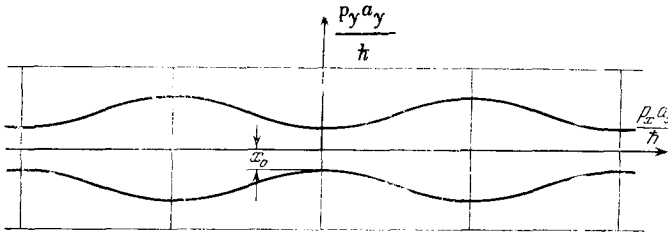

FIG. 13.

FIG. 14.

the continuous spectrum has breaks, whose positions are given by the equations:

$$S_1 = \frac{2\pi\hbar eH}{c} n,$$

where S_1 is the portion of the area traversed by the electron which lies in a unit cell. The width of the gap region is of order $\hbar\omega_H e^{-\frac{\pi}{c} x_0}\sqrt{\frac{R}{x_0}}$ (where x is the half-width of the "isthmus," and R is the radius of curvature at the "isthmus," cf. Fig. 14).

So far we have not included the possibility of transitions between zones. The analysis shows that, in those cases where the trajectories corresponding to the quantum numbers n and p in the zones s and s' intersect, the transition probability is proportional to δ^3, whereas when they do not probability is exponentially small.

This section serves as the basis for classical and quasiclassical treatments. On the other hand, the relatively fine features pointed out here (such as the broadening of levels, gaps in the continuous spectrum, etc.) enable us to explain various features of the de Haas -- van Alphen and other oscillatory effects.

7. QUANTUM THEORY OF SCATTERING OF AN ELECTRON WITH AN ARBITRARY DISPERSION LAW.

The development of a theory of scattering involves the computation of cross sections for various processes and the study of the shape of the wave surface of the scattered particle at large distances from the scattering center. While the first part of the problem (the computation of cross sections) cannot be solved without knowing the structure of the inhomogeneity, the second problem -- the study of the shape of the wave surface at large distances -- can be formulated and solved under very general assumptions concerning the nature of the inhomogeneity, while the asymptotic behavior of the electron wave function turns out to be determined by the shape of the energy surface.

Let us consider the scattering of an electron which is in the state (s_0, p_0), i. e., which has the wave function $\psi^{(0)}_{s_0 p_0}(r) = e^{\frac{i p_0 r}{\hbar}} u_{s_0 p_0}(r)$, by a local inhomogeneity. If we assume that the scat-

tering particle is infinitely heavy (impurity atom, vacancy, etc.), the perturbed electron wave function can be written as follows:[24, 25, 28]

$$\psi_{s_0 p_0}(r) = \psi^{(0)}_{s_0 p_0}(r) - \sum_s \int \frac{C^{sp}_{s_0 p_0} e^{\frac{ipr}{\hbar}}}{\varepsilon_s(p) - \varepsilon_{s_0}(p_0)} d\tau_p. \quad (7.1)$$

The quantities $C^{sp}_{s_0 p_0}$ describe the nature of the scattering center, which is assumed to be at the point r = 0. If the inhomogeneity of the crystal is characterized by a perturbation operator Λ, then in all cases where the perturbation has the character of a δ-function[26, 27]

$$C^{sp}_{s_0 p_0} = \frac{\Lambda^{sp}_{s_0 p_0} u_{sp}(r)}{1 + \sum_s \int \frac{\Lambda^{sp}_{s_0 p_0} d\tau_p}{\varepsilon_s(p) - \varepsilon_{s_0}(p_0)}}.$$

Here the quantities $\Lambda^{sp}_{s_0 p_0}$ are the matrix elements of the operator Λ.

Whenever we can use perturbation theory,

$$C^{sp}_{s_0 p_0} = \Lambda^{sp}_{s_0 p_0} u_{sp}(r).$$

We use the notation

$$I_s(r) = \int \frac{C^{s, p}_{s_0 p_0} e^{\frac{ipr}{\hbar}} d\tau_p}{\varepsilon_s(p) - \varepsilon}; \quad \varepsilon = \varepsilon_{s_0}(p_0). \quad (7.2)$$

The particular form of the integrals $I_s(r)$ enables us to investigate the scattered wave at large distances from the scattering obstacle.

The integration in (7.2) can be carried out by integrating over the energy and over the surfaces of constant energy, so that

$$I_s(r) = \int \frac{I_s(r, \varepsilon') d\varepsilon'}{\varepsilon' - \varepsilon}, \quad (7.3)$$

where

$$I_s(r, \varepsilon') = \int_{\varepsilon_s(p) = \varepsilon'} \frac{C^{sp}_{s_0 p_0} e^{\frac{ipr}{\hbar}}}{|\nabla\varepsilon_s(p)|} dS_{\varepsilon'}, \quad (7.4)$$

$dS_{\varepsilon'}$ is the element of area on the energy surface $\varepsilon_s(p) = \varepsilon'$, while the integral in (7.3) is taken between the limiting energy values permitted for the s'th zone (from $\varepsilon_{s\,min}$ to $\varepsilon_{s\,max}$).

In calculating the asymptotic value of the integrals (7.4) for large r, it is convenient to introduce coordinates on the energy surface $\varepsilon_s(p) = \varepsilon'$ which are related to the lines of intersection of the surface with the planes n·p = const (where n = $\frac{r}{r}$). We introduce the variable u = p·n, and integrate first over the strip on the surface between u and u + du, and then integrate with respect to the variable u (cf. Fig. 15). This gives

$$I_s(r, \varepsilon') = \int j_s(u) e^{\frac{iur}{\hbar}} du,$$

$$j_s(u) du = \int \frac{C^{sp}_{s_0 p_0}}{|\nabla\varepsilon_s(p)|} dS_{\varepsilon'},$$

$$\varepsilon_s(p) = \varepsilon'; \quad u < pn < u + du. \quad (7.5)$$

From this expression it is clear that terms of order $1/r$, which correspond to diverging (scattered) waves, arise from the integration near the jumps in the function f_s (u). As is easily shown, the only points of discontinuity of the function f_s (u) are points where the surface ϵ_s (p) = ϵ' is tangent to a plane perpendicular to the direction of propagation n (cf. Figs 10 and 15). Denoting the points of tangency by p_ν, we get

$$I_s(\mathbf{r},\ \epsilon') \cong \sum_\nu \frac{2\pi C_{s_0 p_0}^{s p_\nu} e^{\frac{i p_\nu r}{\hbar}}}{|\nabla \epsilon_s(p_\nu)|\ \sqrt{|K_\nu|}} \frac{1}{r}, \tag{7.6}$$

where K_ν is the Gauss curvature of the surface ϵ_s (p) = ϵ' at the point p = p_ν.

The points of tangency p_ν are obviously determined by the equations

$$\begin{aligned}\epsilon_s(p_\nu) &= \epsilon'; \\ [\mathbf{n} \times \mathbf{v}_s(p_\nu)] &= 0.\end{aligned} \right\} \tag{7.7}$$

By substituting the expressions (7.6) in formula (7.3), we can verify that for r → ∞ the integrals over energy remain finite only if $\epsilon \equiv \epsilon_{s_0}$ (p_0) lie within the range of energy values admissible in the s'th zone. In this case the integrals (7.3) should be regarded as the limiting values of the integrals

$$I_s(\mathbf{r}) = \int \frac{I_s(\mathbf{r},\,\epsilon')\,d\epsilon'}{\epsilon' - \epsilon + i\gamma} \tag{7.8}$$

for infinitely small damping (γ → +0).

The main part of the integrals (7.3) or (7.8) comes from integration near the pole ($\epsilon' = \epsilon$).

Using this result, we get the asymptotic expression for the perturbed wave function:
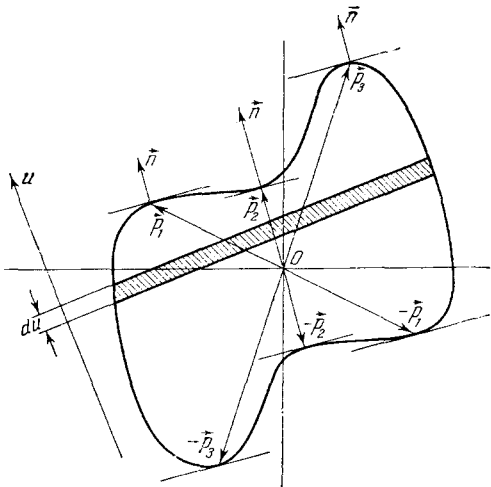

FIG. 15. Section of the surface ϵ_s (P) = ϵ by the plane n ·p = const. P_ν , $- P_\nu$ (ν = 1, 2, 3) are the points of tangency to the supporting plane of the propagation direction n.
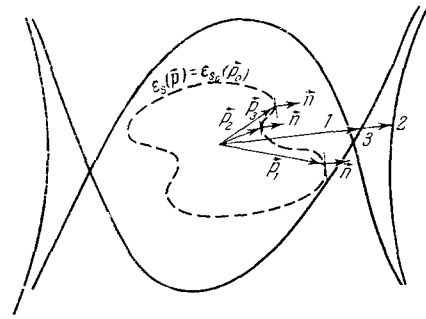

FIG. 16. Section of the wave surface of the scattered electron (solid lines). The dashed line shows the section of the energy surface.

$$\psi_{s_0 p_0}(\mathbf{r}) \sim \psi_{s_0 p_0}^{(0)}(\mathbf{r}) - \frac{(2\pi)^{3/2} i}{r^{1/2}} \sum_{s,\,\nu} \frac{C_{s_0 p_0}^{s,p} e^{\frac{i p_\nu r}{\hbar}}}{|\nabla \epsilon_s(p_\nu)|\ \sqrt{|K_\nu|}}, \tag{7.9}$$

where the values of p_ν are given by Eqs. (7.7), if we replace ϵ' by $\epsilon \equiv \epsilon_{s_0}$ (p_0).

The results obtained here are in agreement with the conclusions of Sec. 4, which were based on the classical (corpuscular) treatment. In fact the procedure for determining p Eqs. (7.7) consists in finding those points on the energy surface where the electron velocity (v_s = $\nabla \epsilon_s$ (p)) coincides in direction with the scattering direction n.

The expression found for the perturbed wave function permits us to draw various conclusions concerning the nature of the scattered waves.

In the majority of cases the wave function of an electron scattered by a single inhomogeneity is a superposition of several waves, the number of waves being equal to the number of possible solutions of (7.7) for $\epsilon' = \epsilon_{s_0}$ (p_0). Each of these waves has its own shape and velocity of propagation (cf. Fig. 16). Even in those cases where the energy of the scattered electron lies within a single zone, the number of scattered waves, as a rule, will be greater than one, because usually the energy surfaces are not convex, but have a complicated shape. The amplitude of each of the scattered waves is determined not only by the dispersion law but also by the characteristics of the scattering center (via the quantities $C_{s_0 p_0}^{sp}$, which can be related to the perturbation produced by the scattering center). The phase of the wave, i. e., the shape of the wave surface, is determined only by the dispersion law; the wave surface for each of the waves is a surface polar to the energy surface ϵ_s (p) = ϵ of the electron.

Knowledge of the wave function for the scattered electron enables us to calculate the cross section

for scattering into solid angle dO in the direction n:

$$d\sigma(n) = \frac{16\pi^4}{|\nabla \varepsilon_{s_0}(p_0)|} \sum_{s,\nu} \frac{|B^{sp_\nu}_{s_0p_0}|^2}{|K_\nu||\nabla \varepsilon_s(p_\nu)|} dO. \quad (7.10)$$

where the quantities $B^{sp\nu}_{s_0p_0}$ are simply related to the coefficients $C^{sp\nu}_{s_0p_0}$.

Each term in formula (7.10) determines the cross section for the process in which the scattered electron has a definite value of quasimomentum and belongs to a definite zone.

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