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INTERACTION OF CONDUCTION ELECTRONS WITH A METAL SURFACE

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CONTENTS

MOST phenomena occurring in a metal with sufficiently large electron mean free path depend substantially on the character of the interaction between the conduction electrons and the boundaries of the sample. This interaction is usually described purely phenomenologically with the aid of the so-called specularity coefficient p, defined in such a way that the fractions of the electrons reflected from the boundary specularly or diffusely are equal to p and 1 – p, respectively. Since the wavelength of the conducting electrons coincides in order of magnitude with the interatomic distance, and the characteristic dimensions of the roughnesses of the boundary are much larger than this quantity, it has been customary to assume that the coefficient p is close to zero or, what is the same thing, that the electron reflection is close to diffuse.

Recently, however, many phenomena have been observed indicating clearly that the reflection of the electrons, at least in some cases, is not diffuse. The most outstanding example are the oscillations, first observed by Khaĭkin[1], of the surface impedance of a metal in weak (on the order of 1–10 Oe) magnetic fields. As shown by Nee and Prange[2], these oscillations can be explained only by assuming that the electrons responsible for the oscillations are reflected practically specularly from the boundary. The splendid agreement between theory and experiment (see[3]) confirms this assumption. Another example is the observation[4] of cyclotron resonances corresponding to electron motion along trajectories and accompanied by reflection from the surface of the metal. We note also that, as shown by Sharvin and Fisher[5], it is possible to produce and focus beams of conducting electrons in a metal.

The most significant fact is that possibilities are opening up presently for a quantitative experimental investigation of the real law governing the reflection of conduction electrons from the surface of a metal. This, in turn, will make it possible to proceed to study the properties of the metal surface itself from a principally new viewpoint. The point is that usually the structure of the surface is investigated with the aid of scattering of light, x-rays, or electrons incident on the surface from vacuum. The study of the scattering of conducting electrons (or other short-wave excitations) has, as we shall show below, a number of fundamental advantages connected with the fact that in this case we are dealing with scattering of quasiparticles of the crystal itself, which "sense" the crystal symmetry much better.

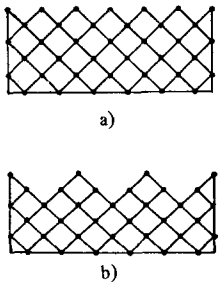

FIG. 1

1. REFLECTION FROM A PERFECT SURFACE

The law of reflection of conduction electrons depends, naturally, on the structure of the metal boundary and on the shape of the roughnesses. It is necessary to distinguish here between roughnesses that are inherent in a perfect surface (i.e., one in thermodynamic equilibrium), and random roughnesses connected with imperfection of the crystal.

We consider first the case of a perfect surface. Let the function $\xi(\rho)$ define the true shape of the crystal, i.e., the distances of the "extreme" atoms from the plane representing the median surface of the sample, ρ being a two-dimensional vector lying in this plane. The law governing the reflection of the electrons is closely related to the properties of the translational symmetry of the function $\xi(\rho)$.

Let us explain the situation first for the simplest case of a two-dimensional quadratic crystal lattice. We assume that the median plane of the sample surface (in this case a straight line) is perpendicular to the $\langle 11 \rangle$ direction. Figures 1a and 1b show two possible surfaces of this crystal with specified direction of the median line. It can be stated that in case 1a the surface has a natural translational symmetry of the given median direction. Indeed, all the crystal properties are periodic on a straight line parallel to the $\langle 11 \rangle$ direction, with a period equal to the diagonal of the unit cell (square). In the case of Fig. 1a, the crystal surface, and particularly the function $\xi(\rho)$, has a translational symmetry with the same period. To the contrary, in the case of the surface shown in Fig. 1b, the symmetry of the function $\xi(\rho)$ is lower than the symmetry of the median line of the surface. The period of the function $\xi(\rho)$ is twice as large as the diagonal of the square. A

lowering of the crystal symmetry occurs in this case on the surface.

In the general case, possible surface structures can be classified in accordance with whether there exists a natural translational symmetry of the given median plane or not, in the following manner. We consider the aggregate of all the possible Bloch functions of the crystal $u_{nk}\exp(ik\cdot r)$, the functions realizing the representations of the corresponding space group. Here k is the quasimomentum and n is the aggregate of the remaining quantum numbers. Any function of the coordinates in the crystal can be expanded in Bloch functions. The Bloch functions with zero value of the quasimomentum constitute the complete set of functions having the natural translational symmetry (periodicity) of the crystal. The presence of a nonzero quasimomentun, generally speaking, removes the natural symmetry of the function, but does not violate it in a plane perpendicular to the direction of the quasimomentum. It is therefore clear that if the crystal boundary has a natural median-plane symmetry, then the function $\xi(\rho)$ should be expandable in Bloch functions with zero projections of the quasimomentum on the median plane:

$$\xi(\rho)=\sum_{k_t=0} A_{nk}u_{nk}e^{ik\rho}, \qquad (1)$$

where the summation is over all values of n and over all k such that the tangential components relative to the median plane k_t vanish; A_{nk} are certain constants.

If the boundary of the crystal does not have a natural symmetry, then the expansion of the type (1) will also include terms with nonzero tangential components of the quasimomentum. The set of these quantities k_{t_1}, k_{t_2}, ... constitutes in this case one of the most important characteristics of the surface structure of the crystal.

We now proceed directly to an explanation of the laws governing the reflection of conduction electrons from the boundary. First, reflection should leave the electron energy unchanged. This follows from the fact that for electrons located near the Fermi surface, at sufficiently low temperatures, the reflection problem is a single-particle problem, i.e., the electron is a good quasiparticle during the entire process of interaction with the surface. Indeed, the single-particle character of the problem could be violated only by processes wherein the quasiparticle in question decayed into other excitations (at zero temperature). It is known that for electrons in the interior of a crystal the probability of such processes is arbitrarily small if the electron energy is sufficiently close to the Fermi energy. The proof of this statement is obtained by using only the energy conservation law and the Pauli principle, both of which also remain valid in the presence of a surface (only the momentum conservation law drops out). It is therefore clear that the presence of a surface does not violate the single-particle character of the problem.

Let ψ_{inc} be the wave function of an electron incident on the surface, and ψ_{ref} the wave function of a reflected electron. In the general case they are connected with each other by a relation of the type

$$\psi_{ref}=\hat{F}(\rho)\psi_{inc}, \qquad (2)$$

where $\hat{F}(\rho)$ is a certain linear operator that depends on the coordinate on the median plane. If the surface has a natural symmetry of the median plane, then this operator has an expansion in Bloch functions of the type (1), containing only functions with $k_t = 0$. But this means that the wave functions of the incident and reflected electrons have the same values of the tangential components of the quasimomentum. We have thus obtained a conservation law for the tangential quasimomentum, completely analogous to the conservation law for the tangential momentum in the reflection of ordinary particles from a level surface. It is important to bear in mind, however, that this law is valid not for any perfect surface, but only for one having a natural symmetry. Thus, k_t is conserved for the structure shown in Fig. 1a but not for the structure of Fig. 1b.

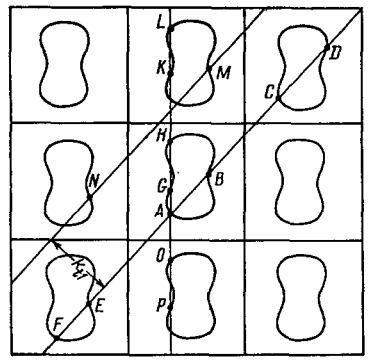

FIG. 2

Using the conservation laws for the energy and the tangential quasimomentum, we can easily determine all the possible states of the reflected electron. Let us draw the equal-energy surface corresponding to the energy of the incident electron and let us repeat it periodically over the entire reciprocal lattice (Fig. 2). Let the point A correspond to the state of the incident electron. We draw through the point A a straight line parallel to the direction of the normal to the surface of the crystal (this is the line k_t = const, line FD in the figure). The points B, D, E... are the intersections of the line with the equal-energy surfaces and determine the possible states of the reflected electron (the remaining intersection points C, F, ... correspond to electrons that move towards the surface and not away from it).

If the normal to the surface has a certain random (irrational) direction relative to the crystallographic axes, then even for a surface having a natural symmetry the number of possible states of the reflected electron is infinite, since all the points B. D, E, ... are in this case not equivalent. This fact is connected in final analysis with the circumstance that for an irrational direction even the most symmetrical surface in the usual sense of the word does not have any periodicity. If particles incident from vacuum were to be reflected from such a surface, we would not obtain any simple picture at all. For the conduction electrons there is a simple criterion that distinguishes surfaces with natural symmetry at any direction of the normal, namely, all the states of the reflected electron can be located on a definite straight line in the reciprocal lattice.

For rational directions of the surface, the number

of possible states of the reflected electron is finite, for in this case there exists only a finite number of nonequivalent intersection points. Thus, for a normal parallel to the line PL on Fig. 2 there are two such points (G and H). The points O, L, ... are equivalent to the point H, and the points K, P, ...to the point G.

If the surface does not have natural symmetry, and is characterized by the aforementioned set of two-dimensional vectors $\mathbf{k}_{t_1}, \mathbf{k}_{t_2}, \ldots$, then the expansion of the operator $\hat{F}(\rho)$ in Bloch functions has the following form:

$$\hat{F}(\rho) = \sum_{\mathbf{k}_t=0} \hat{f}^{(0)}_{n\mathbf{k}} u_{n\mathbf{k}} e^{i\mathbf{k}\rho} + \sum_{\mathbf{k}_t=\mathbf{k}_{t_1}} \hat{f}^{(1)}_{n\mathbf{k}} u_{n\mathbf{k}} e^{i\mathbf{k}\rho} + \sum_{\mathbf{k}_t=\mathbf{k}_{t_2}} \hat{f}^{(2)}_{n\mathbf{k}} u_{n\mathbf{k}} e^{i\mathbf{k}\rho} + \ldots,$$

where $\hat{f}^{(0)}_{n\mathbf{k}}, \hat{f}^{(1)}_{n\mathbf{k}}, \hat{f}^{(2)}_{n\mathbf{k}}$ are certain operators that do not depend on ρ. It is seen from (2) that in this case, besides reflection with conservation of $\mathbf{k}_t$, a change of the tangential quasimomentum, equal to the vectors $\mathbf{k}_{t_1}, \mathbf{k}_{t_2}, \ldots$, is possible. Each of these vectors corresponds to its own straight line parallel to the line $\mathbf{k}_t$ = const. The points of intersection of all the lines with the equal-energy surfaces determine the possible states of the reflected electrons. Thus, if the state of the incident electron is represented by the point A in Fig. 2 (the normal to the boundary is parallel to the lines FD and MN) and there is one nonvanishing $\mathbf{k}_{t_1}$, then the reflections at M, N, ... are possible in addition to the reflections at B, D, E ....

An experimental study of the law governing the reflection of conduction electrons thus makes it possible to determine directly the set of vectors $\mathbf{k}_{t_1}, \mathbf{k}_{t_2}, \ldots$, which determine the structure of the surface. It should be noted that one and the same crystal can have a surface with natural symmetry for some directions of the normal, and without such symmetry for other directions. In addition, when the temperature or the pressure is changed, unique phase transitions are possible, wherein nothing happens in the interior of the crystal and only the symmetry properties of the surface change. All such singularities can be easily explained if the law governing the electron reflection is known.

We note that we are considering throughout reflection of conduction electrons, although everything said here pertains to all other short-wave excitations of the crystal, and particularly to Debye phonons.

2. GLANCING ELECTRONS

The problem of calculating the angular dependence of the reflection coefficient can be solved in the general case for any surface (perfect or not) in the important case when the velocity of the incident electron is almost parallel to the surface (glancing electron). This problem is analogous in many respects to the well known problem of scattering of slow particles in quantum mechanics (see[6]). We emphasize that inasmuch as the quasimomentum does not have the same direction as the velocity, the direction of the quasimomentum of a glancing electron is perfectly arbitrary.

If the reflection of the glancing electron occurs with conservation of the tangential quasimomentum, then one of all the possible states of the reflected electrons has a quasimomentum close to that of the incident electron. Indeed, since the velocity is normal to the equal-energy surface, it is clear that the straight line $\mathbf{k}_t$ = const is almost perpendicular to this normal and crosses the equal-energy surface a second time at a close point. The transition of the electron to this point upon reflection corresponds to specular reflection with a small change of the quasimomentum. It is precisely such a reflection which occurs with overwhelming probability, as we shall show, for a glancing electron reflected from an arbitrary surface of the metal, when, generally speaking, there is no conservation of $\mathbf{k}_t$.

We are interested in the probability of specular reflection only. We consider, accordingly, the electron wave function ψ describing the "mirror reflection channel," in analogy with the introduction of a wave function describing the "input channel" in the theory of inelastic scattering (see[6]). The process of reflection into any other state are analogous in such a description to inelastic processes.

We regard the electron energy $\epsilon(\mathbf{k})$ as a function of $k_x \equiv k$ (the x axis is normal to the surface of the metal, which in turn occupies the region $x < 0$ at a fixed $\mathbf{k}_t$ equal to the value of the tangential momentum of the incident electron. Since the incident electron is glancing and the reflection is accompanied by a small change of momentum, an important role is played by the small region of values of k near a certain value k_0 corresponding to zero velocity component normal to the surface

$$\frac{\partial \varepsilon}{\partial k}\Big|_{k=k_0} = 0.$$

Expanding the energy ϵ in powers of $(k - k_0)$, we obtain

$$\varepsilon = \varepsilon_0(\mathbf{k}_t) + \hbar^2 \frac{(k-k_0)^2}{2m}, \tag{3}$$

where m is a certain effective mass.

This is the form that the electron energy takes far from the boundary. On approaching the boundary, the potential energy U of the interaction between electron and the boundary becomes important. If it is assumed that the characteristic dimension of the roughnesses is of the order of the interatomic distance a, then for $|x| \gg a$ the influence of the roughnesses becomes smoothed out and the potential energy depends only on x. The electron energy is thus equal to

$$\varepsilon = \varepsilon_0(\mathbf{k}_t) + \hbar^2 \frac{(k-k_0)^2}{2m} + U(x),$$

and we can write the following equation for the x-dependent part of the wave function:

$$\left\{\left(i\frac{d}{dx} + k_0\right)^2 + \frac{2m}{\hbar^2}[\varepsilon_0 + U(x) - \varepsilon]\right\}\psi = 0.$$

Introducing a new unknown function $\varphi = \psi \exp(-ik_0 x)$, we transform the last equation into

$$\frac{d^2\varphi}{dx^2} + \left[q^2 - \frac{2m}{\hbar^2}U(x)\right]\varphi = 0, \tag{4}$$

where $\hbar q = \sqrt{2m(\epsilon - \epsilon_0)} = mv_x$, and v_x is the incident-electron velocity component normal to the surface. The condition $qa \ll 1$ is satisfied for a glancing electron.

In the region $1/q \gg |x| \gg a$ we can neglect the two last terms of (4). If this is done we get, in fact,

$$\varphi(x) = A + Bx. \tag{5}$$

where A and B are constants that depend on the structure of the metal boundary.

If we now regard the discarded terms as a perturbation, we readily see that the first of them makes a contribution of the order of $(qx)^2 \ll 1$, and the second of the order $(a/|x|)^{n-2}$, if $U(x) \sim |x|^{-n}$. This contribution is also small if the potential energy decreases more rapidly than x^{-2}, a condition always satisfied in practice.

It is important that the ratio of the constants A and B at small values of q is independent of q. This is clear from the fact that even when $|x| \ll x_0$, where x_0 is given by the equation $\hbar^2q^2 \sim mU(x_0)$ $(x_0 \gg a)$, we can neglect the term q^2 in (4) compared with the potential energy. The quantity q does not enter in the equation at all at such values of x, and all the more when $|x| \sim a$.

When $|x| \gg a$, we can neglect in (4), generally speaking, only the last term. The solution can then be written in the form

$$\varphi(x) = e^{iqx} + Ve^{-iqx}, \tag{6}$$

where V(q) is the sought reflection coefficient. From the condition for "joining" formulas (5) and (6) at $qx \ll 1$, we get

$$V = -1 + \alpha q, \tag{7}$$

where $\alpha = 2iA/B = \alpha' + i\alpha''$.

The probability of specular reflection is determined by the square of the modulus of the reflection coefficient

$$|V|^2 = 1 - 2\alpha' q = 1 - 2\alpha' \frac{mv_x}{\hbar}.$$

Its deviation from unity is thus proportional to the first power of the velocity v_x, or, equivalently, to the first power of the small angle between the electron velocity and its projection on the plane of the metal boundary. For a boundary with atomic-size roughnesses, the parameters α' and α'' have the same order of magnitude as the interatomic distance.

It is important to note that the derivation of (7) was based essentially on two assumptions, first the existence of a channel for specular reflection with a small change of the quasimomentum (small q), and second the possibility of expanding $\epsilon(k)$ in a power series. The first assumption is satisfied not only by glancing electrons but also by electrons belonging to small groups, i.e., in the case when one deals with a small closed section of the Fermi surface. If the function $\epsilon(k)$ is analytic in the corresponding section of k-space (the small group has in this case a quadratic spectrum), then even the reflection of nonglancing electrons is described by formula (7). In the opposite case, for example in the case of bismuth, a special analysis is necessary, with allowance for the concrete form of the singularity. The special sensitivity of the problem to the analytic properties of the function $\epsilon(k)$ is connected with the presence of a classical turning point $V(x_0) = \epsilon$ near the surface.

We assume now that the metal boundary has, besides the atomic roughnesses, also random macroscopic irregularities. In the calculation of the influence of the latter on the electron reflection coefficient, we can neglect the small quantities αq connected with the atomic-size roughnesses. It is then seen from (6) and (7) that the boundary can be considered purely macroscopically, and we can write for it in the condition $\psi = \varphi = 0$. We emphasize that such an approach is valid only for glancing electrons or for small groups with a quadratic spectrum. In the general case the atomic-size roughnesses, which always accompany the macroscopic irregularities, cannot be disregarded.

The boundary condition $\psi = 0$ was used to investigate the interaction of conduction electrons with a rough metal boundary by Greene and O'Donnell[7], Chaplik and Éntin[8], Kaner, Makarov and Fuks[9], Fal'kovskiĭ[10,11], Singhal[12], and Makarov and Fuks[13].

If the amplitude of the irregularities is not too large, then their influence on the motion of the electron can be accounted for by perturbation theory. Let the function $x = \xi(\rho)$, where $\rho = (y, z)$, describe the surface of a metal with random macroscopic irregularities. Choosing the average surface as the $x = 0$ plane, we can always make the average of the random quantity $\xi(\rho)$ equal to zero. The statistical properties of the surfaces are described by the binary correlation function

$$\overline{\xi(\rho)\xi(\rho')} = d^2w(\rho - \rho'), \tag{8}$$

where $d = \sqrt{\overline{\xi^2}}$ is the rms height of the irregularities, and $w(\rho)$ is a correlation function satisfying the condition $w(0) = 1$ and decreasing significantly at distances l on the order of the characteristic "wavelength" of the irregularities.

We rewrite the boundary condition $\psi(\xi, \rho) = \varphi(\xi, \rho) = 0$, by expanding in powers of ξ accurate to terms of second order inclusive:

$$\varphi(\rho) + \frac{\partial\varphi}{\partial x}\xi(\rho) + \frac{1}{2}\frac{\partial^2\varphi}{\partial x^2}\xi^2(\rho) = 0, \tag{9}$$

where all the quantities are taken at $x = 0$.

In the zeroth approximation in ξ, the wave function takes, in accord with (6), (7), and (8), the form

$$\varphi = e^{ik_t\rho}\{e^{iq(k_t)x} - e^{-iq(k_t)x}\},$$

where $\hbar q(k_t) = mv_x$ is a function of the tangential momentum k_t at a fixed energy. In the next-higher approximations, the wave function contains reflected waves with different values of the tangential momentum. However, by virtue of the fact that $\xi(\rho)$ changes little over atomic distances, the momenta of the incident and reflected electrons should be close to each other. Transitions to other sections of the Fermi surface are therefore impossible, so that the connection between the normal and tangential quasimomenta is determined by one and the same function $q(k_t)$. We seek the wave function in the form

$$\varphi = e^{ik_t\rho}\{e^{iq(k_t)x} - e^{-iq(k_t)x}\} + \int \frac{d^2k_t'}{(2\pi)^2} F(k_t')\, e^{ik_t'\rho - iq(k_t')x}, \tag{10}$$

where $F(k_t)$ is an unknown function. Substituting (10) in the condition (9) and using successive approximations, we obtain in the second approximation

$$F(k_t') = -2iq(k_t)\xi(k_t - k_t') + 2q(k_t)\int \frac{d^2k_t''}{(2\pi)^2} q(k_t'')\xi(k_t - k_t'')\xi(k_t'' - k_t'); \tag{11}$$

here $\xi(k_t)$ is the Fourier component of the function $\xi(\rho)$:

$$\xi(\rho) = \int \frac{d^2k_t}{(2\pi)^2}\xi(k_t)\, e^{ik_t\rho}.$$

To calculate the wave function averaged over the ensemble of functions ξ, we substitute (11) in (10) and average the terms quadratic in ξ in accordance with (8). The linear terms vanish upon averaging. As a result we obtain

$$\overline{\varphi} = e^{ik_t\varrho}\{e^{iq(k_t)x} + V(\mathbf{k}_t)\, e^{-iq(k_t)x}\},$$

where the reflection coefficient is equal to

$$V(\mathbf{k}_t) = -1 + \frac{d^2}{2\pi^2}\, q(\mathbf{k}_t) \int d^2\mathbf{k}_t' q(\mathbf{k}_t')\, w(\mathbf{k}_t' - \mathbf{k}_t), \qquad (12)$$

$w(\mathbf{k}_t)$ is the Fourier component of the correlation function, which determines the distribution of the inhomogeneities over the "wavelength" and is normalized by the condition

$$\int \frac{d^2\mathbf{k}_t}{(2\pi)^2}\, w(\mathbf{k}_t) = 1. \qquad (13)$$

A formula similar to (12) for the formally identical problem of scattering of electromagnetic waves by an uneven surface was obtained by Bass [14].

Since the inhomogeneities in question have characteristic dimensions greatly exceeding the interatomic distance, the function $w(\mathbf{k}_t)$ differs from zero only at small values of the argument. Therefore, if $q(\mathbf{k}_t)$ is not too small, namely $q(\mathbf{k}_t) \gg (la)^{-1/2}$, we can replace $w(\mathbf{k}_t)$ in formula (12) by $(2\pi)^2 \delta(\mathbf{k}_t)$. We then have

$$V = -1 + 2(qd)^2. \qquad (14)$$

In the inverse limiting case $q(\mathbf{k}_t) \ll (la)^{-1/2}$, we can put $q(\mathbf{k}_t) = 0$ when calculating the integral in (12). The dependence of q on $\mathbf{k}_t'$ can easily be determined by expanding the quantity $\epsilon_0(\mathbf{k}_t')$ in (3) in powers of $\mathbf{k}_t' - \mathbf{k}_t$, i.e., by putting $\epsilon_0(\mathbf{k}_t') = \hbar \mathbf{v}_t(\mathbf{k}_t' - \mathbf{k}_t)$, where $\mathbf{v}_t$ is the tangential component of the incident-electron velocity. As a result we obtain

$$\hbar q(\mathbf{k}_t') = \sqrt{2m\hbar \mathbf{v}_t(\mathbf{k}_t' - \mathbf{k}_t)}.$$

Substituting this in (12) and carrying out the simple integration, we obtain the reflection coefficient (the function w is assumed to be isotropic):

$$V = -1 + v_x d^2 (1 + i) \left(\frac{16m^3 v_t}{\pi^3\hbar^3 l}\right)^{1/2} \Gamma^2\left(\frac{3}{4}\right) \int_0^\infty \varkappa^{3/2} f(\varkappa)\, d\varkappa, \qquad (15)$$

where $\Gamma(x)$ is the gamma function; we have introduced in place of w the corresponding dimensionless function $f(\kappa) = (2\pi l^2)^{-1} w(\kappa/l)$ of the dimensionless argument κ, so that the integral in (15) is of the order of unity.

Formula (15) shows that for extremely glancing electrons the probability of nonspecular reflection, in accord with the general formula (7), is proportional to the first power of the normal velocity component. Comparison of formulas (15) and (7) also shows that the constant α, which characterizes the macroscopic inhomogeneities of the boundary, is of the order of $d^2/(la)^{1/2}$. Thus, if the macroscopic inhomogeneities are such that $d^4/l \gg a^3$, then they make the main contribution, and the reflection coefficient is determined by formula (15). In the opposite limiting case, atomic-size roughnesses, which are always present on the macroscopically uneven boundary, become more significant, and the reflection coefficient is determined by formula (7) with $\alpha \sim a$.

As shown above, formula (12) can also be used for nonglancing electrons, if one deals with the reflection of electrons belonging to small (regular) groups. For irregularities with characteristic "wavelength" l much larger than the inverse parameter $(2p_0)$ of the Fermi-surface section corresponding to the group under consideration, formulas (14) and (15) remain valid as before, the former holding when $q \gg (p_0/l)^{1/2}$, and the latter when $q \ll (p_0/l)^{1/2}$. Since p_0 is much smaller than the reciprocal interatomic distance, the inequality $p_0 l \ll 1$ may be realized for the macroscopic irregularities. We then obtain from (12) the following expression for the reflection coefficient (the effective mass m is assumed for simplicity to be isotropic):

$$V = -1 + v_x d^2 \frac{2m}{\hbar l}\left\{\frac{1}{3}(p_0 l)^3 f(0) + i\int_0^\infty \varkappa^2 f(\varkappa)\, d\varkappa\right\}. \qquad (16)$$

The probability of nonspecular reflection is determined mainly by the real part of the coefficient V. Comparison of (16) with (7) shows that in this case the contribution of the atomic roughnesses to the indicated probability can be neglected if $d^2 l^2 \gg a/p_0^3$.

Fal'kovskii [10] derived for the distribution function of glancing electrons a boundary condition that describes their interaction with a rough metal surface, and used the result to investigate the influence of the surface properties on the high-frequency impedance of a metal in the absence of a magnetic field. Under strongly anomalous skin-effect conditions, when the electron mean free path $(v\tau)$ greatly exceeds the depth δ of the skin layer, the main contribution to the impedance is made, as is well known [15], by the glancing electrons. Since the law of reflection of glancing electrons is close to specular, the surface impedance Z is close to the known value Z_0 (see [15]) calculated for a rigorously specular boundary, and differs from it by an amount

$$Z - Z_0 \sim Z_0 \frac{d^2}{l^{1/2} a^{3/2}} \frac{\delta}{v\tau}$$

when $v\tau/\delta \gg (l/a)^{1/2} \ln(l/a)$ and

$$Z - Z_0 \sim Z_0 \left(\frac{v\tau d}{\delta l}\right)^2 \ln\left\{\frac{\delta}{v\tau}\left(\frac{l}{a}\right)^{1/2}\right\}$$

when $v\tau/\delta \ll (l/a)^{1/2} \ln(l/a)$.

The surface impedance is connected in a strictly defined manner with the surface characteristics l and d.

3. WIDTHS OF MAGNETIC SURFACE LEVELS

The surface-impedance oscillations of a metal in a weak magnetic field, observed by Khaĭkin [1], are resonances corresponding to transitions between different magnetic surface levels [2]. These levels appear for a glancing electron moving near the surface of a metal in a magnetic field along a trajectory of the type shown in Fig. 3. The sections of trajectories between successive collisions with the boundary are approximately circles with radius $R = v_y/\Omega$, where $\Omega = eH/mc$, m is the effective mass that enters in formula (3), and the magnetic field is directed along the z axis. The area of the segment shown shaded in the figure is equal to $(2/3)R^2\theta^3$. According to the quasiclassical quantization rule, the magnetic flux through this area should equal an integer number (n) of flux quanta

$$\frac{2}{3} R^2\theta^3 H = \frac{2\pi\hbar c}{e} n,$$

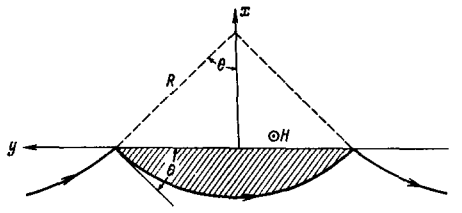

FIG. 3

from which we obtain the possible values of the angle θ:

$$\theta_n = \left(3\pi \frac{\hbar\Omega}{mv_y^2} n\right)^{1/3}. \quad (17)$$

The energy levels are obtained by substituting in the formula $\epsilon = \epsilon_0(k_t) + \hbar^2 q^2/2m$ the values of q defined by $\hbar q = mv_y\theta$:

$$\varepsilon = \varepsilon_0(\mathbf{k}_t) + \left\{\frac{m}{2}\left(\frac{3\pi}{2} v_y \hbar\Omega n\right)^2\right\}^{1/3}. \quad (18)$$

Oscillations are observed in fields on the order of 1--10 Oe. According to (17), such values of the magnetic field correspond to angles $\theta \sim 10^{-2}$--10^{-3}, so that we are indeed dealing with glancing electrons.

Perfectly defined values of (18) for the energy levels were obtained assuming complete specular reflection of the electrons from the boundary. Actually the electron always has a nonzero probability of nonspecular reflection, and consequently the exact stationary levels are transformed into quasistationary ones with a finite decay probability, i.e., finite width.

The widths of magnetic surface levels for a metal with a rough boundary were calculated by Prange and Nee [16], Kaner, Makarov, and Fuks [9], Fischbeck and Mertsching [17], and Singhal [12]. The most consistent and complete theory was developed by Fal'kovskiĭ [9], and then by Makarov and Fuks [13].

To establish a quantitative connection between the width of the magnetic surface levels and the electron reflection coefficient, it suffices to compare the wave function Ve^{-iqx} of the reflected electron with its value $-e^{-iqx}$ in the case of total specular reflection, i.e., in the case when the condition $\psi = 0$ is satisfied on the boundary. We see that as a result of a single reflection the wave function acquires an additional factor $(-V)$. In a time t, the electron experiences $N = t/T$ reflections, where $T = 2\theta/\Omega$ is the time between collisions with the surface, and therefore the additional factor in the wave function is equal to

$$(-V)^N = e^{N\ln(-V)} \approx e^{-N(1+V)} = \exp\left\{-i\frac{t}{\hbar}\left[\frac{\hbar\Omega}{2i\theta}(1+V)\right]\right\}.$$

We have used here the fact that the coefficient V for the glancing electrons is close to -1. Since the wave function is proportional to $\exp(-i\epsilon t/\hbar)$ (ϵ is the energy), it follows that the additional factor is equivalent to the addition of the complex quantity $[(\hbar\Omega)/(2i\theta)](1 + V)$ to the energy. Its imaginary part determines the sought level width

$$\gamma = \frac{\hbar\Omega}{2\theta}\operatorname{Re}(1+V). \quad (19)$$

In addition, a change takes place in the real part of the energy, i.e., a level shift by an amount

$$\delta\varepsilon = \frac{\hbar\Omega}{2\theta}\operatorname{Im}(1+V). \quad (20)$$

Substituting the reflection coefficient in the form (7), in (19) and (20), we obtain

$$\gamma = \frac{mv_y\alpha'}{2}\Omega, \quad \delta\varepsilon = \frac{mv_y\alpha''}{2}\Omega, \quad (21)$$

from which we see that the roughnesses of the atomic scale lead to a level broadening and shift proportional to the first power of the magnetic field. The broadening and shift due to the macroscopic irregularities, for sufficiently weak magnetic fields $\Omega \ll (a/l)^{3/2}(\epsilon_F/n\hbar)$, are also proportional to the first power of H. Indeed, in this case, as seen from (17), the angles θ are small compared with $(a/l)^{1/2}$ and we can use formula (15) for the reflection coefficient. As a result we obtain

$$\gamma = \delta\varepsilon = \Omega d^2\left(\frac{4m^3v_tv_y^2}{\pi^3\hbar l}\right)^{1/2}\Gamma^2\left(\frac{3}{4}\right)\int_0^\infty \varkappa^{3/2} f(\varkappa)\, d\varkappa. \quad (22)$$

If $\Omega \gg (a/l)^{3/2}(\epsilon_F/n\hbar)$, then substitution of the coefficient V from (14) in (19) yields

$$\gamma = \Omega^{4/3}\left(\frac{3\pi n}{\hbar^2} m^5 v_y^4\right)^{1/3} d^2. \quad (23)$$

The level shift is in this case much smaller than the width.

For formula (23) to be valid, it is actually necessary to impose an additional upper bound on the field, $\Omega \ll (\hbar v_t n/ml^3)^{1/2}$. The point is that when $\Omega \gtrsim (\hbar v_t n/ml^3)^{1/2}$ the path v_tT traversed by the electron between successive collisions with the metal surface becomes of the same order as or smaller than the correlation length l. The condition of statistical independence of the different collisions of the electron with the surface, assumed in the derivation of formulas (19) and (20), is then violated. If there is a correlation between the different collisions, then there is no direct connection between the level width and the reflection coefficient. Nonetheless, the width can be expressed in terms of the correlation function of the irregularities $f(\kappa)$. In the limiting case $\Omega \gg (\hbar v_t n/ml^3)^{1/2}$, calculations (see [11,13]) lead to the following formula:

$$\gamma = 2\pi\Omega^2 l\frac{(mv_y d)^2}{\hbar v_t}\int_0^\infty f(\varkappa)\, d\varkappa. \quad (24)$$

Thus, when the field is increased, the level width due to the macroscopic irregularities is at first proportional to H, then to $H^{4/3}$, and finally to H^2.

When it comes to the magnetic surface levels of the electrons belonging to the small groups, for large-scale irregularities ($p_0 l \gg 1$) formula (22) is valid when $\Omega \ll (\hbar^2 p_0/m^2 l^3 n^2)^{1/2}$, formula (23) when $(\hbar^2 p_0/m^2 l^3 n^2)^{1/2} \ll \Omega \ll (\hbar^2 p_0 n/m^2 l^3)^{1/2}$, and formula (24) when $\Omega \gg (\hbar^2 p_0 n/m^2 l^3)^{1/2}$.

For small-scale macroscopic irregularities ($a \ll l \ll 1/p_0$), the level width and the shift are obtained by substituting (16) in (19) and (20):

$$\gamma = \frac{1}{3}\Omega(dl)^2 mv_y p_0^3 f(0), \quad \delta\varepsilon = \Omega d^2\frac{mv_y}{l}\int_0^\infty \varkappa^2 f(\varkappa)\, d\varkappa. \quad (25)$$

In this case the width is much smaller than the shift.

A quantitative experimental investigation of the width of magnetic surface levels was carried out by Koch and Murray [18] on gallium and tin samples. In the region of not too small values of the magnetic field, the measured width of the resonances varied quadratically with the magnetic field, in full agreement with

(24). In weaker fields, a weaker field dependence was observed, also in agreement with the predictions of the theory. In addition, a special investigation was made in[18] of the state of the surface (the parameters l and d were measured). Unfortunately, the Fermi surfaces of gallium and tin have not been investigated with sufficient thoroughness, so that measurements of the surface levels could lead only to estimates of the parameters of the energy spectra of the electrons responsible for the oscillations. There exist, however, a number of metals (for example, bismuth or copper), whose Fermi surfaces are fully known and for which oscillations in weak fields have been observed. Measurements of the level widths in such cases would lead to quantitative conclusions concerning the surface state of the metal.

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