INFLUENCE OF ROUGH BOUNDARY OF A METAL ON THE MAGNETIC SURFACE LEVELS

N. M. MAKAROV and I. M. FUKS

Institute of Radiophysics and Electronics, Ukrainian Academy of Sciences

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The influence of statistical surface roughnesses of the boundary of a metal on the spectrum and damping of the magnetic surface electron states is investigated by the Green's function technique. It is shown that the results of the phenomenological theory derived in a previous paper by Kaner and coworkers[7] follow from the general formulas of the microscopic theory by successive scattering acts of electrons by an uneven surface are independent of one another. The damping of the surface states first increases in proportion to the magnetic field strength H and then in proportion to $H^{4/3}$. In the opposite limiting case of strong correlation of the successive reflections, the damping is proportional to H^2. Formulas are derived for the level shift of the surface electrons, and an illustrative physical interpretation of the results is presented.

1. INTRODUCTION

IN 1960, M. Khaĭkin observed oscillations of the surface impedance of metals in weak magnetic fields[1]. Subsequently, Nee and Prange[2] explained this phenomenon as being the result of transitions under the influence of a high-frequency field between magnetic surface levels. In a constant and homogeneous magnetic field **H** parallel to the boundary of the sample, the electrons whose orbit centers lie outside the metal at a distance approximately equal to the radius of the electron trajectory are reflected many times from the surface and drift along it (Fig. 1). Such electrons are called skipping. Their motion along the normal to the interface between the metal and the vacuum is finite and periodic and is therefore quantized. The quantum states of the skipping electrons are called magnetic surface levels. The oscillations of the impedance in a weak field actually constitute cyclotron resonance with the magnetic surface levels.

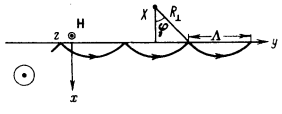


FIG. 1

The possibility of such a treatment of the oscillations is based on the fact that the reflection of the electrons should be specular. In other words, the metal-vacuum interface should be an ideal plane. Random irregularities on the surface of the metal, even microscopic ones, lead to a partly diffuse scattering of the skipping electrons. The result is an additional shift and an additional damping of the magnetic surface levels, causing the resonance to become smeared out. The damping due to the scattering of the electrons by the surface of the metal is a function of the magnetic field and of the microscopic parameters of the boundary of the sample (the heights and lengths of the roughnesses). Therefore the surface damping can be separated from the ordinary volume damping. We note that recently there appeared experimental papers (e.g.,[3,4]) devoted to a clarification of the dependence of the surface damping of the electronic states on the magnitude of the magnetic field H. The undoubted interest in the study of the influence of the roughness of the boundary on the line shape of the Khaĭkin oscillations is connected with the possibility of the investigation of the fine structure of metallic surfaces.

A qualitative discussion of this question is contained in[5,6]. Subsequently, a detailed analysis was presented by Kaner and the authors[7]. That paper is based on the fact that in the quasiclassical approximation the average wave function of the electron at the surface of the metal can be represented in the form of a sum of two plane waves—incident and reflected—with a known reflection coefficient V that depends on the microscopic parameters of the boundary. It should be noted that such an approach to the problem, although sufficiently evident, requires proof and a derivation on the basis of a consistent microscopic theory. In the present paper we investigate by the Green's function method the influence of the statistical roughnesses of the boundary of the metal on the spectrum and damping of the magnetic surface electronic states. This makes it possible to obtain not only rigorous criteria for the validity of the results of[7] and to obtain for them a clear physical interpretation, but also to investigate in detail those limiting cases when the phenomenological approach developed in[7] is not applicable. This is all the more necessary also because certain conclusions of a recent paper by Fal'kovskiĭ[8] contradict the results of[7].

The question of scattering of electrons by a rough boundary of a sample is closely connected with the problem of diffraction of waves by statistically rough surfaces. By now, a number of new solutions of this problem were obtained by using methods that take multiple scattering of waves into account[9,10]. The fact that the change of the spectrum is the consequence of multiple scattering of electrons by a surface makes it possible to use the methods of diffraction theory, developed in particular for the problem of the change of the spectrum of natural modes in a rough waveguide[11].

2. FORMULATION OF PROBLEM. AVERAGE GREEN'S FUNCTION

We consider a metal bounded by an uneven surface

$x = \xi(\mathbf{r})$. We shall assume the roughnesses to be random, and the constant and homogeneous magnetic field **H** to be parallel to the averaged sample surface x = 0 (the yz plane). The x axis is directed towards the interior of the metal, and the z axis along the **H** vector. The planar radius vector **r** has coordinates y and z (Fig. 2).

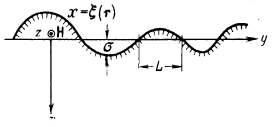


FIG. 2

By $\xi(\mathbf{r})$ we mean a random function of the vector **r** with zero mean value

$$\langle \xi(\mathbf{r}) \rangle = 0. \tag{2.1}$$

Assuming the roughnesses to be statistically homogeneous, we can write the binary correlation function $\langle \xi(\mathbf{r})\xi(\mathbf{r}') \rangle$ in the form

$$\langle \xi(\mathbf{r})\xi(\mathbf{r}') \rangle = \sigma^2 \mathscr{W}(\mathbf{r}-\mathbf{r}'), \tag{2.2}$$

where $\sigma = \langle \xi^2(\mathbf{r}) \rangle^{1/2}$ is the rms height of the roughnesses (variance), $\mathscr{W}(\mathbf{r})$ is the correlation function. From the definition (2.2) it follows that $\mathscr{W}(0) = 1$, $\mathscr{W}(-\mathbf{r}) = \mathscr{W}(\mathbf{r})$, and finally $\nabla\mathscr{W}(\mathbf{r}) = 0$ when $\mathbf{r} = 0$. In addition, the function $\mathscr{W}(\mathbf{r})$ tends to zero as $r \to \infty$. The latter property follows from the obvious fact that at large distances the heights of the roughnesses do not correlate. We introduce the characteristic correlation radius L, the horizontal dimension of the inhomogeneities. We define it as the distance over which the function $\mathscr{W}(\mathbf{r})$ decreases appreciably.

1. The problem of determining the spectrum of the surface electronic states reduces to finding the Green's function of the Schrödinger equation averaged over the ensemble of realizations of the random function $\xi(\mathbf{r})$. Assuming for simplicity the electron dispersion law to be quadratic and isotropic, we obtain for the Green's function $\mathscr{G}(x, \mathbf{r}; x_0, \mathbf{r}_0)$ the following equation

$$\left[-\frac{\hbar^2}{2m}\Delta - i\hbar\Omega x\frac{\partial}{\partial y} + \frac{m\Omega^2}{2}x^2 - \varepsilon \right] \mathscr{G}(x, \mathbf{r}; x_0, \mathbf{r}_0) = -\delta(\mathbf{r}-\mathbf{r}_0)\delta(x-x_0) \tag{2.3}$$

with boundary conditions

$$\mathscr{G}(x \to \infty, \mathbf{r}; x_0, \mathbf{r}_0) = 0, \quad \mathscr{G}(x = \xi(\mathbf{r}), \mathbf{r}; x_0, \mathbf{r}_0) = 0. \tag{2.4}$$

We have introduced here the following notation: ϵ—energy, m—effective mass, $\Omega = eH/mc$—cyclotron frequency, e—absolute value of the electron charge, $2\pi\hbar$—Planck's constant, c—velocity of light. The vector potential of the magnetic field **H** is chosen in the form $\mathbf{A} = \{0, Hx, 0\}$.

Let the surface of the metal $x = \xi(\mathbf{r})$ differ little from the plane x = 0. Then the second boundary condition can be expanded in terms of the small parameter ξ:

$$\mathscr{G}(0, \mathbf{r}; x_0, \mathbf{r}_0) + \xi(\mathbf{r})\mathscr{G}'(0, \mathbf{r}; x_0, \mathbf{r}_0) = 0, \tag{2.5}$$

where the prime denotes the partial derivative with respect to x. The approximate boundary condition (2.5) approximates well the exact condition if its first term is much larger than the second. To this end it is necessary that the "projection" of the de Broglie wavelength of the electron on the x axis, which equals $1/k_x$, be much larger than the characteristic height σ of the roughnesses:

$$(k_x\sigma)^2 \ll 1. \tag{2.6}$$

We note incidentally that the boundary condition (2.5) appears also when account is taken of the interaction of the electrons with the surface short-range scattering centers (see, e.g., [12]).

2. Before we proceed to determine the average Green's function, let us find the Green's function of the unperturbed problem, in which the metal-vacuum interface is the plane x = 0. This function $\mathscr{G}_0(x, \mathbf{r}; x_0, \mathbf{r}_0)$ should satisfy equation (2.3) and the boundary conditions (2.4) and (2.5) with $\xi = 0$. From the spatial homogeneity of the unperturbed problem with respect to the variables **r** and $\mathbf{r}_0$ it follows that $\mathscr{G}_0$ depends only on the difference $\mathbf{r} - \mathbf{r}_0$. It can therefore be sought in the form of an expansion in plane waves:

$$\mathscr{G}_0(x, \mathbf{r}; x_0, \mathbf{r}_0) = \int_{-\infty}^{\infty} \frac{d^2\mathbf{p}}{(2\pi\hbar)^2} G_0(x, x_0; \mathbf{p}) \exp\left\{ \frac{i}{\hbar}\mathbf{p}(\mathbf{r}-\mathbf{r}_0) \right\},$$

where the two-dimensional momentum **p** with components p_y and p_z is canonically conjugate to the variable **r**. For the Green's function $G_0(x, x_0; \mathbf{p})$ we obtain from (2.3) the equation

$$\left[-\mu^2\frac{d^2}{dx^2} + \frac{1}{4}\left(\frac{x-X}{\mu}\right)^2 - \eta \right] G_0(x, x_0; \mathbf{p}) = -\delta(x-x_0)/\hbar\Omega, \tag{2.8}$$

where

$$\eta = \frac{\varepsilon - p_z^2/2m}{\hbar\Omega}, \qquad X = -\frac{cp_y}{eH}, \qquad \mu = \left(\frac{\hbar c}{2eH}\right)^{1/2}. \tag{2.9}$$

The quantity $\eta\hbar\Omega$ represents the energy of the transverse (to the vector **H**) motion of the electron, **X** is the projection of the coordinates of the center of rotation of the electron on the x axis (Fig. 1), and μ is the magnetic length.

The unperturbed Green's function $G_0(x, x_0; \mathbf{p})$ satisfying Eq. (2.8) with the condition $G_0 = 0$ at x = 0 and $x \to \infty$ can be found with the aid of two linearly independent solutions of the homogeneous equation (Eq. (2.8) without the right-hand side). One solution should equal zero on the unperturbed surface of the metal, and the second should vanish at $x \to \infty$. As a result we obtain

$$G_0(x, x_0; \mathbf{p}) = \frac{\Gamma(-\eta+1/2)}{\mu\hbar\Omega\sqrt{2\pi}} D_{\eta-1/2}^{-1}\left(-\frac{X}{\mu}\right) \cdot \times \begin{cases} D_{\eta-1/2}\left(\frac{x_0-X}{\mu}\right)\mathscr{D}(x) & \text{for } x < x_0, \\ D_{\eta-1/2}\left(\frac{x-X}{\mu}\right)\mathscr{D}(x_0) & \text{for } x > x_0; \end{cases} \tag{2.10}$$

$$\mathscr{D}(x) = D_{\eta-1/2}\left(\frac{x-X}{\mu}\right)D_{\eta-1/2}\left(\frac{X}{\mu}\right) - D_{\eta-1/2}\left(-\frac{x-X}{\mu}\right)D_{\eta-1/2}\left(-\frac{X}{\mu}\right).$$

Here $\Gamma(x)$ is the Euler Gamma function, and the functions of the parabolic cylinder $D_{\eta-1/2}((x-X)/\mu)$ and $D_{\eta-1/2}(-(x-X)/\mu)$ are two linearly independent solutions of the homogeneous equations (2.8), with $D_{\eta-1/2}((x-X)/\mu)$ vanishing at $x \to \infty$.

The poles of $G_0(x, x_0; \mathbf{p})$ correspond to the spectrum of the electrons in the problem with a smooth separation boundary and, according to (2.10), are determined by the equation

$$D_{\eta-1/2}(-X/\mu)=0. \quad (2.11)$$

At fixed values of X (the coordinates of the rotation center) the dispersion equation (2.11) gives the condition for the quantization of the transverse electron energy

$$\eta=\eta(n, X), \quad (2.12)$$

and at fixed positive η we obtain

$$X=X_n(\eta). \quad (2.13)$$

The quantum number n = 1, 2, 3, ... is the number of the zero of the parabolic-cylinder function. Equation (2.11) has real solutions (2.13) only for real $\eta \geq 1/2$. The roots lie in the following region of variation of X:

$$-2\mu\sqrt{\eta}<X<\infty, \quad (2.14)$$

and their number is equal to the integer part of $\eta + 1/2$ (n = 1, 2, 3, ... $[\eta + 1/2]$). In addition, at a fixed value of η, $X_n(\eta)$ increases with increasing n; the maximum value of the X coordinate is reached at $n_{max} = [\eta + 1/2]$. The meaning of the inequality (2.14) becomes physically obvious if it is recognized that $2\mu\sqrt{\eta} \equiv R_\perp$ is the radius of rotation of the electron in the plane perpendicular to the magnetic field H (Fig. 1). When $X < -R_\perp$, the electron trajectory is located entirely outside the metal, and consequently there exist no such states.

The unperturbed electronic states corresponding to the solutions of Eq. (2.11) are divided into two different groups. One of them is made up of electrons whose orbit centers lie in the interior of the metal at a distance larger than the radius $R_\perp$ of the orbit:

$$2\mu\sqrt{\eta}<X<\infty. \quad (2.15)$$

Such electrons are not scattered by the interface, and we shall call them volume electrons. The second group includes the "surface" electrons, which collide during each turn with the boundary of the sample (Fig. 1). The X coordinate of the surface electrons lies in the range

$$-2\mu\sqrt{\eta}<X<2\mu\sqrt{\eta}. \quad (2.16)$$

Among all the solutions (2.13) of Eq. (2.11), only one can be located in the interval (2.15). If at the same time η is a half-integer, then such a solution is $X = \infty$. Equation (2.11) has no volume solution if η lies far from half-integer values.

The spectrum of the unperturbed electronic states in the quasi-classical approximation was analyzed in detail in[7]. For volume electrons the X coordinate is proportional to $[-\ln(\eta - n + 1/2) + \text{const}]^{1/2}$, and for surface electrons the dispersion equation (2.11) is written in the quasi-classical approximation ($n \gg 1$) in the form

$$\eta\left[\arccos\left(-\frac{X}{2\mu\sqrt{\eta}}\right)+\frac{X}{2\mu\sqrt{\eta}}\left(1-\frac{X^2}{4\mu^2\eta}\right)^{1/2}\right]=\pi\left(n-\frac{1}{4}\right). \quad (2.17)$$

3. Let us turn to the determination of the average Green's function $\langle \mathcal{G}(x, r; x_0, r_0)\rangle$, the poles of which give the sought spectrum of the perturbed electronic states. It was shown in[9,10] that if the Green's function satisfies the boundary condition (2.5), then its mean value satisfies the following non-local boundary condition (see formula (10a) of[10])[1]:

$$\langle \mathcal{G}(0, \mathbf{r}; x_0, \mathbf{r}_0)\rangle+\int_{-\infty}^{\infty} d^2\mathbf{r}'\mathcal{M}(\mathbf{r}-\mathbf{r}')\langle \mathcal{G}'(0, \mathbf{r}'; x_0, \mathbf{r}_0)\rangle=0, \quad (2.18)$$

where $\mathcal{M}(\mathbf{r} - \mathbf{r}')$ is the analog of the mass operator, for which there is given in[10] a diagram technique perfectly analogous to that used in the theory of volume scattering. Since the roughnesses are statistically homogeneous and $\mathcal{M}$ depends on the difference $\mathbf{r} - \mathbf{r}'$, the average Green's function should also depend only on $\mathbf{r} - \mathbf{r}_0$. This circumstance enables us to seek it in the form (2.7). The Fourier component $\langle G(x, x_0; \mathbf{p})\rangle$ of the average Green's function should satisfy Eq. (2.8). We therefore represent it in the form of a sum of the particular solution $G_0(x, x_0; \mathbf{p})$ and the general solution of the homogeneous equation:

$$\langle G(x, x_0; \mathbf{p})\rangle = G_0(x, x_0; \mathbf{p}) - A(x_0; \mathbf{p}) D_{\eta-1/2}\left(\frac{x-X}{\mu}\right). \quad (2.19)$$

We note that expression (2.19) satisfies the requirement of regularity at $x \to \infty$. The unknown constant $A(x_0, \mathbf{p})$ is determined from the boundary condition (2.18), which in the momentum representation is written in the form

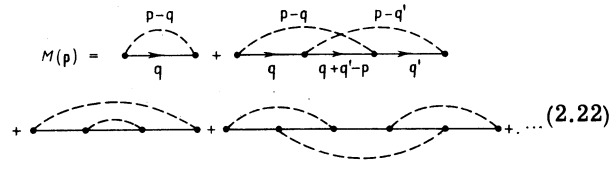
$$\langle G(0, x_0; \mathbf{p})\rangle + M(\mathbf{p})\langle G'(0, x_0; \mathbf{p})\rangle = 0. \quad (2.20)$$

Substituting (2.19) in (2.20) we obtain the final result for the average Green's function in the p representation

$$\langle G(x, x_0; \mathbf{p})\rangle = G_0(x, x_0; \mathbf{p}) - \frac{G_0'(0, x_0; \mathbf{p}) M(\mathbf{p}) D_{\eta-1/2}((x-X)/\mu)}{D_{\eta-1/2}(-X/\mu) + \mu^{-1} D'_{\eta-1/2}(-X/\mu) M(\mathbf{p})} \quad (2.21)$$

Here the prime at the parabolic-cylinder function denotes the derivative with respect to the argument.

In concluding this section, we present a graphic representation for the Fourier transform of the mass operator, which characterizes the expansion of M(p) in powers of σ^2:



(2.22)

We see that all the diagrams consist of three elements—a solid line, a dashed line, and a point. The dashed line is in correspondence with the Fourier component of the correlation function $\mathcal{W}(\mathbf{r})$:

$$\underset{\mathbf{p}}{\dashrightarrow} = W(\mathbf{p}) \equiv \int_{-\infty}^{\infty} \frac{d^2\mathbf{r}}{2\pi\hbar} \mathcal{W}(\mathbf{r}) \exp\left(-\frac{i}{\hbar}\mathbf{pr}\right). \quad (2.23)$$

We note that W(p) is an even, real, and positive-definite function. The solid line denotes the second derivative with respect to x and x_0 of the unperturbed Green's function at x_0, $x \to 0$, $x_0 > x$, multiplied by $\mu^2\hbar\Omega$. According to (2.10), this quantity is equal to

$$\underset{\mathbf{p}}{\longrightarrow} = -\frac{1}{\mu} D'_{\eta-1/2}\left(-\frac{X}{\mu}\right) \Big/ D_{\eta-1/2}\left(-\frac{X}{\mu}\right). \quad (2.24)$$

Finally, the point corresponds to the average height of the roughnesses σ, and also to the momentum conservation law: the sum of the momenta entering the point equals to the sum of the outgoing momenta; the sum of the momenta outgoing from the first point of each term in (2.22) and entering the last point should be equal to **p**. Integration $\int_{-\infty}^{\infty} d^2q/2\pi\hbar$ is carried out over all the

[1] In [9,10] this result was obtained for the Green's function of the Helmholz equation with the boundary condition (2.5). It is seen however from the derivation given in [10] that formula (2.18) is valid for the Green's function of any Hermitian differential operator of second order.

intermediate momenta q. Each diagram has an even number of points connected in succession by solid lines. In addition, the points are connected pairwise by dashed lines. It should be borne in mind here that the series (2.22) contained only such diagrams which cannot be broken up into two unconnected parts by breaking one solid line.

We note that (2.22) contains not only diagrams whose beginning and end are connected by a dashed line (diagrams of the first and third type). It follows therefore that Eq. (4.10) of[8] for the mass operator is inexact, and corresponds to allowance for only the simple vertex in the Feynman diagrams, namely, no account is taken of diagrams of the type of the second and fourth terms in (2.22). It is easy to show, however, that the second and third terms give, generally speaking, contributions of the same order to the series (2.22) for M(p). These terms are important for estimating the limits of applicability of the approximation employed below.

3. SPECTRUM AND DAMPING OF SURFACE ELECTRONIC STATES

1. According to formula (2.21), the dispersion equation for the determination of the spectrum of the electrons is given in our case by

$$D_{\eta-1/2}(-X/\mu)+\frac{1}{\mu}D'_{\eta-1/2}(-X/\mu)M(\mathbf{p})=0. \tag{3.1}$$

The quantization conditions are determined by the roots of this equation $\eta = \eta(n, X, p_z)$, which, generally speaking, do not coincide with the solutions (2.12) of the unperturbed Eq. (2.11). With the aid of (2.9) and the new rules for the quantization for η we can determine the spectrum of the electrons that are scattered by the rough boundary of the metal:

$$\varepsilon = \varepsilon_n(X, p_z) + \delta\varepsilon. \tag{3.2}$$

Here $\epsilon_n(X, p_z)$ are the unperturbed energy levels corresponding to the dispersion equation (2.11), and the complex quantity $\delta\epsilon$ determines the change of the spectrum (Re $\delta\epsilon$) and the damping ($-$ Im $\delta\epsilon$), due to the nonspecular reflection of the electrons. Assuming the shift and broadening of the levels to be much smaller than the distance between neighboring energy levels ($|\delta\epsilon| \ll |\epsilon_{n+1} - \epsilon_n|$), we shall solve (3.1) by the perturbation method. As a result we obtain for $\delta\epsilon$

$$\delta\varepsilon = -\hbar\Omega\frac{\partial\eta(n,X)}{\partial X}M(\mathbf{p}). \tag{3.3}$$

Thus, the determination of the correction $\delta\epsilon$ reduces to a calculation of the Fourier component of the mass operator. Within the framework of the assumptions made above we can confine ourselves in the series (2.22) for M(p) to the simplest (first) diagram:

$$M(\mathbf{p}) = -\frac{\sigma^2}{2\pi\hbar\mu}\int_{-\infty}^{\infty} d^2\mathbf{q}\, W(\mathbf{p}-\mathbf{q})\frac{D'_{\tilde{\eta}-1/2}(cq_y/\mu eH)}{D_{\tilde{\eta}-1/2}(cq_y/\mu eH)},$$
$$\hbar\Omega\tilde{\eta} = \varepsilon - q_z^2/2m. \tag{3.4}$$

We shall discuss below in detail the character of the approximations made thereby. The integrand in (3.4) has simple poles, which are determined by the zeroes of the function of the parabolic cylinder and, according to (2.14), lie in the region bounded by the inequalities

$$|q_z| \leqslant q_0 \equiv \left[2m\left(\varepsilon - \frac{\hbar\Omega}{2}\right)\right]^{1/2}, \quad -\infty < q_y \leqslant (2m\varepsilon - q_z^2)^{1/2}. \tag{3.5}$$

Taking this circumstance into account, we transform the integral (3.4) into

$$M(\mathbf{p}) = -\frac{\sigma^2}{2\pi\hbar\mu}\int_{-\infty}^{\infty} dq_z \int_{-\infty}^{\infty} dq_y\, W(p_y - q_y;\ p_z - q_z)\frac{D'_{\tilde{\eta}-1/2}(cq_y/\mu eH)}{D_{\tilde{\eta}-1/2}(cq_y/\mu eH)}$$
$$-i\frac{\sigma^2}{4\mu^2}\int_{-q_0}^{q_0} dq_z \sum_{n=1}^{[\tilde{\eta}+1/2]} W(p_y - q_y^n;\ p_z - q_z), \tag{3.6}$$

where q_y^n are the solutions of the unperturbed equation (2.11) at $\eta = \tilde{\eta}$ and $X = -cq_y/eH$. The first term in (3.6) determines the level shift Re $\delta\epsilon$, and the second the damping of the levels.

Since the influence of the surface of the sample on the spectrum of the volume electrons is exponentially small even in the case of a plane boundary[7], we shall investigate $\delta\epsilon$ only for surface electrons. It is seen from (3.6) that the damping of the surface electron states is determined by the sum of the probabilities of the transition due to scattering by the rough boundary both in the surface states ($|q_y^n| \leq (2m\epsilon - q_z^2)^{1/2}$) and in the volume ones, corresponding to the last term in the sum (3.6). Indeed, each term of this sum contains the factor $W(\mathbf{p} - \mathbf{q})$, which determines the probability of scattering from p into q in the Born approximation[13]. In the quasi-classical approximation, the summation in (3.6) can be carried out only over the poles corresponding to the surface states, since the probability of transition to volume states is exponentially small. In fact; the electron after colliding with the surface continues to move along a circular arc and ultimately again collides with the boundary of the sample. In other words, in the quasi-classical approximation scattering from the surface states leads only to transitions to surface states.

2. Let us proceed to investigate those limiting cases in which the general formula (3.6) can be greatly simplified. If the inequality

$$|\partial q_y^n/\partial n| \ll 2\pi\hbar/L \tag{3.7}$$

is satisfied, then in the sum (3.6) $W(p_y - q_y^n;\ p_z - q_z)$ is a slowly-varying function of the number n, making it possible to replace the sum in the quasi-classical approximation by the integral

$$\sum_n W(p_y - q_y^n;\ p_z - q_z) \approx -\int_{-\sqrt{2m\varepsilon - q_z^2}}^{\sqrt{2m\varepsilon - q_z^2}} dq_y \left(\frac{\partial q_y^n}{\partial n}\right)^{-1} W(p_y - q_y;\ p_z - q_z).$$

The integral in the sense of the principal value in the range $-(2m\epsilon - q_z^2)^{1/2} \leq q_y \leq (2m\epsilon - q_z^2)^{1/2}$ can be neglected here. Using the quantization condition (2.17) and the quasi-classical asymptotic forms of the parabolic-cylinder function, we can readily derive the relations

$$\left(\frac{\partial q_y^n}{\partial n}\right)^{-1} = \frac{2i\mu}{\pi\hbar}\frac{D'_{\tilde{\eta}-1/2}(cq_y/\mu eH)}{D_{\tilde{\eta}-1/2}(cq_y/\mu eH)} = -\frac{2\mu^2}{\pi\hbar^2}(2m\varepsilon - q_y^2 - q_z^2)^{1/2}. \tag{3.8}$$

As a result, the formula (3.6) for M(p) is transformed into

$$M(\mathbf{p}) = -i\frac{\sigma^2}{2\pi\hbar^2}\int_{-\infty}^{\infty} d^2\mathbf{q}\, W(\mathbf{p}-\mathbf{q})\sqrt{2m\varepsilon - q^2}. \tag{3.9}$$

Substituting (3.9) in (3.3) and recognizing that from (2.17) it follows that

$$\mu\frac{\partial\eta(n,X)}{\partial X}=-\left(1-\frac{X^2}{4\mu^2\eta}\right)^{1/2}\sqrt{\eta}\Big/\arccos\left(-\frac{X}{2\mu\sqrt{\eta}}\right).$$

we obtain for $\delta\epsilon$ the final expression in the limiting case (3.7):

$$\delta\varepsilon=-i\frac{\hbar\Omega}{2\varphi}(1+V). \tag{3.10}$$

We have introduced here the following notation:

$$V=-1+\frac{\sigma^2k_x}{\pi\hbar^2}\int_{-\infty}^{\infty}d^2q\sqrt{2m\varepsilon-q^2}W(\mathbf{p}-\mathbf{q}) \tag{3.11}$$

is the average coefficient of reflection of the plane wave with wave vector (k_X, p/h) from a statistically uneven surface, first obtained by Bass[14];

$$k_x=\frac{1}{\hbar}(2m\varepsilon-p^2)^{1/2}=\frac{\sqrt{\eta}}{\mu}\sin\varphi \tag{3.12}$$

is the projection of the wave vector of the de Broglie electron wave on the x axis, and

$$\varphi=\arccos(-X/2\mu\sqrt{\eta}) \tag{3.13}$$

is the glancing angle of the electron in the plane perpendicular to the magnetic field **H** at the instant when the electron collides with the surface of the sample (Fig. 1).

From (3.10) we get directly the formulas (4.14) of the paper by Kaner and the authors[7], which were obtained under the assumption that the wave function of the electron near the boundary of the metal can be represented in the form of a sum of two plane waves—incident and reflected—with a reflection coeffficient V. From the foregoing derivation of formula (3.10) it follows that such an analysis is adequate if the inequality (3.7) is satisfied; this inequality can be written with the aid of (3.8) and (3.12) in the form

$$L\ll 2R_\perp\sin\varphi. \tag{3.14}$$

We recall that $R_\perp\equiv 2\mu\sqrt{\eta}$ is the radius of the orbit of the electron in a plane perpendicular to the magnetic field **H** (Fig. 1). The inequality (3.14) denotes that the distance between two successive collisions of the electron with the surface of the metal $\Lambda = 2R_\perp\sin\varphi$ (Fig. 1) greatly exceeds the correlation radius of the roughnesses L. It is obvious here that successive acts of scattering of the electron by the interface are independent. This, in fact, was the basis of the derivation of (4.14) in[7].

3. When the correlation radius L is much larger than the de Broglie wavelength k^{-1} ($k=\sqrt{2m\epsilon}/\hbar$) and the angles of encounter of the electron with the surface are not very small, then we obtain from (3.11)

$$1+V=2(k_x\sigma)^2[1+iO\{W(\hbar k_x^2/2k)\}] \tag{3.15a}$$

for $kL\gg 1$ and $(k_X/k)^2\gg 2/kL$. For extremely small encounter angles we have

$$1+V=k_x\sigma^2\sqrt{\frac{k}{L}}e^{i\pi/4}\left(-2\sqrt{\frac{2}{\pi}}\int_0^\infty\frac{d\rho}{\sqrt{\rho}}\frac{dw(\rho)}{d\rho}\right) \tag{3.15b}$$

for $kL\gg 1$ and $(k_X/k)^2\ll 2/kL$. Finally, for small-scale roughnesses the asymptotic form of the reflection coefficient is

$$1+V=\frac{k_x\sigma^2}{L}\left\{\frac{2}{3}(kL)^3\int_0^\infty w(\rho)\rho\,d\rho-2i\int_0^\infty\frac{d\rho}{\rho}\frac{dw(\rho)}{d\rho}\right\} \tag{3.15c}$$

for $kL\ll 1$. The correlation coefficient $w(\rho)\equiv\mathcal{W}(\rho L)$ changes here over an interval on the order of unity in terms of the dimensionless variable ρ, so that the integrals of $w(\rho)$, which enter in (3.15b) and (3.15c), are constants close to unity. The asymptotic formulas given above pertain to the simplest case of isotropic roughnesses, when $\mathcal{W}(\mathbf{r})$ depends only on r. A generalization of these results for anisotropic roughnesses (with the correlation radius dependent on the direction) reduces to an inessential change of the coefficients in (3.15a)–(3.15c).

Substituting (3.15a)–(3.15c) in (3.10), we obtain explicit expressions for the level shift (Re $\delta\epsilon$) and the damping ($-$Im $\delta\epsilon$) of the surface electronic states. In[8] it was concluded that the damping and the shift of the surface levels are quantities of the same order. From the formulas given above it follows that this, generally speaking, is not the case: when $kL\gg 1$ and $(k_X/k)^2\gg 2/kL$, the shift is smaller than the damping by at least a factor $\exp(k_X^2L/4k)$[2)], and when $kL\ll 1$ the damping is smaller by a factor $(kL)^{-3}$ than the shift. Only in the particular case when $kL\gg 1$ and the encounter angles are extremely small do we have $-$Im $\delta\epsilon$ = Re $\delta\epsilon$.

We recall that the results (3.10) and (3.11) were obtained considering only the simplest diagram in the series (2.22) for M(**p**). Allowance for the next higher diagrams, proportional to σ^4, makes it possible to estimate the resultant error. Without writing out the rather cumbersome general formulas (the corrections to (3.4) of next higher order in σ^2), we present the corresponding inequalities that ensure validity of formula (3.4) in the limiting cases considered above:

$$(k_x\sigma)^2\ll 1 \text{ for } kL\gg 1 \text{ and } (k_x/k)^2\gg 2/kL; \tag{3.16a}$$

$$k\sigma^2/L\ll 1 \text{ for } kL\gg 1 \text{ and } (k_x/k)^2\ll 2/kL; \tag{3.16b}$$

$$(\sigma/L)^2\ll 1 \text{ for } kL\ll 1. \tag{3.16c}$$

The first of these inequalities coincides with Eq. (2.6), the physical meaning of which has already been discussed. The last inequality is equivalent to the requirement that the surface be gently sloping—the ratio σ/L must be of the order of the angles of inclination of the surface relative to the plane x = 0 (Fig. 2). For $kL\gg 1$ and glancing incidence of the electron on the metal-vacuum interface, the inequality (3.1a) is replaced by the stronger one (3.16b). This is connected with the fact that in the case of glancing incidence there is an increase in the probability of multiple diffraction of the de Broglie wave by the roughnesses of the surface upon collision of the electron with the boundary of the sample. These processes can be neglected when the height of the roughnesses σ is much smaller than the dimension of the Fresnel zone $(L/k)^{1/2}$.

We note, finally, that the conditions (3.16) ensure validity of the inequality

$$|1+V|\ll 1. \tag{3.17}$$

As seen from formula (3.10), the width and shift of the levels are certainly small here compared with the distance between them $\epsilon_{n+1}-\epsilon_n\approx\pi\hbar\Omega/\varphi$, as was assumed in solving the dispersion equation (3.1).

[2)] This estimate pertains to a Gaussian correlation function $\mathcal{W}(r)=\exp(-r^2/L^2)$. In the case of a non-Gaussian but analytic function $\mathcal{W}(r)$, the estimate remains exponential as before.

4. The preceding two items pertain to the case of uncorrelated successive reflections of the electron, when the inequality (3.7) is satisfied. Let us consider now the inverse limiting case of strong correlation

$$\left|\frac{\partial q_y^n}{\partial n}\right| \gg \frac{2\pi\hbar}{L}, \qquad \left|\frac{\partial q_y^n}{\partial q_z}\right| \frac{2\pi\hbar}{L} . \tag{3.18}$$

Then the function $W(\mathbf{p}-\mathbf{q})$ is "sharp" ($\Delta q \sim \Delta p \sim 2\pi\hbar/L$) and we can confine ourselves in the sum (3.6) to a single term, while the limits of integration with respect to dq_z can be regarded as infinite. The integral in the sense of principal value turns out to be exponentially small (and not in accord with a power law, as in[8]) the more the inequalities (3.18) are satisfied, so that for $M(\mathbf{p})$ we obtain

$$M(\mathbf{p}) = -i\frac{\sigma^2}{4\mu^2}\int_{-\infty}^{\infty} dq_z W(\theta q_z, q_z) = -i\frac{\sigma^2 L}{2\mu^2\zeta}\int_0^{\infty} w(\rho)\,d\rho,$$
$$\zeta^2 = 1+\theta^2, \quad \theta = \partial q_y^n/\partial q_z. \tag{3.19}$$

Substituting this expression in formula (3.3) we arrive at the following result:

$$\delta\varepsilon = -i\hbar\Omega\frac{k_x\sigma^2 L}{2\mu^2\varphi\zeta}\int_0^{\infty} w(\rho)\,d\rho. \tag{3.20}$$

The inequalities (3.18) can be transformed with the aid of relations (2.17), (3.8), and (3.12) to the form

$$L \gg \Lambda, \qquad \Lambda_z = 2\frac{cp_z}{eH}\varphi. \tag{3.21}$$

Here Λ_z is the distance traversed by the electron along the z axis between two successive collisions. We see that (3.21) are equivalent to the requirement $L \gg (\Lambda^2+\Lambda_z^2)^{1/2} \equiv \Lambda_\zeta$. In other words, formula (3.20) was obtained under the condition that the distance between neighboring points of reflection of the electron from the surface of the metal is much smaller than the correlation radius of the roughnesses.

It follows from (3.20) that the damping is proportional to L in this limiting case, whereas the inequalities (3.18) do not impose an upper limit on the correlation radius. The required limitations are obtained from the condition implied in the derivation of (3.19)

$$W(0, q_z) \gg \left|\delta q_y^n \frac{\partial W(0, q_z)}{\partial q_y}\right|$$

which leads to inequality

$$(\sigma L)^2/8\pi\mu^4 \ll 1. \tag{3.22}$$

For a given limitation on L, the smearing of the levels (3.20) is always much smaller than the distance between them.

4. DISCUSSION OF RESULTS

1. The foregoing results were obtained under the condition (2.6) $(k_x\sigma)^2 \ll 1$, which can be satisfied as a rule only for skipping electrons. Indeed, for typical metals $k = \sqrt{2m\epsilon}/\hbar \sim 10^8$ cm^{-1}, so that for $\varphi \gtrsim 1$ the indicated inequality is violated even for roughnesses of atomic dimensions. Therefore in the discussion of the results we shall pay principal attention to the skipping electrons for which $\varphi \ll 1$. For simplicity we assume that the energy of motion of the electron in a plane perpendicular to the magnetic field, $\eta\hbar\Omega = \epsilon - p_z^2/2m$, is of the order of the Fermi energy ϵ_F. From (2.17) at small glancing angles φ we obtain the following quantization condition:

$$\sin\varphi_n \approx \varphi_n = \left[\frac{3\pi}{2}\frac{\hbar\Omega}{\varepsilon_F}\left(n-\frac{1}{4}\right)\right]^{1/3} \propto H^{1/3}. \tag{4.1}$$

Let us investigate the dependence of the level shift and damping on the magnetic field H, bearing in mind that for typical metals $kL \gg 1$. Weak magnetic fields

$$(H/H_0)^2 \ll (kL)^{-3}[3\pi(n-1/4)]^{-2}, \tag{4.2}$$

where $H_0 = 2\sqrt{2}\hbar ck^2/e$ correspond to extremely small glancing angles $\varphi_n^2 \ll 2/kL$. Substituting the asymptotic expression (3.15b) for the reflection coefficient V in formula (3.10), we obtain the shift and width of the levels:

$$\mathrm{Re}\,\delta\varepsilon = -\mathrm{Im}\,\delta\varepsilon = k\sigma^2\sqrt{\frac{k}{\pi L}}\,\Gamma\left(\frac{3}{4}\right)\hbar\Omega \propto H. \tag{4.3}$$

Here and henceforth the values of the numerical coefficients are given for $\mathcal{W}(\mathbf{r}) = \exp(-r^2/L^2)$.

With increasing magnetic field, the glancing angle φ_n increases and becomes larger than $(2/kL)^{1/2}$. We assume, on the other hand, that the magnetic field is sufficiently small to satisfy the inequality (3.14), i.e.,

$$(kL)^{-3}[3\pi(n-1/4)]^{-2} \ll (H/H_0)^2 \ll (kL)^{-3}[3\pi(n-1/4)]. \tag{4.4}$$

Then, using formula (3.15a), we obtain for the level width

$$\delta\varepsilon = -i(k\sigma)^2\varphi_n\hbar\Omega \propto H^{4/3}. \tag{4.5}$$

We see that in the indicated interval of magnetic fields (4.4) the damping is $\varphi_n\sqrt{kL} \gg 1$ times larger than in the region (4.2).

With further increase of H, the distance between two successive reflections of the electron becomes smaller than the correlation radius L. Therefore in the region of magnetic fields

$$(kL)^{-3}[3\pi(n-1/4)] \ll (H/H_0)^2 \ll (k^2\sigma L)^{-2}, \tag{4.6}$$

corresponding to the inequalities (3.21) and (3.22), the damping is determined by formula (3.20)

$$\delta\varepsilon = -i\frac{k\sigma^2 L\sqrt{\pi}}{4\mu^2}\hbar\Omega \propto H^2. \tag{4.7}$$

The level width in this case is larger by $L/2R_\perp\varphi_n \gg 1$ times than in the preceding case (cf. (4.5)).

Thus, with increasing magnetic field the damping increases first linearly, then like $H^{4/3}$[7], and finally, in the region (4.6) of sufficiently strong fields, in proportion to H^2. The relation $\delta\epsilon \propto H^2$ for cylindrical Fermi surface was recently obtained by Mertsching and Fischbeck[15] as a result of application of quantum-mechanical perturbation theory to the scattering problem (Born approximation)[3)].

2. The fact that at large correlation radii the damping increases linearly with L (formula (3.20) or (4.7)) is at first glance quite unexpected. Indeed, with increasing L, the surface becomes more gently sloping and the scattering of the electrons on it approaches specular. This seeming contradiction can be readily eliminated

[3)] We are grateful to the authors of [15] for the opportunity of becoming acquainted with their results prior to publication.

on the basis of the following simple geometrical consideration.

When $kL \gg 1$ and $\varphi^2 \gg 2/kL$, the change of the glancing angle φ in the collision of an electron with the interface can be neglected, since the reflection takes place from a locally flat surface. In other words, the electron remains in the same quantum state, and the role of the roughnesses reduces to a change in the phase of the wave function by an amount $2k_x\xi(\mathbf{r}_s)$ when the electron collides with the boundary at the point $\mathbf{r}_s$. After N collisions with the surface, the wave function of the electron acquires the form

$$\psi = \psi_0 \exp\Big[2ik_x \sum_{s=1}^{N} \xi(\mathbf{r}_s)\Big], \tag{4.8}$$

where ψ_0 is the wave function of the unperturbed problem ($\xi = 0$).

If successive reflections of the electron are not correlated (3.14), i.e., $|\mathbf{r}_s - \mathbf{r}_{s+1}| \gtrsim \Lambda \gg L$, then the random quantities $\xi(\mathbf{r}_s)$ are independent, making it possible to write

$$\Big\langle \exp\Big[2ik_x \sum_{s=1}^{N} \xi(\mathbf{r}_s)\Big]\Big\rangle = \langle \exp(2ik_x\xi)\rangle^N = e^{-2(k_x\sigma)^2 N}. \tag{4.9}$$

We have assumed here that $\xi(\mathbf{r})$ has a normal distribution. For $(k_x\sigma)^2 \ll 1$, the average wave function decreases appreciably at $N \gg 1$. In this case the number of collisions during the time t is equal to

$$N = \Omega t / 2\varphi \tag{4.10}$$

and for the average wave function we have

$$\langle\psi\rangle = \psi_0 \exp\Big[-(k_x\sigma)^2 \frac{\Omega}{\varphi} t\Big]. \tag{4.11}$$

Thus, the relaxation time of the surface electronic states τ, due to scattering by the rough boundary, turns out to be

$$\frac{1}{\tau} = -\frac{\operatorname{Im}\delta\varepsilon}{\hbar} = (k_x\sigma)^2 \frac{\Omega}{\varphi}. \tag{4.12}$$

This result coincides exactly with formulas (3.10) and (3.15a), which were obtained from the microscopic theory.

In the opposite limiting case (3.21), when $L \gg \Lambda_\zeta$, successive reflections cannot be regarded as independent. The random quantities $\xi(\mathbf{r}_s)$ and $\xi(\mathbf{r}_{s+\nu})$ (the heights of the roughnesses of the s-th and $s + \nu$-th reflection points) then correlate if $|\nu| \le \nu_0 = L/\Lambda_\zeta$. Assuming for estimates that the correlation function is in the form of a step

$$\mathscr{W}(\mathbf{r}) = 1 \text{ for } r < L \text{ and } \mathscr{W}(\mathbf{r}) = 0 \text{ for } r \geqslant L,$$

we can transform the phase ψ in (4.8) into

$$\sum_{s=1}^{N} \xi(\mathbf{r}_s) = \sum_{j=1}^{n} \sum_{s=j-\nu_0}^{j+\nu_0} \xi(\mathbf{r}_s) = 2\nu_0 \sum_{j=1}^{n} \xi(\mathbf{r}_j). \tag{4.13}$$

Here $n = N/2\nu_0$ is the number of independent groups of intercorrelated reflection points, and the quantities $\xi(\mathbf{r}_j)$ are in this case independent. Therefore averaging over the wave function of the electron can be carried out in the same manner as in (4.9), as a result of which we obtain

$$\langle\psi\rangle = \psi_0 \exp[-4(k_x\sigma)^2 \nu_0 N]. \tag{4.14}$$

When $(k_x\sigma)^2\nu_0 \ll 1$ we can use for N formula (4.10).

From this we get for the relaxation time

$$\frac{1}{\tau} = -\frac{\operatorname{Im}\delta\varepsilon}{\hbar} = 2(k_x\sigma)^2 \frac{L\Omega}{\Lambda_\zeta \varphi}. \tag{4.15}$$

This formula is in full accord with the previously obtained result (3.20), if it is recognized that for the assumed model we have $\int_0^\infty w(\rho)d\rho = 1$.

3. The influence of the rough boundary on the damping of the magnetic surface levels was investigated experimentally by Koch and Murray[4] on samples of tin and gallium for small electronic groups ($k \sim 10^5$ cm^{-1}) at characteristic roughness dimensions $\sigma \sim 10^{-5}$ cm and $L \sim 10^{-3}$ cm. The inequalities (4.6) are satisfied in this case for fields of the order of several Oe up to $H \lesssim 20$ Oe, which should lead to a quadratic dependence of the level widths on the magnetic field in accord with formula (4.7). In weaker fields, when the left-hand inequality in (4.6) is violated, the width of the levels (4.5) is proportional to $H^{4/3}$. These results are in qualitative agreement with the data of[4].

In the case of small values $k \lesssim 10^5$ cm^{-1} and small-scale roughnesses of the interface, the inequality $kL \ll 1$ may be satisfied. Then the width shift of the levels are determined by formulas (3.10) and (3.15c). This case may be of definite interest in that respect that the level shift

$$\operatorname{Re}\delta\varepsilon = \sqrt{\pi}\frac{k\sigma^2}{L}\hbar\Omega \propto H \tag{4.16}$$

is much larger than their width

$$-\operatorname{Im}\delta\varepsilon = {}^1/_6 (k\sigma)^2 (kL)^2 \hbar\Omega \propto H, \tag{4.17}$$

and the dependence on the magnetic field is linear.

In conclusion we note that in all the cases considered by us the scattering of the electrons by the surface hardly differed from specular—this is precisely the meaning of the limitations under which $|\delta\epsilon| \ll |\epsilon_{n+1} - \epsilon_n|$. In the opposite limiting case of diffuse scattering, as shown in[7], the damping reaches its maximum value

$$\delta\varepsilon = -i\frac{\hbar\Omega}{2\varphi_n} \propto H^{2/3}, \tag{4.18}$$

which is comparable with the distance between the levels. The spectrum of the surface electronic states is in this case practically continuous.

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