

RESONANCE WIDTH ON MAGNETIC SURFACE LEVELS

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The two-particle Green function for electrons on magnetic surface levels, averaged over an ensemble of random irregularities of the metal boundary, is calculated. It is shown that the width of resonance transitions in a high frequency electromagnetic field is not identical to the sum of the level widths and is defined by the transport scattering cross section. In a comparatively strong magnetic field, or for sufficiently smooth irregularities, the transport width of the transition is much smaller and depends on the magnetic field strength in other ways than the total width. The shape of the resonance curve is analyzed by taking into account scattering by the boundary irregularities in a metal with a spherical or cylindrical Fermi surface.

1. INTRODUCTION

WHEN a metallic sample is placed in a constant magnetic field, two different types of electronic states are produced. Besides the usual volume states corresponding to the Landau level, there exists electrons that collide with the boundary of the metal. In a magnetic field parallel to the surface of the sample, the motion of such "surface" electrons has a periodic character, and is consequently quantized. These quantum states are called magnetic surface levels. In weak magnetic fields (1–10 Oe), the frequencies of the transitions between levels lie in the microwave band (10^{10} – 10^{11} Hz). The transitions induced by the electromagnetic field lead to the resonant oscillations of the surface impedance of metals, first observed experimentally by Khaikin^[1]. This is the interpretation proposed by Nee and Prange^[2] for the oscillations of the surface impedance in weak magnetic fields. Recently, Koch and co-workers carried our extensive experimental investigations of this phenomenon in many metals. Since the surface states are the result of multiple collisions between the electrons and the boundary of the metal, microscopic surface inhomogeneities play a very important role in the spectrum and in the damping of the magnetic surface levels. The role of the roughnesses was discussed qualitatively by Prange and Nee^[7] and by Fischbeck and Mertsching^[8]. A detailed study of the influence of random inhomogeneities of the metal boundary on the spectrum and damping of the surface stage was carried out in^[9], using the results of the theory of wave diffraction by surfaces with random roughnesses (cf. e.g.,^[10,11]). Subsequently, the principal results of^[9] were derived again by Fal'kovskii^[12], who used a diagram technique developed by Chaplik and Éntin^[13]. It should be noted that the problem of the influence of roughnesses on the surface electronic states in a magnetic field has many features in common with the problem of the spectrum and damping of waves in an irregular waveguide with rough walls^[14]. The magnetic field plays here the role of the second wall in a flat waveguide, forming together with the metal surface an "electronic" waveguide. This analogy was used by Makarov and Fuks^[15] in an analysis of the influence of

surface roughnesses on the spectrum and damping of magnetic surface states.

In all the aforementioned theoretical papers, they calculated the surface-level broadening, which is obviously determined by the total cross section for the scattering of the electron by the random inhomogeneities. In the experiments one usually measures the width of the resonant-absorption peaks, which is determined actually not by the total but by the transport scattering cross section. One can expect the difference between the two to become particularly strong when a strong correlation exists between the successive reflections of the electrons from the surface. In other words, when the inhomogeneity length on the surface exceeds the distance between two successive collisions of the electron with the boundary, the transport scattering cross section becomes much smaller than the total cross section. The experimental widths of the resonant transitions can therefore not be compared, generally speaking, with the sum of the total widths of the levels between which the transition takes place.

We investigate in the present paper the influence of a rough metal surface on the width of the resonant transition between magnetic surface levels. Unlike the cited studies, where formulas were obtained for the damping of the average single-particle Green's functions, we calculate here the damping of two-particle Green's functions.

2. FORMULATION OF PROBLEM. GENERAL RELATIONS

We consider a metal placed in a constant and homogeneous magnetic field \mathbf{H} parallel to the central surface of the sample ($x = 0$). The x axis is directed into the interior of the metal and the z axis along the vector \mathbf{H} . Assume that a plane monochromatic electromagnetic wave $\vec{\mathcal{E}} = \vec{\mathcal{E}}(x)e^{-i\omega t}$ propagates in the metal in a direction normal to the surface. The real part of the surface impedance is proportional to the dissipative loss Q (per unit time). In the approximation linear in the field $\vec{\mathcal{E}}$, this loss can be calculated from the formula

$$Q = \frac{2\pi e^2}{\hbar\omega} \sum_{n,m} (f_m - f_n) |\langle n | \sqrt{\vec{\mathcal{E}}}(x) | m \rangle|^2 \delta(\omega_{nm} - \omega), \quad (2.1)$$

where $f_n = f(E_n)$ is the equilibrium distribution function over the quantum states $|n\rangle$ with allowance for the interaction of the electrons with the scatterers, E_n are the exact energy levels, \hat{v} is the electron-velocity operator, $\hbar\omega_{nm} = E_n - E_m$, and e is the absolute value of the electron charge. The matrix elements $\langle n|\hat{v}\mathcal{E}(\mathbf{x})|m\rangle$ in (2.1) are conveniently expressed in terms of the Green's functions

$$\mathcal{G}_{\pm}(E, \mathbf{R}, \mathbf{R}') = \sum_n \frac{\psi_n^*(\mathbf{R})\psi_n(\mathbf{R}')}{E - E_n \pm i\epsilon}, \quad (2.2)$$

where $\psi_n(\mathbf{R})$ are the eigenfunctions of the electronic Hamiltonian with allowance for the external electromagnetic fields; ϵ is an infinitesimally small positive quantity indicating the direction of circling around the poles in the complex E plane; the asterisk denotes complex conjugation. Transformations of formula (2.1), similar to those given by Edwards^[16] for the static case, enable us to rewrite the expression for Q in the form

$$Q = \frac{e^2}{2\pi\omega} \int_0^{\infty} dE (f - f) \int_{-\infty}^{\infty} d\mathbf{R} d\mathbf{R}' \tilde{\mathcal{G}}(\mathbf{R}, \mathbf{R}') (\hat{v}(\mathbf{R})\mathcal{E}(\mathbf{x})) \times (\hat{v}^*(\mathbf{R}')\mathcal{E}^*(\mathbf{x}')) \mathcal{G}(\mathbf{R}', \mathbf{R}). \quad (2.3)$$

Here $\mathcal{G} = \mathcal{G}_- - \mathcal{G}_+$ is the causal Green's function, and the tilde over a function means that the argument E (which will henceforth be omitted) is shifted by an amount $\hbar\omega$:

$$f = f(E + \hbar\omega); \quad \tilde{\mathcal{G}}(\mathbf{R}, \mathbf{R}') = \mathcal{G}(E + \hbar\omega; \mathbf{R}, \mathbf{R}')$$

etc.

We now perform a Fourier transformation with respect to the coordinates y and z , which are parallel to the central surface of the metal:

$$\mathcal{G}(\mathbf{R}, \mathbf{R}') = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(\mathbf{p}, \mathbf{p}'; x, x') \exp\left\{\frac{i}{\hbar}(\mathbf{p}\mathbf{r} - \mathbf{p}'\mathbf{r}')\right\} d\mathbf{p} d\mathbf{p}', \quad (2.4)$$

where \mathbf{r} denotes a two-dimensional radius-vector in the $\{y, z\}$ plane, and analogously for the velocity vector \hat{v} :

$$\int_{-\infty}^{\infty} e^{i\mathbf{p}\mathbf{r}/\hbar} \hat{v}(\mathbf{R}) e^{-i\mathbf{q}\mathbf{r}'/\hbar} d\mathbf{r} = (2\pi\hbar)^2 \delta(\mathbf{p} - \mathbf{q}) \mathbf{v}(\mathbf{q}, x). \quad (2.5)$$

Substituting (2.4) and (2.5) in (2.3), we obtain

$$Q = \int_0^{\infty} \int_0^{\infty} dx dx' \mathcal{K}_{ij}(x, x') \mathcal{E}_i(x) \mathcal{E}_j^*(x'). \quad (2.6)$$

Here $\mathcal{K}_{ij}(x, x')$ denotes the kernel of the dissipative-conductivity-operator:

$$\mathcal{K}_{ij}(x, x') = \frac{e^2 \hbar^4}{2\pi\omega} \int_0^{\infty} dE (f - f) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{p} d\mathbf{p}' \quad (2.7)$$

$$\times \tilde{G}(\mathbf{p}, \mathbf{p}'; x, x') v_i(\mathbf{p}, x) v_j^*(\mathbf{p}', x') G(\mathbf{p}', \mathbf{p}; x', x).$$

The problem consists of investigating the singularities of the kernel \mathcal{K}_{ij} at frequencies ω close to the resonant frequencies ω_{nm} of the transitions between the states numbered n and m .

3. SPECTRUM AND DAMPING OF SINGLE-PARTICLE STATES

In the simplest case of a spherical Fermi surface, the Schrödinger equation for the Green's function takes the form

$$\left[-\mu^2 \frac{d^2}{dx^2} + \frac{1}{4} \left(\frac{x-X}{\mu}\right)^2 - \eta\right] G(\mathbf{p}, \mathbf{p}'; x, x') = -\frac{\delta(\mathbf{p}-\mathbf{p}')\delta(x-x')}{\hbar\Omega(2\pi\hbar)^2} \quad (3.1)$$

Here $\Omega = e\hbar/mc$ is the cyclotron frequency, m the effective electron mass, $\mu = (2e\hbar/\hbar c)^{-1/2}$ is the magnetic length, $X = -cp_y/e\hbar$ is the x -coordinate of the center of the electron orbit, and $\hbar\Omega\eta = E - p_z^2/2m$. We note that Eq. (3.1) is actually valid not only in the case of a spherical Fermi surface, but also for a larger class of equal-energy surfaces whose interceptions with the $p_z = \text{const}$ plane are circles. The only difference is that the quantity $\eta\hbar\Omega$ should be taken to mean the energy $E_{\perp}(p_z)$ of the transverse electron motion (in a plane perpendicular to the magnetic field \mathbf{H}). In particular, for a cylindrical Fermi surface parallel to the z axis we have $\eta = E/\hbar\Omega$, where E is the total electron energy.

The boundary conditions for Eq. (3.1) are that the Green's function vanish at $x, x' \rightarrow \infty$ and on the surface of the metal. We specify the metal-vacuum interface in the form

$$x = \zeta(\mathbf{r}), \quad \langle \zeta(\mathbf{r}) \rangle = 0. \quad (3.2)$$

The function $\zeta(\mathbf{r})$ is a random function of two spatial coordinates with zero mean value, and the angle brackets denote averaging over the ensemble and its realizations. Assuming the surface roughnesses to be spatially-homogeneous, we introduce also the correlation function of the roughnesses

$$\langle \zeta(\mathbf{r})\zeta(\mathbf{r}') \rangle = \mathcal{W}(\mathbf{r} - \mathbf{r}'). \quad (3.3)$$

The value of \mathcal{W} at $\mathbf{r} = \mathbf{r}'$ determines the mean-squared height (variance) σ of the roughnesses, and the distance L over which $\mathcal{W}(\mathbf{r})$ decreases significantly determines the correlation length (radius).

In the weak non-specularity approximation, when the surface roughnesses can be regarded as perturbations, the boundary condition on the surface of the metal can be written in the form

$$\mathcal{G}(\mathbf{r}, \mathbf{r}'; 0, x') + \zeta(\mathbf{r})\mathcal{G}'_x(\mathbf{r}, \mathbf{r}'; 0, x') = 0, \quad (3.4)$$

where the prime at the Green's function denotes differentiation with respect to x . Changing over in this condition to the Fourier components, we obtain

$$G(\mathbf{p}, \mathbf{p}'; 0, x') + \int_{-\infty}^{\infty} \zeta(\mathbf{p} - \boldsymbol{\kappa}) G'_x(\boldsymbol{\kappa}, \mathbf{p}'; 0, x') d\boldsymbol{\kappa} = 0, \quad (3.5)$$

where $\zeta(\mathbf{p} - \boldsymbol{\kappa})$ denotes the Fourier transform of the random function $\zeta(\mathbf{r})$.

The averaging of expression (2.7) for \mathcal{K}_{ij} reduces to a calculation of the mean value of the product of two Green's functions. In the calculation of the integrals with respect to the momenta \mathbf{p} and \mathbf{p}' in (2.7), the main contribution is made only by the pole parts of the G -functions, which can be written in the form

$$G(\mathbf{p}, \mathbf{p}'; x, x') \approx \mathcal{D}(x, x'; X, X') g(\mathbf{p}, \mathbf{p}'), \quad (3.6)$$

where

$$\mathcal{D}(x, x'; X, X') = (2\pi/\hbar^2\Omega) \times D_{\eta-1/2}\left(\frac{x-X}{\mu}\right) D'_{\eta-1/2}\left(\frac{x'-X'}{\mu}\right) \left\{ D'_{\eta-1/2}\left(-\frac{X}{\mu}\right) D'_{\eta-1/2}\left(-\frac{X'}{\mu}\right) \right\}^{-1}. \quad (3.7)$$

Here $D_{\eta-1/2}$ are parabolic-cylinder functions and are the eigenfunctions of Eq. (3.1) without the right-hand side, $D'_{\eta-1/2}$ denotes the derivative of $D_{\eta-1/2}$ with respect to the argument $\eta' = \eta(p'_z)$, and $X' = X(p'_y)$

$= -cp'_y/eH$. Substitution of (3.6) in the boundary condition (3.5) leads to the following integral equation for the function $g(\mathbf{p}, \mathbf{p}')$ with a random kernel

$$g(\mathbf{p}, \mathbf{p}') = g_0(\mathbf{p}) \left\{ \delta(\mathbf{p} - \mathbf{p}') - \int \zeta(\mathbf{p} - \boldsymbol{\kappa}) g(\boldsymbol{\kappa}, \mathbf{p}') d\boldsymbol{\kappa} \right\}, \quad (3.8)$$

where

$$g_0(\mathbf{p}) = D_{\eta-\frac{1}{2}}(-X/\mu) / \mu D_{\eta-\frac{1}{2}}(-X/\mu). \quad (3.9)$$

An equation for the function $g(\mathbf{p}, \mathbf{p}')$ in the form (3.8) was obtained by Chaplik and Ėntin^[13] in an investigation on the conductivity of a thin film with rough boundaries. They formulated a diagram technique for the calculation of the average Green's function $\langle g(\mathbf{p}, \mathbf{p}') \rangle$. Analogous calculations of the spectrum of natural modes in a waveguide with random inhomogeneities were also performed in^[14,17,18]. The methods and results of these investigations were applied to the problem of the spectrum of magnetic surface levels by Makarov and Fuks^[15] and by Fal'kovskii^[12]. We present here only the final expression for the average single-particle Green's function

$$\langle g(\mathbf{p}, \mathbf{p}') \rangle = g(\mathbf{p}) \delta(\mathbf{p} - \mathbf{p}'), \quad g(\mathbf{p}) = \frac{g_0(\mathbf{p})}{1 + g_0(\mathbf{p})M(\mathbf{p})}. \quad (3.10)$$

The function $M(\mathbf{p})$ is the analog of the mass operator. In the first Born approximation in terms of the small parameters of the non-specularity of the scattering, $M(\mathbf{p})$ is connected with the spatial spectrum of the roughnesses

$$W(\mathbf{p}) = \frac{1}{(2\pi\hbar)^2} \int \mathcal{W}(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} d\mathbf{r} \quad (3.11)$$

by the relation

$$M(\mathbf{p}) = \int g_0(\mathbf{q}) W(\mathbf{p} - \mathbf{q}) d\mathbf{q}. \quad (3.12)$$

If we disregard the irregularities on the surface of the metal, i.e., we assume that $\zeta = 0$ and $M = 0$, then the spectrum of the unperturbed surface states is determined from the dispersion equation

$$D_{\eta-\frac{1}{2}}(-X/\mu) = 0. \quad (3.13)$$

At a fixed transverse electron energy $E_{\perp}(\mathbf{p}_z) = \eta\hbar\Omega$, this equation leads to a quantization of the X -coordinate of the center of the orbit:

$$X = X_n(\eta) = -cp_n^n / eH. \quad (3.14)$$

In the quasiclassical approximation, the dispersion equation (3.13) takes the form

$$\eta[\arccos(-\xi) + \xi(1 - \xi^2)^{1/2}] = \pi(n - 1/4) \quad (3.15)$$

where $\xi = X/2\mu\eta^{1/2}$, and n are natural numbers. From this it is easy to obtain, in particular, the formulas

$$\frac{\partial X_n}{\partial \eta} = -\frac{\mu}{\eta^{1/2} \sin \varphi_n}, \quad \frac{\partial X_n}{\partial n} = \frac{\pi\mu}{\varphi_n \eta^{1/2}}, \quad (3.16)$$

where φ_n denotes the quantized value of the angle of encounter of the electron with the metal boundary ($x = 0$) in the yz plane:

$$\varphi_n = \left[\frac{3\pi}{2\eta} \left(n - \frac{1}{4} \right) \right]^{1/2}. \quad (3.17)$$

As seen from (3.10), allowance for the scattering of the electrons by random surface inhomogeneities leads to a shift of the poles of the average Green's function

$g(\mathbf{p})$ in comparison with the poles (3.13) of the unperturbed function $g_0(\mathbf{p})$. The real part of the mass operator, $\text{Re } M(\mathbf{p}_n) = M_n^{(r)}$ determines the shift of the energy levels

$$\delta E_n = - \left(\frac{\partial X_n}{\partial E_{\perp}} \right)^{-1} M_n^{(r)}, \quad (3.18)$$

and the imaginary part $\text{Im } M(\mathbf{p}_n) = M_n^{(i)}$ determines their width:

$$\Gamma_n = \left(\frac{\partial X_n}{\partial E_{\perp}} \right)^{-1} M_n^{(i)}. \quad (3.19)$$

4. TWO-PARTICLE GREEN'S FUNCTION. WIDTH OF RESONANT TRANSITIONS

We proceed now to calculate the conductivity tensor $\langle \mathcal{K}_{ij}(\mathbf{x}, \mathbf{x}') \rangle$ averaged over the ensemble of realizations of the random roughnesses.

1. If we substitute the expression (3.6) for $G(\mathbf{p}, \mathbf{p}'; \mathbf{x}, \mathbf{x}')$ in (2.7), we obtain mean values of the products of two single-particle Green's functions in the form

$$\langle g(\mathbf{p}, \mathbf{p}') \bar{g}(\mathbf{p}', \mathbf{p}) \rangle = (2\pi\hbar)^{-2} S \Delta(\mathbf{p}, \mathbf{p}'). \quad (4.1)$$

Here S is the metal surface area exposed to the electromagnetic wave. By starting from (3.8), we can obtain for $\Delta(\mathbf{p}, \mathbf{p}')$ an analog of the Bethe-Salpeter equation, which takes in the simplest ladder approximation the form

$$\Delta(\mathbf{p}, \mathbf{p}') = g(\mathbf{p}) \bar{g}(\mathbf{p}') \left\{ \delta(\mathbf{p} - \mathbf{p}') + \int W(\mathbf{p} - \boldsymbol{\kappa}) \Delta(\boldsymbol{\kappa}, \mathbf{p}') d\boldsymbol{\kappa} \right\}. \quad (4.2)$$

It is convenient to represent the averaged Green's functions $g(\mathbf{p})$ in the form of differences between the retarded and advanced Green's functions $g_+(\mathbf{p})$ and $g_-(\mathbf{p})$, respectively, whose poles lie on opposite sides of their real axis:

$$g_{\pm}(\mathbf{p}) = \{ [g_0(\mathbf{p})]^{-1} + M^{(r)}(\mathbf{p}) \pm iM^{(i)}(\mathbf{p}) \}^{-1}. \quad (4.3)$$

We represent in the same manner the non-averaged function $g(\mathbf{p}, \mathbf{p}') = g_+(\mathbf{p}, \mathbf{p}') - g_-(\mathbf{p}, \mathbf{p}')$, which is connected with the causal function $G = G_+ - G_-$ by relation (3.6).

It is easy to see that in the pole approximation the main contribution to the integral (2.7) is made by only two terms:

$$\begin{aligned} \langle g_+(\mathbf{p}, \mathbf{p}') \bar{g}_-(\mathbf{p}', \mathbf{p}) \rangle &= (2\pi\hbar)^{-2} S \Delta_+(\mathbf{p}, \mathbf{p}'), \\ \langle g_-(\mathbf{p}', \mathbf{p}) \bar{g}_+(\mathbf{p}, \mathbf{p}') \rangle &= (2\pi\hbar)^{-2} S \Delta_+^*(\mathbf{p}', \mathbf{p}). \end{aligned} \quad (4.4)$$

An equation for $\Delta_+(\mathbf{p}, \mathbf{p}')$ is obtained from (4.2) directly and takes the form (cf. ^[13])

$$\Delta_+(\mathbf{p}, \mathbf{p}') = g_+(\mathbf{p}) \bar{g}_-(\mathbf{p}') \left\{ \delta(\mathbf{p} - \mathbf{p}') + \int_{-\infty}^{\infty} W(\mathbf{p} - \boldsymbol{\kappa}) \Delta_+(\boldsymbol{\kappa}, \mathbf{p}') d\boldsymbol{\kappa} \right\}. \quad (4.5)$$

Using expressions (3.9) and (3.10), we can expand the functions $g_{\pm}(\mathbf{p})$ in the "partial fractions" in the form

$$g_{\pm}(\mathbf{p}) = \sum_n [X_n(E, p_{\perp}) - X + M_n^{(r)} \pm iM_n^{(i)}]^{-1}, \quad (4.6)$$

where the summation is over all the surface states with given total energy E .

2. The spectrum of the unperturbed frequencies ω_{nm}^0 of the resonant transitions of a metal with a specular surface is determined from the condition that the pair of poles of the functions $g_0(\mathbf{p})$ and $\bar{g}_0(\mathbf{p})$ coincide:

$$X_m(E, p_z) - X_n(E + \hbar\omega_{nm}^0, p_z) = 0. \quad (4.7)$$

If we use the quasiclassical quantization condition (3.15) and the ensuing formulas (3.16), then we obtain for ω_{nm}^0 the following formula:

$$\omega_{nm}^0 = \Omega\pi(n - m) / \varphi_n. \quad (4.8)$$

It is valid as the transitions occur between sufficiently close levels, so that $|n - m| \ll n$ and $\hbar\omega_{nm}^0 \ll E_n$. The orbits of the electrons that interact most effectively with the high-frequency electromagnetic field lie entirely in a skin layer of thickness δ , and are characterized by glancing angles $\varphi_n \sim (\delta/R)^{1/2}$, where $R = v/\Omega$ is the Larmor radius. It follows therefore that only glancing electrons with $\varphi_n \ll 1$ become effective in weak magnetic fields ($H = 1-10$ Oe). This is indeed the reason why the frequencies ω_{nm}^0 of transitions even between neighboring levels greatly exceed the cyclotron frequency Ω and lie in the microwave band. The resonant frequency closest to ω_{nm}^0 corresponds to a transition between states numbered $n + 1$ and $m + 1$. Starting from (4.8) and (3.17), we can easily obtain the following estimate for the distance between resonances of neighboring series:

$$\omega_{n+1, m+1}^0 - \omega_{n, m}^0 \approx \omega_{nm}^0 / 3n. \quad (4.9)$$

3. In the case of a surface that is not very rough, when the reflection of the electrons from the metal boundary can be regarded as nearly specular, the contributions to the integrals of the function $\Delta_+(\mathbf{p}, \mathbf{p}')$ with respect to \mathbf{p} and \mathbf{p}' are made, as before, only by a small vicinity of the point of the double pole:

$$p_y^n \approx p_y'^n \approx -\frac{eH}{c} X_n(E) \approx -\frac{eH}{c} X_m(E + \hbar\omega). \quad (4.10)$$

The function $\Delta_+(\mathbf{p}, \mathbf{p}')$ is the "sharpest" among all the remaining functions of \mathbf{p} and \mathbf{p}' in the integral (2.7). This enables us to take the smooth functions outside the integral with respect to $dp_y dp_y'$ at the point p_y^n . As to the integrals with respect to the longitudinal momenta p_z and p_z' , the main contribution to them is made by the vicinity of the extremal frequencies $\omega_{nm}(p_z) = \omega_{nm}^{\text{ext}}$ and consequently, all the functions in (2.7), with the exception of $\Delta_+(\mathbf{p}, \mathbf{p}')$, can be taken outside the integrals with respect to dp_z and dp_z' at the point $p_z = p_z' = p_{nm}^{\text{ext}}$ corresponding to the extremal transition frequency. We note that in this sense the cylindrical Fermi surface is not exceptional, since the integrands in (2.7) do not depend on p_z and p_z' at all in this case, and they can be taken outside the integral with respect to dp_z and dp_z' . Thus, an analysis of the dependence of the dissipative conductivity kernel \mathcal{K}_{ij} on the frequency ω reduces to an investigation of the integral

$$J(\omega) = \int [\Delta_+(\mathbf{p}, \mathbf{p}') + \Delta_+(\mathbf{p}', \mathbf{p})] d\mathbf{p} d\mathbf{p}' = 2 \text{Re} \int \Delta_+(\mathbf{p}, \mathbf{p}') d\mathbf{p} d\mathbf{p}'. \quad (4.11)$$

4. Returning to the integral equation (4.5), let us determine the conditions under which we can confine ourselves in the calculation of the integral (4.11) in the product

$$g_+(\mathbf{p}) g_-(\mathbf{p}) = \sum_{s,j} [(X_j - X + M_j)(X_s - X + M_s^*)]^{-1} \quad (4.12)$$

to only one term with $s = n$ and $j = m$, corresponding to

a resonant transition between the levels n and m . Integrating (4.12) with respect to p_y , we obtain

$$\Phi(p_z) = \int g_+(\mathbf{p}) g_-(\mathbf{p}) dp_y = \frac{2\pi eH}{ic} \sum_{s,j} [X_j - X_s + M_j - M_s^*]^{-1}. \quad (4.13)$$

We introduce the frequency ω_{nm} of the transition between the averaged states n and m as a solution of the equation

$$X_m(E) - X_n(E + \hbar\omega_{nm}) + M_m^{(*)} - M_n^{(*)} = 0. \quad (4.14)$$

From (4.14) we obtain with the aid of formulas (3.16) and (3.18) at $n - m \ll n$

$$\hbar\omega_{nm} = \hbar\omega_{nm}^0 + \delta E_n - \delta E_m. \quad (4.15)$$

Then the principal (resonant) term ($s = n, j = m$) in the sum (4.13) can be written in the form

$$\Phi(p_z) \approx \frac{i\pi\hbar}{\mu^2} \left(\frac{\partial X_n}{\partial E} \right)^{-1} [\hbar(\omega - \omega_{nm}) - i\Gamma_{nm}]^{-1}. \quad (4.16)$$

Here $\Gamma_{nm} = \Gamma_n + \Gamma_m$ is the total width of the levels between which the transition takes place; the widths Γ_{nm} are determined by the total cross sections for the scattering of electrons by the rough surface, and are connected with the imaginary part of the mass operator M by relation (3.19).

When estimating the contribution of the remaining (nonresonant) terms to the sum over s and j in (4.13), it is necessary to take into account only those surface states for which the electronic trajectories do not lie entirely in the skin layer. In the quasiclassical approximation, this sum can be replaced by an integral, which can be easily estimated by using relations (3.16):

$$\sum_{s,j} [X_j - X_s + M_j - M_s^*]^{-1} \lesssim N \frac{\pi\eta^{1/2}}{\mu\varphi}. \quad (4.17)$$

Here N is the number of states whose orbits lie inside the skin layer ($0 < X_j + 2\mu\eta^{1/2} \lesssim \delta$). Comparing (4.16) in (4.17), we arrive at an inequality that enables us to confine ourselves in the sum (4.13) to the resonant terms only:

$$|\hbar(\omega - \omega_{nm}) + i\Gamma_{nm}| \ll \omega_{nm} / N. \quad (4.18)$$

Thus, the deviation from resonance $\omega - \omega_{nm}$ and the total level width Γ_{nm} should be smaller than the distances between neighboring resonances of adjacent series (compare with the estimate (4.9)). On the other hand, it is obvious that this is the only case of interest, for otherwise the neighboring absorption lines overlap and cannot be resolved as individual resonances. It should also be noted here that the transition frequencies ω_{nm}^0 and ω_{nm} , which are respectively solutions of (4.7) and (4.14), depend, generally speaking, on a continuous quantum number, namely the longitudinal momentum p_z . For this reason, integration with respect to the momenta p_z and p_z' in (4.11) smears out the resonant dependence of \mathcal{K}_{ij} on ω even in the case of specular reflection of the electrons from the metal boundary. An exception in this respect is the case of a cylindrical Fermi surface, when the functions $g_0(\mathbf{p})$ and $g(\mathbf{p})$ (and consequently also $M(\mathbf{p})$) depend only on p_y and do not depend on p_z .

5. We proceed, finally, to calculate the integral (4.11). To this end, we integrate both halves of (4.5) with respect to $d\mathbf{p}'$ and introduce a new unknown function $\psi(\mathbf{p})$

$$\int_{-\infty}^{\infty} \Delta_+(p, p') dp' = \psi(p) g_+(p) \bar{g}_-(p). \quad (4.19)$$

From (4.5) we obtain for $\psi(p)$ the equation

$$\psi(p) = 1 + \int W(p - \kappa) g_+(\kappa) \bar{g}_-(\kappa) \psi(\kappa) d\kappa. \quad (4.20)$$

We now integrate (4.19) with respect to dp and recognize that the product $g_+(p) \bar{g}_-(p)$ is a "sharp" function of p_y and differs from zero only in the narrow interval

$$|\delta p_y|_s \approx \frac{eH}{c} |M_n^{(i)} - M_m^{(i)}|$$

about the point

$$p_y^n = -\frac{eH}{c} [X_n(E_\perp) + M_n^{(r)}].$$

This enables us to take the function $\psi(p)$ outside the integral with respect to dp_y , so that we obtain for $J(\omega)$ from (4.19)

$$J(\omega) = 2 \operatorname{Re} \int \psi(p_y^n, p_z) \Phi(p_z) dp_z, \quad (4.21)$$

where $\Phi(p_z)$ is given by (4.16). We now put in (4.20) $p_y = p_y^n$ and recognize that $W(p - \kappa)$ is a much smoother function of p_y than $g_+(p) \bar{g}_-(p)$. Indeed, the width of the function W with respect to the variable p_y can be estimated at $|\delta p_y|_W \approx \hbar/L$, where L is the correlation interval of the roughnesses.

The inequality $|\delta p_y|_g \ll |\delta p_y|_W$, as shown in^[15] (see formula (3.22) of^[15]), should always be satisfied provided the shifts and the widths of the levels are smaller than the distances between them. This makes it possible to take $W(p_y - \kappa_y, p_z - \kappa_z)$ in (4.20) outside the integral with respect to $d\kappa_y$ at $\kappa_y = p_y^n$. As the result we arrive at the equation

$$\psi(p_y^n, p_z) = 1 + \int_{-\infty}^{\infty} W[p_y^n(p_z) - p_y^n(\kappa_z); p_z - \kappa_z] \Phi(\kappa_z) \psi(p_y^n, \kappa_z) d\kappa_z. \quad (4.22)$$

We have explicitly taken it into account here that p_y^n depends on the transverse energy E_\perp and is therefore a function of p_z . In the simplest case of a cylindrical Fermi surface, the function Φ does not depend on the longitudinal momentum p_z , so that we readily obtain from (4.21) and (4.22)

$$J(\omega) = 2p_f \operatorname{Re} [\Phi^{-1} - \bar{W}(0)]^{-1}, \quad (4.23)$$

where p_f is the dimension of the Fermi cylinder along the p_z axis, and we have introduced the notation

$$\bar{W}(p_y) \equiv \int_{-\infty}^{\infty} W(p_y, p_z) dp_z. \quad (4.24)$$

Substituting in (4.23) the explicit form of Φ from (4.16), we find that the dependence of the conductivity on the frequency ω near the frequencies ω_{nm} of the resonant transitions in a metal with a cylindrical Fermi surface are described by a Lorentz curve

$$J(\omega) = \frac{2p_f \pi \hbar}{\mu^2} \left| \frac{\partial X_n}{\partial E_\perp} \right|^{-1} \frac{\gamma_{nm}}{\hbar^2 (\omega - \omega_{nm})^2 + \gamma_{nm}^2}, \quad (4.25)$$

where

$$\gamma_{nm} = \Gamma_{nm} - \frac{\pi \hbar}{\mu^2} \left| \frac{\partial X_n}{\partial E_\perp} \right|^{-1} \bar{W}(0). \quad (4.25a)$$

If the transverse energy E_\perp depends on p_z , the most effective electrons are those near $p_z = p_z^{\text{ext}}$. This makes

it possible to expand the p_z -dependent transition frequency $\omega_{nm}(p_z)$ in (4.16) about the extremal point p_z^{ext} . For concreteness we assume $p_z^{\text{ext}} = 0$ and imply this argument in all the functions that follow:

$$\omega_{nm}(p_z) \approx \omega_{nm} + \frac{1}{2} \omega_{nm}'' p_z^2, \quad \omega_{nm}'' \equiv \frac{\partial^2}{\partial p_z^2} \omega_{nm}(p_z). \quad (4.26)$$

This leads to the following dependence of Φ on p_z :

$$\Phi(p_z) \approx \frac{2\pi i}{\mu^2 |\omega_{nm}''|} \left(\frac{\partial X_n}{\partial E_\perp} \right)^{-1} [\Delta - i\nu - s p_z^2]^{-1}, \quad (4.27)$$

where

$$\Delta = \frac{2(\omega - \omega_{nm})}{|\omega_{nm}''|}, \quad \nu = \frac{2\Gamma_{nm}}{\hbar |\omega_{nm}''|}, \quad s = \frac{\omega_{nm}''}{|\omega_{nm}''|}. \quad (4.27a)$$

When solving at (4.22), we consider two opposite limiting cases.

a) Let $\Phi(p_z)$ be a much "sharper" function of p_z than W , i.e.,

$$\hbar/L \approx |\delta p_z|_W \gg |\delta p_z|_\Phi \approx |\Delta - i\nu|^{1/2}. \quad (4.28)$$

Then, as shown by simple estimates, the second term in the first part of (4.22) can be neglected when satisfaction of the inequality (4.28) is approached, i.e., we can put $\psi(p_y^n, p_z) \approx 1$. As a result we obtain for $J(\omega)$ from (4.21)

$$J(\omega) = C \left[\frac{(\Delta^2 + \nu^2)^{1/2} + s\Delta}{2(\Delta^2 + \nu^2)} \right]^{1/2}, \quad C = \frac{(2\pi)^2}{\mu^2 |\omega_{nm}''|} \left| \frac{\partial X_n}{\partial E} \right|^{-1} \quad (4.29)$$

Thus, in the case of resonance at the extremal frequencies ω_{nm}^{ext} , the dependence of the conductivity on the frequency ω has a different character than in the case of a cylindrical Fermi surface.

b) In the limiting case that is the opposite of (4.28), the function W is the "sharpest" in comparison with Φ and ψ , so that we get from (4.22)

$$\psi(p_y^n, p_z) = [1 - \Phi(p_z) \bar{W}(0)]^{-1}. \quad (4.30)$$

Substituting (4.30) in (4.21) and integrating with respect to dp_z , we arrive again at formula (4.29), with the only difference that Γ_{nm} in the definition (4.27a) of the parameter ν must be replaced by γ_{nm} in accordance with formula (4.25a).

In concluding this section, we note that integration with respect to the energy E in (2.7) also leads to additional smearing of the resonance (cf.^[19]) in the frequency band

$$\Delta\omega \approx \omega(T + \hbar\omega) / E_f. \quad (4.31)$$

This smearing, however, can be neglected and $(f - f)/\hbar\omega$ in (2.7) can be replaced by $-\delta(E - E_f)$, if

$$\hbar\omega(T + \hbar\omega) / E_f \ll \gamma_{nm}. \quad (4.32)$$

5. DISCUSSION OF RESULTS

The shapes of the absorption lines due to transitions between magnetic surface levels are described by expressions (4.25) in (4.29) derived in the preceding section. The first of them pertains to a cylindrical Fermi surface and the second to resonance at extremal frequencies.

1. We consider first the simpler case of a cylindrical Fermi surface. First, it follows from (4.25) and (4.15) that the roughnesses lead to a shift of the resonant frequency ω_{nm} relative to the unperturbed frequency

ω_{nm}^0 , owing to the level shifts δE_n and δE_m . Second, and more important, the width γ_{nm} of the resonance curve is generally not equal to the sum of the widths $\Gamma_{nm} = \Gamma_n + \Gamma_m$ of the levels between which the transition takes place. The width Γ_n of each level, as shown earlier^[15], is determined by the sum of the probabilities of the electron transition as a result of incoherent scattering by the surface from the state $|n\rangle$ into all possible surface states (including the same state $|n\rangle$, but with a random phase):

$$\Gamma_n = \frac{\pi\hbar}{2\mu^2} \left| \frac{\partial X_n}{\partial E_\perp} \right|^{-1} \sum_{k=1}^{[n+1/2]} \overline{W}(p_v^n - p_v^k). \quad (5.1)$$

If we introduce in place of the total damping Γ_n the analog of the "transport" damping γ_n , then we can rewrite (4.25a) in the form

$$\gamma_n = \gamma_n + \gamma_m. \quad (5.2)$$

The expression for γ_n differs from (5.1) only in the absence of the term with $k = n$. This means that the cross section for the scattering into this state is excluded from the "transport" damping, just as in classical kinetics scattering through a zero angle makes no contribution to the transport cross section. Using the quasiclassical asymptotic expressions (3.16) for $\partial X_n / \partial E$ and recognizing that in weak magnetic fields the resonance is ensured only by glancing electrons ($X \approx R$), we obtain for γ_n

$$\gamma_n = \frac{\pi\hbar^2}{2\mu^4} \left(\frac{E}{2m} \right)^{1/2} \sum_{k \neq n} \overline{W}(p_v^n - p_v^k). \quad (5.3)$$

If the inequality

$$|\partial p_v^n / \partial n| \ll \hbar / L, \quad (5.4)$$

is satisfied, then $\overline{W}(p_v^n - p_v^k)$ in the sum (5.3) is a slowly varying function of the number k , so that the sum can be replaced in the quasiclassical approximation by an integral. Then the "transport" damping γ_n obviously does not differ from the total damping Γ_n , and consequently the resonance width γ_{nm} is equal to the sum of the widths $\Gamma_n + \Gamma_m$ of the levels between which the transition takes place. The dependence of the total width Γ_n on the state of the surface and on the value of the magnetic field was investigated in detail earlier^[15].

The inequality (5.4) means that the distance between two successive collisions of the electron with the surface of the metal greatly exceeds the correlation radius of the roughnesses. The successive acts of electron scattering are statistically independent and there is no correlation between the "fluctuations" of the energies E_n and E_m of the different states. The limiting case opposite to (5.4) ($|\partial p_v^n / \partial n| \gg \hbar / L$) corresponds to a strong correlation of the successive reflections. In this case the surface roughnesses are so gently sloping that the main cause of the level broadening is incoherent scattering of the electron into the same state (i.e., specular reflection but with a random phase):

$$\overline{W}(0) \gg \overline{W}(p_v^n - p_v^k), \quad n \neq k, \quad (5.5)$$

It follows therefore that the transport damping

$$\gamma_n = \frac{\pi\hbar^2}{\mu^4} \left(\frac{E}{2m} \right)^{1/2} \overline{W}(a_n H^{1/2}), \quad (5.6)$$

$$a_n^3 \equiv (\pi e \hbar / c)^2 [3(n - 1/2)(2mE)^{1/2}]^{-1}$$

is in this case much smaller than the total Γ_n , and the width γ_{nm} of the resonant transition between levels turns out to be smaller than the width of each level. The reason for this fact is that in the case of long gently-sloping roughnesses the random positions of the energy levels (with sufficiently close numbers, e.g. for all glancing electrons) turn out to be correlated. The entire system of levels fluctuates in this case as a whole, so that the distance between the levels is practically unchanged in spite of the large spread (Γ_n) of these fluctuations. It is seen from (5.6) that the character of the dependence of γ_n (and consequently of γ_{nm}) on the magnetic field H strongly influences the explicit form of the spatial spectrum $\overline{W}(p)$ of the surface roughnesses. For example, in the case of a Gaussian correlation function of the roughnesses

$$\mathcal{W}(r) = \sigma^2 \exp\left(-\frac{r^2}{L^2}\right), \quad \overline{W}(p) = \frac{\sigma^2}{2\hbar} \left(\frac{L}{\pi}\right)^{1/2} \exp\left(-\frac{p^2 L^2}{4\hbar^2}\right) \quad (5.7)$$

it follows from (5.6) that

$$\gamma_n = AH^2 \exp\left[-\frac{\alpha_n^2 L^2}{4\hbar^2} H^{1/2}\right], \quad A = \frac{2\pi e^2 \sigma^2}{\hbar c^2} \left(\frac{EL}{2\pi m}\right)^{1/2}. \quad (5.8)$$

At the same time, the total damping is $\Gamma_n = AH^2$ and is practically independent of the explicit form of the correlation function.

2. In the case of resonance at the extremal transition frequencies, as follows from (4.29), the absorption line shape differs significantly from a Lorentz curve. This is due to the fact that a relatively small group of electrons, with longitudinal momenta in the interval $|\delta p_z| \Phi \approx |\Delta - i\nu|^{1/2}$, takes part in the resonance (see formula (4.27)). Since the frequencies ω_{nm} of the transitions between states with different numbered n and m depend on p_z in this case, the resonance becomes smeared out even when the electron reflection is specular. In the absence of scattering ($\nu = 0$), the absorption becomes infinite in proportion to $|\Delta|^{-1/2}$ as $\Delta \rightarrow 0$, and has a sharply asymmetrical form. Allowance for the roughnesses leads to a shift and to a smearing of the resonance maximum. A simple test of the extremum of (4.29) shows that the maximum shifts from $\Delta = 0$ by an amount $\Delta_0 = s\nu/3^{1/2}$, i.e., the resonant frequency ω_{res} satisfies the relation

$$\hbar(\omega_{\text{res}} - \omega_{nm}^0) = \delta E_n - \delta E_m + \gamma_{nm} s / \sqrt{3} \quad (5.9)$$

Consequently, unlike the case of a cylindrical Fermi surface, the position of the absorption maximum is connected not only with the average displacement of the energy levels $\delta E_n - \delta E_m$, but also with their transport width γ_{nm} . The value of $J(\omega)$ at the maximum is

$$J(\omega_{\text{res}}) = \frac{C}{\nu^{1/2}} \left(\frac{3}{4}\right)^{3/4} \approx 0.8 \frac{C}{\nu^{1/2}}. \quad (5.10)$$

We emphasize that when the inequality (4.28) is satisfied the parameter ν in (4.29) is determined by the total level width Γ_{nm} , whereas in the opposite limiting case the definition of ν contains the transport damping γ_{nm} . This is connected with the fact that in the former case, upon single scattering of an electron by the rough surface, the characteristic change of the z -component of the momentum by an amount $|\delta p_z| \overline{W} \approx \hbar / L$ is so large that the electron is no longer resonant after the scattering. Therefore scattering into a state with the same

number (but with a different p_z) also contributes to the width of the resonance. On the other hand, if the opposite inequality $|\delta p_z|_{\Phi} \gg |\delta p_z|_W$ is satisfied, then Γ_{nm} must be replaced by γ_{nm} for the same reasons as in the case of a cylindrical Fermi surface.

3. We have confined ourselves above to an analysis of the smearing of a resonance by magnetic surface levels in the case of a single-parameter spatial spectrum of the roughnesses, when there is only one macroscopic parameter L over which the correlation function $\mathcal{W}(\mathbf{r})$ changes significantly. There can actually be superimposed on such roughnesses also roughnesses of atomic scale, due to the natural roughness of the crystal surface. If this "small ripple" is in thermodynamic equilibrium, then, as shown by Andreev^[20], the reflection of the conduction electrons becomes locally specular, i.e., the diffuse character of the scattering is connected only with the macroscopic roughnesses considered above.

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