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Microscopic theory of conduction electron scattering from a random metal surface with mildly sloping asperities

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Abstract. A new integral boundary condition for the conduction electron distribution function, which describes electron scattering from a statistically rough surface at arbitrary values of the Rayleigh parameter, is derived and analysed. The average slope of asperities is assumed to be small. The method of passing to the limit of Born and Kirchhoff approximations is demonstrated. It is proved that electron reflection from a mildly sloping surface asperity is always nearly specular. An exception is the case of a narrow range of small incidence angles with respect to the boundary, for which the diffusivity of electron scattering may be caused by the shadowing effect. As an example, the role of electron–surface scattering for the normal, anomalous and infrared skin effect is analysed from a unified standpoint. For the anomalous skin effect, the change in the kind of surface scattering of the electrons with small incidence angles is shown to lead to non-monotonic frequency and temperature dependences of the metal impedance already in the leading approximation in the anomality parameter. In contrast to the known earlier microscopic boundary conditions, the new condition enables one to analyse a series of kinetic effects in which the electrons participate with large incidence angles with respect to the sample boundary.

1. Introduction

In investigating kinetic properties of bounded metal samples, the problem of the description of conduction electron scattering by surface defects is known to arise. The solution of the problem within the framework of quasiclassical theory is reduced to the formulation of a boundary condition for the electron distribution function.

The simplest form of such a boundary condition has been suggested by Fuchs [1]. In Fuchs' model, surface properties are characterized by the single phenomenological parameter ρ, having the meaning of electron specular reflection probability. This model adequately describes the limiting cases of diffuse ($\rho = 0$) and specular ($\rho = 1$) reflection. For the remaining cases, one should make allowance for both the dependence of ρ on the electron momentum and the possibility of electron scattering in non-specular directions. According to this, the boundary condition is transformed into an integral relation with respect to momenta. The scattering probability is determined by a scattering indicatrix dependent on the electron momenta before and after the interaction with the boundary, as well as on parameters of surface defects.

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Two approaches can be singled out in the theory of surface scattering of quasiparticles. The first one refers to the case of the scattering indicatrix employed whose explicit form is either not specified (see e.g. [2–4]) or chosen from model arguments [5, 6]. However, such an approach does not solve the question of metal kinetic coefficients as a function of boundary microscopic parameters; therefore it is phenomenological itself.

The second approach is developed on the basis of quantum scattering theory. It allows one to determine the dependences of conductivity, impedance and other kinetic coefficients on boundary parameters, electromagnetic wave frequency, temperature, intensities of external fields, etc. Various examples of the microscopic boundary conditions can be found elsewhere [7–12].

The most widespread surface defects are asperities. The electron scattering indicatrix for a rough surface was calculated earlier in two limiting cases, viz. the Born approximation, $k_x\zeta \ll 1$ [8], and the Kirchhoff approximation, $k_x\zeta \gg 1$ [9]. The limits of validity of the former or latter limiting cases are determined by the Rayleigh parameter $k_x\zeta$, the product of root-mean-square asperity height ζ and normal (with respect to the average metal surface) component of the electron wavevector k_x (the x axis is directed inside the metal).

In typical metals with well treated surfaces, ζ and the electron de Broglie wavelength k_F^{-1} are, as a rule, of the same order ($k_F \sim 10^8$ cm^{-1} being a conduction electron wavevector on the Fermi surface). Therefore the Born approximation $k_x\zeta \ll 1$ can be justified only for electrons with small incidence angles φ with respect to the sample boundary. Such electrons determine a whole series of well known effects in metal physics, e.g. direct-current size effects in thin metal samples, anomalous skin effect, Azbel'–Kaner cyclotron resonance, radiofrequency size effects and quantum oscillations of impedance in weak magnetic fields. Originally the theory of above-listed phenomena was constructed in the Fuchs' model [1, 13–19]. Further theoretical development is related to the use of the Born approximation [11, 12, 20–22].

However, there is a rather wide variety of electromagnetic phenomena caused by electrons with arbitrary angles $\varphi \sim 1$ of electron impact with the boundary. One can attribute to them the skin effect in the infrared frequency range, static skin effect, doppleron oscillations of impedance, transverse electron focusing in a magnetic field, etc. The influence of surface–electron scattering on these effects has so far been studied theoretically only in the framework of the phenomenological approach [4, 6, 23–25]. There was no microscopic theory because in this case the Rayleigh parameter is of the order of unity ($k_x\zeta \sim 1$), and neither the Born nor Kirchhoff approximation is valid. Meanwhile, the microscopic analysis of the phenomena in the intermediate region $k_x\zeta \sim 1$ turns out to be of importance not only itself, but also from the application viewpoint. Thus, for instance, in experiments [26] the possibility of investigation of phase transitions in 2D systems of hydrogen and deuterium on a tungsten surface using a static skin effect was demonstrated.

The formulation of the microscopic theory of surface scattering at arbitrary Rayleigh parameter values was held back by the absence of an adequate theory of wave diffraction by a rough boundary. Recently such a theory, asymptotically exact with respect to the parameter

$$\gamma/\varphi \sim k_F\zeta/k_xL \ll 1 \tag{1}$$

was suggested in a series of papers by Voronovich [27, 28] (L being the mean length of the asperities). It should be stressed that inequality (1) can hold only for surfaces with

mildly sloping asperities ($\gamma = \zeta/L \ll 1$). This is the case for the possibility, realized in [28], of constructing an asymptotic series for the surface scattering amplitude in powers of the parameter (1) independent of wavelength. Actually, mildly sloping surface asperities ($\gamma \ll 1$) can be regarded as a strongly anisotropic bulk scatterer. The characteristic range of action of such a potential is of the order ζ in one direction and L in another. Precisely because of the strong anisotropy of the potential, one managed to solve the quantum-mechanical scattering problem for an arbitrary value of Rayleigh parameter.

In the present paper, on the basis of the method developed earlier [28], the collision integral of electrons with a rough metal surface was calculated in the quadratic approximation in parameter (1). Note that both Born and Kirchhoff approximations naturally imply multiparameter expansions including, besides the limitation on the Rayleigh parameter, an independent requirement of small obliquity of asperities ($\gamma \ll 1$). The collision integral derived in this paper is a one-parameter expansion in γ/φ. The investigation [29] of metal surfaces with a scanning tunnelling microscope has demonstrated that the slope of boundary asperities γ in the samples being utilized in current experiments is actually small ($\gamma \simeq 10^{-2}$–10^{-4}). Therefore there is good reason to believe that the derived collision integral describes the interaction of electrons with the metal surface with sufficient accuracy.

So far there has been the widespread opinion that the behaviour of electron reflection from a rough metal surface is first determined by the Rayleigh parameter. It was believed that, if $k_x\zeta \geqslant 1$, i.e. the incidence angle $\varphi \sim 1$, then the reflection is diffuse. If $k_x\zeta \ll 1$, i.e. $\varphi \to 0$, then the reflection is nearly specular. Perhaps, one of the most significant results of the present paper is the refutation of such a viewpoint. An analysis of the obtained surface collision integral allows us to infer that for an arbitrary value of the Rayleigh parameter the electron reflection is nearly specular, provided that the condition (1) holds. This condition suggests that the incidence angle φ is large enough ($\gamma = \zeta/L \ll \varphi \sim k_x/k_F \leqslant 1$). Thus for surfaces with $\gamma \ll 1$ the region of very small incidence angles remains unexplored; in this region the condition (1) becomes invalid ($\varphi < \gamma \ll 1$). Assuming that reflection is diffuse in this region, the diffusivity is caused by the shadowing effect, well known in diffraction theory [30] but, unfortunately, studied incompletely.

In the last section of this paper we have considered a skin-effect problem and analysed the conclusions to which the above assumptions lead. Apparently, the shadowing effect may turn out to be essential only under the anomalous skin-effect conditions when electrons with a small incidence angle play the main role. The metal impedance for the anomalous skin-effect conditions is well known to be independent of temperature. The assumption of a diffuse scattering probability in the small incidence angle domain leads to the conclusion of the existence of the flat temperature dependence of surface impedance already within the leading approximation in the anomality parameter.

2. Boundary condition for the electron distribution function

The distribution function of electrons in a bounded sample is determined from a Boltzmann kinetic equation. Its general solution contains an integration constant, to find which one needs to formulate a boundary condition on the metal–vacuum interface.

Let us consider a metal half-space bounded by a rough surface $x = \xi(\boldsymbol{r})$, $\xi(\boldsymbol{r})$ being a random function of 2D position vector $\boldsymbol{r} = \{y, z\}$. The average surface coincides with coordinate plane $x = 0$, the x axis being directed into the metal.

To calculate metal macroscopic characteristics (e.g. conductivity, impedance, etc) one needs to use the distribution function averaged over surface random asperities. Therefore the boundary condition is formulated at the metal averaged surface, $x = 0$. Such a boundary condition manifests the relation between the averaged distribution functions of the electrons flying away from $f(k_x, \boldsymbol{k})$ and impinging on $f(-k_x, \boldsymbol{k})$, the metal surface. In general, the relation between $f(-k_x, \boldsymbol{k})$ and $f(k_x, \boldsymbol{k})$ can be written as a linear integral relationship

$$f(k_x, \boldsymbol{k}) = \int_{k' \leq k_F} \frac{d^2\boldsymbol{k}'}{(2\pi)^2} Q(\boldsymbol{k}, \boldsymbol{k}') f(-k'_x, \boldsymbol{k}'). \tag{2}$$

Since the scattering by static defects is elastic, the energy conservation law

$$k_x^2 + k^2 = k_x'^2 + k'^2 = k_F^2 \tag{3}$$

holds.

For simplicity, here and below the dispersion law for electrons is assumed to be quadratic and isotropic, $\boldsymbol{k} = \{k_y, k_z\}$ being a 2D wavevector. The equality (3) determines the dependence of normal component k_x on $k = |\boldsymbol{k}|$, and of k'_x on $k' = |\boldsymbol{k}'|$ ($k_x(k) > 0$ and $k'_x(k') > 0$).

Apparently, the integral kernel $Q(\boldsymbol{k}, \boldsymbol{k}') = Q(\boldsymbol{k}', \boldsymbol{k})$ is a probability density of a transition from the state $\boldsymbol{k}'$ to $\boldsymbol{k}$ as the electron hits the surface. Since for the equilibrium distribution function the boundary condition (2) should be an identity, the probability density satisfies an ordinary normalization condition

$$\int_{k' \leq k_F} \frac{d^2\boldsymbol{k}'}{(2\pi)^2} Q(\boldsymbol{k}, \boldsymbol{k}') = 1. \tag{4}$$

The condition (4) implies the absence of particle flux through the surface $x = 0$. Therefore, usually, instead of the kernel $Q(\boldsymbol{k}, \boldsymbol{k}')$, one introduces the kernel $V(\boldsymbol{k}, \boldsymbol{k}')$ according to the formula

$$Q(\boldsymbol{k}, \boldsymbol{k}') = \delta(\boldsymbol{k} - \boldsymbol{k}') \left(1 - \int_{q \leq k_F} \frac{d^2\boldsymbol{q}}{(2\pi)^2} V(\boldsymbol{k}, \boldsymbol{q})\right) + V(\boldsymbol{k}, \boldsymbol{k}'). \tag{5}$$

Substituting expression (5) into formula (2), we come to the following canonical form of the boundary condition

$$f(k_x, \boldsymbol{k}) = f(-k_x, \boldsymbol{k}) - \int_{k' \leq k_F} \frac{d^2\boldsymbol{k}'}{(2\pi)^2} V(\boldsymbol{k}, \boldsymbol{k}')[f(-k_x, \boldsymbol{k}) - f(-k'_x, \boldsymbol{k}')]. \tag{6}$$

This form of the boundary condition representation is more convenient for analysis and applications for two reasons. First, equality (6) implies that the particle flux conservation law holds without any additional requirement like the normalization condition (4). Secondly, in the right-hand part (6) 'specular' (first) and 'diffuse' (second) terms are explicitly singled out. The diffuse term is written as a difference between the incoming and outgoing terms, i.e. they represent an integral of electron–surface collisions.

To compute the kernel $Q(\boldsymbol{k}, \boldsymbol{k}')$ (and the kernel $V(\boldsymbol{k}, \boldsymbol{k}')$ related by equation (5)), the problem should be solved of electron wavepacket scattering by a statistically rough surface $x = \xi(\boldsymbol{r})$. The solution of this problem would lead to establishing the relation between the kernel Q and the amplitude S of plane-wave scattering from a rough surface. We do not wish to touch upon the mathematical details, as it is rather obvious that the

transition probability manifests itself through the second-order moment of S. The exact formula is of the form

$$\langle S(\boldsymbol{k}, \boldsymbol{q}) S^*(\boldsymbol{k}, \boldsymbol{q}') \rangle = (2\pi)^{-2} Q(\boldsymbol{k}, \boldsymbol{q}) \delta(\boldsymbol{q} - \boldsymbol{q}'). \tag{7}$$

Angular brackets here denote averaging over the ensemble of realizations of the random quantity $\xi(\boldsymbol{r})$ and the star symbol represents complex conjugation. The delta-function in the right-hand part of equation (7) is a consequence of statistical homogeneity of the metal surface.

Thus the problem of surface–electron scattering is reduced to finding the scattering amplitude S and calculating the correlator (7). A general mathematical theory of the S-matrix has been derived by Voronovich [27–28]. In [28] the scattering amplitude has been computed in the quadratic approximation in γ/φ, viz.

$$S(\boldsymbol{k}, \boldsymbol{q}) = -\frac{(k_x q_x)^{1/2}}{k_x + q_x} \int_{-\infty}^{\infty} \frac{\mathrm{d}^2 \boldsymbol{r}}{(2\pi)^2} \exp[-\mathrm{i}(k_x + q_x)\xi(\boldsymbol{r}) + \mathrm{i}(\boldsymbol{q} - \boldsymbol{k}) \cdot \boldsymbol{r}]$$

$$\times \left(2 + \mathrm{i} \int_{-\infty}^{\infty} \frac{\mathrm{d}^2 \boldsymbol{k}'}{(2\pi)^2} \xi(\boldsymbol{k}') \exp(\mathrm{i}\boldsymbol{k}' \cdot \boldsymbol{r}) [k_x(\boldsymbol{k} + \boldsymbol{k}')\right.$$

$$\left. + k_x(\boldsymbol{k} - \boldsymbol{k}') - k_x - q_x]\right). \tag{8}$$

Here

$$k_x(\boldsymbol{k} \pm \boldsymbol{k}') = [k_F^2 - (\boldsymbol{k} \pm \boldsymbol{k}')^2]^{1/2} \qquad q_x = k_x(\boldsymbol{q}) = (k_F^2 - q^2)^{1/2}$$

$$\xi(\boldsymbol{k}) = \int_{-\infty}^{\infty} \mathrm{d}^2 \boldsymbol{r}\, \xi(\boldsymbol{r}) \exp(-\mathrm{i}\, \boldsymbol{k} \cdot \boldsymbol{r}).$$

Let us regard the random function $\xi(\boldsymbol{r})$ ensemble as Gaussian. Construct a bilinear form (7) of scattering amplitudes (8) and perform averaging. As a result, we get the expression for Q, which, as can immediately be checked, satisfies the normalization condition (4). Omitting intermediate calculations, we present here the ultimate expression for the kernel of surface collision integral:

$$V(\boldsymbol{k}, \boldsymbol{k}') = -4\zeta^2 k_x k_x' 2\pi \int_0^{\infty} r \mathrm{d}r \mathcal{W}'(r) \frac{J_1(|\boldsymbol{k} - \boldsymbol{k}'| r)}{|\boldsymbol{k} - \boldsymbol{k}'|} \exp\{[-\zeta^2(k_x + k_x')^2][1 - \mathcal{W}(r)]\}. \tag{9}$$

Here $J_1(x)$ is a first-order Bessel function, $\mathcal{W}(r)$ is a binary correlation function of asperity heights determined according to the formula

$$\langle \xi(\boldsymbol{r}) \xi(\boldsymbol{r}') \rangle = \zeta^2 \mathcal{W}(|\boldsymbol{r} - \boldsymbol{r}'|) \tag{10}$$

and the prime on $\mathcal{W}(r)$ in equation (9) denotes a derivative with respect to r. The correlation function has a maximum at $r = 0$. The characteristic scale of $\mathcal{W}(r)$ decrease coincides with a mean roughness length L.

The boundary condition (6) with kernel (9) holds for an arbitrary value of the Rayleigh parameter $k_x\zeta$. Its region of validity is limited only by the inequality (1).

3. Analysis of the boundary condition

Let us investigate the obtained boundary condition (2) and (9) versus the Rayleigh parameter $k_x\zeta$ and find out how it changes into the known boundary conditions [8, 9].

Within the Born approximation, as

$$k_x\zeta \ll 1 \tag{11}$$

the exponent in the integrand (9) can be set to unity. As a result, the kernel $V(k, k')$ takes the form [8]

$$V(k, k') = 4\zeta^2 k_x k_x' W(|k - k'|). \tag{12}$$

Here

$$W(k) = \int_{-\infty}^{\infty} d^2 r\, \mathcal{W}(r) \exp(-i\, k \cdot r) \tag{13}$$

is a Fourier image of the correlation function $\mathcal{W}(r)$. Obviously, $W(0) \sim L^2$, L^{-1} being a characteristic scale of $W(k)$ decrease.

Within the Kirchhoff approximation, as

$$k_x\zeta \gg 1 \tag{14}$$

the main contribution to the integral (9) is given by the vicinity of point $r = 0$, so it should be calculated by the Laplace method. In so doing, the difference $1 - \mathcal{W}(r)$ is replaced by $r^2|\mathcal{W}''(0)|/2$, and $\mathcal{W}'(r) \simeq -r|\mathcal{W}''(0)|$. Performing the integration, we obtain

$$V(k, k') = \frac{8\pi k_x k_x'}{\zeta^2 (k_x + k_x')^4 |\mathcal{W}''(0)|} \exp\left(-\frac{|k - k'|^2}{2\zeta^2 (k_x + k_x')^2 |\mathcal{W}''(0)|} \right). \tag{15}$$

In the boundary condition (6) the function $V(k, k')$ (15) is sharper than the distribution function $f(-k_x', k')$. It suggests that the collision integral in equation (6) can be written in the Fokker–Planck approximation, expanding it in powers of small momentum transfer, $k - k'$. Thus the boundary condition (6) takes the differential form

$$f(k_x, k) = f(-k_x, k) + 2\zeta^2 |\mathcal{W}''(0)| (k_x^2 \nabla^2 - 2k\nabla) f(-k_x, k). \tag{16}$$

Here ∇ and ∇^2 are a two-dimensional gradient and Laplacian, respectively, in k-space. The relationship (16) for the limiting case (14) has first been obtained in [9].

Generally speaking, the behaviour of electron–surface scattering is determined not by the Rayleigh parameter $k_x\zeta$ but by the relation between the angular width ϕ of the scattering indicatrix (9) and the angle $\varphi \sim k_x/k_F$ of the electron impact with the metal boundary. In the boundary condition (6) these quantities respectively determine the variance scale of the integral kernel $V(k, k')$ and distribution function $f(-k_x', k')$.

A detailed analysis of equation (9) as a function of wavevector k' for constant k demonstrates that the characteristic angular range, within which the probability $V(k, k')$ is essentially non-zero (i.e. an angular width of scattering indicatrix), is determined by the following interpolation formula:

$$\phi \simeq (1 + k_x\zeta)/(1 + k_x L). \tag{17}$$

This formula holds at arbitrary values of $k_x\zeta$ and $k_x L$ obeying the inequality (1).

Consider first the case of flat electron impingement on the metal surface, when

$$\gamma \ll \varphi \ll \phi. \tag{18}$$

The distribution function $f(-k_x', \boldsymbol{k}')$ under integration (6) turns out to be sharper than the kernel $V(\boldsymbol{k}, \boldsymbol{k}')$. Therefore the effective region of integration in the incoming term in equation (6) is significantly less than in the outgoing one, hence 'income' can be neglected. Thus the case of flat impingement (18) is equivalent to the τ approximation in bulk scattering theory, and the boundary condition (6) degenerates into the algebraic Fuchs condition [1] with a specularity parameter ρ depending on the electron momentum and parameters of the rough boundary:

$$\rho = 1 - \int_{k' \leqslant k_F} \frac{\mathrm{d}^2 k'}{(2\pi)^2} V(\boldsymbol{k}, \boldsymbol{k}'). \tag{19}$$

Since the inequalities (18) can hold only as $k_x \zeta \ll 1$, the transition probability $V(\boldsymbol{k}, \boldsymbol{k}')$ in expression (19) is determined by the Born approximation formula (12).

In the opposite limiting case of steep impingement

$$\gamma < \phi \ll \varphi \tag{20}$$

the indicatrix $V(\boldsymbol{k}, \boldsymbol{k}')$ is sharper. Therefore the difference of the distribution functions can be expanded in powers of small wavevector transfer, $\boldsymbol{k} - \boldsymbol{k}'$. It suggests that if the impingement is steep (20), the collision integral in equation (6) could be calculated within the Fokker–Planck approximation. Naturally, for the kernel $V(\boldsymbol{k}, \boldsymbol{k}')$ the general formula (9) should be used, not the asymptote (15), which is valid only in the Kirchhoff approximation.

After this procedure, we obtain the differential boundary condition that coincides precisely with the equality (16). Such coincidence confirms the above statement that for electron scattering from a rough surface the physically different situations differ not in the Rayleigh parameter $k_x \zeta$, but by the relationship between the typical incidence angle $\varphi \sim k_x / k_F$ and the scattering indicatrix width (17).

The property of major significance for the boundary condition (6) with integral kernel (9) is that throughout its region of validity (1) it corresponds to nearly specular reflection from a rough metal surface. Actually, it is easy to see that for all the considered cases the 'diffuse' (integral) term in equation (6) appears to be small compared to $f(-k_x, \boldsymbol{k})$. For instance, as the impingement of electrons is steep (20), the second term in equation (6) indicative of the degree of diffusivity is proportional to the small parameter $(\gamma/\varphi)^2$ of the theory. It should be noted, in this respect, that smallness of the integral term in equation (6) as compared to $f(-k_x, \boldsymbol{k})$ does not imply the possibility of its allowance through the step-by-step approximation method. It is caused by the fact that the probability of surface electron scattering should be compared not with unity but with the probability of bulk scattering, which enters into the kinetic equation and can also be small.

From the above, the non-obvious statement follows that the possibility of diffuse reflection of electrons can appear only in the region of extremely small incidence angles, where the condition (1) fails. Here (at $\varphi < \gamma \ll 1$), owing to the shadowing effect (see [30]), the large-angle scattering probability increases; it may lead to diffusivity.

The shadowing effect value is determined not only by the parameter γ/φ, but also by the relation between root-mean-square asperity height ζ and the size of the Fresnel zone $(L/k_F)^{1/2}$. If

$$\zeta^2 k_F/L \ll 1 \tag{21}$$

then electrons with angles $\varphi < \gamma$ 'go round' the asperities and get into the geometrical shadow region [19]. In this case their scattering from the surface is described by the Born approximation; hence it is nearly specular.

Thus the conditions

$$\zeta/L \ll 1 \qquad \zeta^2 k_F/L \ll 1 \tag{22}$$

provide almost specular reflection of electrons with any incidence angles φ. For the possibility of diffuse reflection to arise, rather large obliquity of asperities is needed,

$$\zeta/L \gtrsim 1 \tag{23}$$

or the inequalities

$$k_x/k_F < \zeta/L \ll 1 \qquad L/\zeta^2 k_F \lesssim 1 \tag{24}$$

must hold simultaneously.

In connection with the above, one should mention the experiments by Tsoi [31], as well as by van Kempen *et al* [29] on transverse electron focusing in a magnetic field. In [31] they have observed nearly specular reflection of electrons incident on bismuth at angles $\varphi \simeq \pi/2$. As was established in experiments [29], reflection of the electrons from the (001) plane in silver is much closer to specular than from the (011) plane. An investigation carried out therein for the structure of silver planes by means of a scanning tunnelling microscope has revealed that the mean slope of asperities ζ/L on the (011) plane is essentially larger than at (001). The listed experimental facts can be naturally explained in terms of the suggested theory.

4. A skin effect in metals with rough surfaces

Let us demonstrate an application of the boundary condition (6) and (9) to the simple and well investigated example of a skin effect in metals. Earlier allowance for surface–electron scattering in skin-effect theory was made in the Born approximation (11) and the Kirchhoff approximation (14) (see the review in [11]). An attempt to go beyond these approximations was made in [5], wherein the boundary condition was written in the general form (2). However, the transition probability $Q(k, k')$ was determined phenomenologically, without referring to the microscopic approach. The boundary condition (6) and (9) suggested in this paper enables one to obtain microscopically founded results for the metal impedance in the whole domain of frequencies for different kinds of skin effect: normal, anomalous and infrared. Without dwelling on the details of standard computations, we present the ultimate expressions for the impedance.

4.1. Weak spatial dispersion

$$|l_\omega/\delta| \ll 1 \tag{25}$$

$$l_\omega = v_F/(\nu - i\omega) \qquad \delta = (c/\omega_p)(1 + i\nu/\omega)^{1/2}. \tag{26}$$

Here l_ω is an effective free path length of electrons; δ is the complex depth of the skin layer; v_F, ν and ω_p are the Fermi velocity, frequency of bulk collisions and plasma frequency of the conduction electron gas; ω is an electromagnetic wave frequency; and c is the velocity of light.

The metal impedance in the leading approximation is determined by the complex frequency $\nu - i\omega$, and the impact of surface scattering manifests itself in small corrections to the parameter (25):

$$Z = -(4\pi i\omega\delta/c^2)[1 + \tfrac{3}{16}(1-\rho)l_\omega/\delta]. \tag{27}$$

In the formula (27) the effective diffusivity coefficient is proportional to the scattering transport cross section

$$1 - \rho = \frac{8\pi}{k_F^4}\int_{k,k'\leqslant k_F} \frac{d^2k\, d^2k'}{(2\pi)^4}(k^2 - k\cdot k')V(k,k'). \tag{28}$$

In the limiting cases of large-scale and small-scale asperities, formula (28) is simplified to the following asymptotes:

$$1 - \rho = 2\xi^2|W''(0)| \qquad k_F L \gg 1 \tag{29}$$

$$1 - \rho = 32\xi^2 k_F^4 W(0)/15\pi \qquad k_F L \ll 1. \tag{30}$$

In the low-frequency region ($\omega \ll \nu$), i.e. for the normal skin effect, the correction in equation (27) related to surface scattering plays no essential role since it only slightly changes the imaginary part of the impedance. As for the region of high frequencies referring to infrared metal optics,

$$\nu, \omega_{ir} \ll \omega \ll \omega_p \qquad \omega_{ir} = \omega_p(v_F/c) \tag{31}$$

the metal impedance in the leading approximation is purely imaginary. It means that there is no electromagnetic wave energy dissipation. For this reason the strict allowance for the surface electron relaxation is of great importance, since it, together with bulk relaxation, determines the absorption capacity

$$A = \frac{c}{\pi}\operatorname{Re} Z = \frac{2\nu}{\omega_p} + \frac{3v_F}{4c}(1-\rho). \tag{32}$$

For weak spatial dispersion (25) the main contribution to conductance is due to electrons with incidence angles about $\varphi \sim 1$. The condition (1) for the validity of the suggested theory is satisfied directly for such electrons. Consequently, their reflection from the metal surface throughout the whole domain (25) is almost specular.

4.2. Strong spatial dispersion

$$|\delta/l_\omega| \ll 1. \tag{33}$$

For strong spatial dispersion (i.e. an anomalous skin effect), the impedance Z is sensitive to the kind of surface electron scattering already in the leading approximation in parameter (33). In [14] the dependence of impedance has been calculated versus the phenomenological specularity parameter ρ. Let us write the expansion of function $Z(\rho)$ for the nearly specular reflection ($1 - \rho \ll 1$):

$$Z(\rho) = \tfrac{16}{9}\pi\sqrt{3}(\omega\delta/c^2)[1 + \tfrac{5}{54}(1-\rho)]\exp(-\pi i/3) \tag{34}$$

$$\delta = (4c^2 v_F/3\pi\omega\omega_p^2)^{1/3}. \tag{35}$$

The diffuse additional term to the impedance can also be calculated through the microscopic boundary condition (6) and (9), and the diffusivity effective coefficient for the anomalous skin effect can thus be determined. After standard but cumbersome computations we get

$$1-\rho=\frac{324}{5\sqrt{3}}\frac{l_\omega^2}{\delta^2}\exp\left(\frac{i\pi}{3}\right)\int_{k,k'\le k_F}\frac{d^2k\,d^2k'}{(2\pi)^4}V(k,k')\int_0^\infty\frac{x\,dx}{(x^3-i)[k_F^2+(xl_\omega k_x/\delta)^2]}$$

$$\times\int_0^\infty\frac{x'\,dx'}{(x'^3-i)}\left(\frac{k^2}{k_F^2+(x'\,l_\omega k_x/\delta)^2}-\frac{\boldsymbol{k}\cdot\boldsymbol{k}'}{k_F^2+(x'\,l_\omega k_x'/\delta)^2}\right). \tag{36}$$

Formula (36) is convenient for numerical calculations within a wide frequency domain corresponding to the anomalous skin effect

$$\omega_n=\nu^3/\omega_{tr}^2\ll\omega\ll\omega_{tr}. \tag{37}$$

Analytical expressions for $(1-\rho)$ can be derived in limiting cases of flat and steep impingement. Turning from one case to another is made by varying the frequency ω, since it affects the incidence angle of effective electrons $|\delta/l_\omega|$, and hence the ratio φ/ϕ.

If the condition of steep impingement holds (20), then the integral over $\boldsymbol{k}'$ in formula (36) is calculated in the Fokker–Planck approximation, and the formula

$$1-\rho=a\left(\frac{l_\omega}{\delta}\right)^2\frac{\xi^2}{L^2}\exp\left(-\frac{i\pi}{3}\right)\int_0^\infty x^3w(x)\,dx \tag{38}$$

follows for the diffusivity coefficient, where $w(x)=L^{-2}W(x/L)$ is a dimensionless correlation coefficient decreasing at the distance $\Delta x\sim 1$,

$$a=\frac{1}{5}\left(\frac{12}{\pi}\right)^3\int_0^1\frac{x^2\,dx}{(1-x^2)(x^2+x+1)}\left(\frac{x^2+1}{x^2-1}\ln x-1\right)\approx 0.33.$$

As can be seen from equation (38), the diffusivity effective coefficient is proportional in this case to the small parameter (1) squared. Note that the formulae (29) and (38) were obtained earlier (see the review in [11]).

For flat impingement (18) the last term in equation (36) can be omitted. It is equivalent to neglecting the incoming term of the collision integral (6). As a result, the diffusivity coefficient takes the form

$$1-\rho=\frac{24\pi^2(3\pi)^{1/2}}{5\Gamma^2(1/4)}\frac{\delta}{l_\omega}\frac{\xi^2k_F}{L}(k_FL)^{1/2}\exp\left(\frac{i\pi}{6}\right)\int_0^\infty x^{3/2}w(x)\,dx. \tag{39}$$

Under the conditions of anomalous skin effect (33), electrons with small incidence angles, $\varphi\sim|\delta/l_\omega|$, are effective. If the condition (1) holds for them, then the scattering from the metal surface is nearly specular and the above-listed formulae for $1-\rho$ are valid. If the inequality (1) fails (see condition (24)), then, owing to the shadowing effect, one can expect a sharp increase in the probability of diffuse scattering. In the region relevant to the conditions (24) there is no quantitative theory yet. However, a qualitative analysis of impedance behaviour is possible here.

The incidence angle φ changes as the wave frequency ω or temperature T (i.e. the relaxation frequency) changes. If, as a result of this change of φ, the inequality (1) transforms into the inequality (24), then for one sample both specular and diffuse

scattering of electrons can be realized. Inasmuch as the impedance Z for diffuse scattering is 9/8 times larger than for specular, then in the temperature domain corresponding to the transition a smooth temperature dependence arises. Meanwhile, the impedance frequency dependence becomes non-monotonic. Note that the dependence $Z(T)$ manifests itself already in the leading approximation in the anomality parameter δ/l_ω, not in the temperature corrections [32, 33] studied earlier.

In order to determine the frequency range corresponding to the shadowing effect and possible diffuse scattering of electrons, let us take into account that the incidence angle $\varphi \sim |\delta/l_\omega|$ has a minimum $\varphi = \varphi_{\min}$ at $\omega \sim \nu$. If $\varphi_{\min} > \zeta/L$, then the reflection is nearly specular throughout the whole frequency range (37), so the non-monotonic frequency or temperature dependence does not emerge. The last inequality implies that

$$\omega_{ir}(\zeta/L)^{3/2} < \nu < \omega_{ir}. \tag{40}$$

For a typical metal with $\omega_{ir} \sim 10^{13}\ s^{-1}$ and $\nu \sim 10^9\ s^{-1}$, condition (40) holds provided that $\zeta/L < 10^{-3}$. This is rather a rigorous requirement to the quality of surface treatment. If it does not hold, then the frequency range emerges in which the impact of the shadowing effect is noticeable. Actually, if the left-hand inequality (40) is replaced by the inverse one, i.e. at

$$\nu < \omega_{ir}(\zeta/L)^{3/2} < \omega_{ir} \tag{41}$$

in the frequency domain

$$\omega_n(L/\zeta)^3 < \omega < \omega_{ir}(\zeta/L)^{3/2} \tag{42}$$

then the condition (1) fails. Owing to the shadowing effect, the probability of diffuse electron scattering is increased here. Thus, for instance, if $\zeta/L \sim 10^{-2}$. $\nu \sim 10^9\ s^{-1}$ and $\omega_{ir} \sim 10^{13}\ s^{-1}$, then in the frequency ω domain of 10^7 to $10^{10}\ s^{-1}$ the reflection could be diffuse though throughout the rest of the frequency domain of ω_n to ω_{ir} the reflection could be nearly specular.

To observe the change from specular reflection to diffuse reflection, it would be more convenient to study the temperature, rather than frequency, dependence. In the region of sufficiently low temperatures, when the condition (41) holds, the reflection is diffuse. As the temperature increases, the relaxation frequency ν and incidence angle φ increase. In the temperature domain where $\nu = \nu^* \sim \omega_{ir}(\zeta/L)^{3/2}$ the kind of electron scattering changes from diffuse to specular, with the impedance decreasing by a factor of 9/8. As the temperature increases further, the leading approximation impedance will not change until the condition (37) of anomalous skin effect fails. Sequentially, in the region of normal skin effect the quantity $Z(T)$ starts to increase. The indicated monotonicity in the dependence $Z(T)$ should exist at any wave frequency ω less than ω_{ir}. However, the most convenient for observations is a frequency $\omega = \nu^*$. At this frequency the temperature range in which the scattering changes from diffuse to specular is most narrow.

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