Theory of the surface scattering of electrons in metals with gently sloping surface irregularities

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The derivation and analysis are given of a new integral boundary condition for the distribution of electrons scattered by a randomly rough surface with arbitrary values of the Rayleigh parameter. It is assumed that on the average the surface irregularities are gently sloping. It is shown how the results can be reduced to the limits of the Born and Kirchhoff approximations. It is shown that the reflection of electrons from a rough surface with gently sloping irregularities is always close to the specular case. The only exception is a narrow range of angles of electron paths relative to the surface where electrons may be scattered diffusely because of the shadow effect. Under anomalous-skin-effect conditions a change in the nature of the surface scattering of electrons reaching the surface at low angles gives rise to a nonmonotonic frequency dependence and a weak temperature dependence of the impedance of a metal even in the lowest approximation with respect to the anomaly parameter. In contrast to the already known microscopic boundary conditions, the new condition makes it possible to analyze a number of transport phenomena including those involving electrons incident at large angles on a boundary.

1. INTRODUCTION

The problem of the elastic scattering of conduction electrons by a rough metal surface is closely related to the problem of wave diffraction by randomly irregular surfaces. Therefore, the main results of the theory of this surface scattering of electrons have been derived for the two limiting cases typical of the wave approach: the Born and semiclassical approximations. The ranges of validity of these approximations are determined by the value of the Rayleigh parameter $k_x\zeta$, which represents the product of the rms height of ζ of the irregularities of the normal (relative to the average surface of the investigated metal) component of the electron wave vector k_x (when the x axis is directed into the sample).

There are several effects in the physics of metals (such as the anomalous skin effect, cyclotron resonance, Khaĭkin oscillations, etc.), which are due to a small group of electrons moving almost parallel to the boundary of a sample (these are known as grazing electrons). For this group of electrons the condition $k_x\zeta \ll 1$ may be satisfied because of the smallness of the arrival angle φ and, therefore, the Born approximation may be valid.

The opposite limiting case $k_x\zeta \gg 1$ (Kirchhoff approximation) is of less practical importance, because the height of the surface irregularities ζ and the de Broglie wavelength of an electron $2\pi/k_F$ are usually of the same order of magnitude ($k_F \sim 10^8$ cm^{-1} is the wave vector on the Fermi surface). It would therefore seem that the surface can always be made more rough by increasing the height ζ and, therefore, the Rayleigh parameter. However, the Kirchhoff approximation can be used subject to the additional condition that the average slope of the irregularities $\gamma = \zeta/L$ is small (L is the average length of the irregularities) and roughening of the metal surface inevitably increases the parameter γ. Therefore, the Kirchhoff case is usually only of theoretical interest.

A theory of the surface scattering of electrons is not yet available for a wide range of the Rayleigh parameter $k_x\zeta \sim 1$. This is unfortunate, because this range is extremely important since many electrodynamic phenomena in metals, which are sensitive to the nature of the surface scattering, are associated with electrons arriving at the surface at angles of $\varphi \sim 1$. These phenomena include the skin effect in the infrared range of frequencies, the static skin effect, transverse electron focusing, Doppler oscillations in metal plates, etc.

Development of a microscopic theory of these phenomena has been hindered by the absence of a satisfactory model of wave diffraction by a rough surface with an arbitrary value of the Rayleigh parameter. Such a model, asymptotically exact in terms of the parameter

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

was recently developed in a series of papers published by Voronovich.[1-3] We must draw attention to the fact that the inequality (1) can be satisfied only for surfaces with gently sloping irregularities ($\gamma \ll 1$). This has made it possible to find an asymptotic series[1-3] for the amplitude of the surface scattering in terms of the parameter (1), which is independent of the wavelength. In fact, gently sloping ($\gamma \ll 1$) surface irregularities can be regarded as forming a strongly anisotropic bulk scatterer. The characteristic radius of action of the potential of such a scatterer along one direction is of order ζ, whereas along the surface it is of the order of L. It is this strong anisotropy of the potential that makes it possible to solve the quantum-mechanical problem of the scattering for an arbitrary value of the Rayleigh parameter $k_x\zeta$.

We employ the method developed by Voronovich[1-3] and calculate the collision integral for electrons reaching a rough surface of a metal. We do this to second order in the parameter (1). The Born and the Kirchhoff approximations are many-parameter expansions which not only impose re-

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strictions on the value of the Rayleigh parameter, but also an independent requirement that the surface irregularities should be gently sloping ($\gamma \ll 1$). The integral parameter obtained below, however, is a one-parameter expansion in γ/φ. Studies of metal surfaces with the aid of a tunnel microscope[4] showed that the slope γ of the surface irregularities of samples used in modern experiments is indeed small ($\gamma \sim 10^{-2}$–10^{-4}). Therefore, there are grounds for assuming that our collision integral describes sufficiently accurately the interaction of electrons with a real surface of a metal.

Up to now it has been held widely (see, for example, Ref. 5) that the nature of the scattering of electrons from a rough surface of a metal is governed primarily by the Rayleigh parameter. It has been assumed that for $k_x\zeta \geqslant 1$, i.e., that if the angle of arrival is $\varphi \to \pi/2$, then the reflection is diffuse, but for $k_x\zeta \ll 1$, i.e., if $\varphi \to 0$, then the reflection is nearly specular. One of the most important results of the present study is a refutation of this point of view. An analysis of our surface collision integral led us to the conclusion that, apart from the dependence on the value of the Rayleigh parameter, the reflection of electrons is nearly specular if the condition (1) is obeyed. This condition means that the arrival angle φ is sufficiently large ($\gamma \ll \varphi \leqslant 1$; $\varphi \sim k_x/k_F$). We can expect diffuse scattering of electrons from a boundary with gently sloping irregularities ($\gamma \ll 1$) only in the range of very low arrival angles, i.e., when the condition (1) is disobeyed. The reason for the diffuse scattering is obviously the shadow effect, well known from the theory of diffraction,[5] but not yet fully understood.

2. BOUNDARY CONDITION FOR THE ELECTRON DISTRIBUTION FUNCTION

The electron distribution function for a bounded sample is found from the Boltzmann transport equation. Its general solution contains integration constants, which can be found by formulating the boundary conditions at the metal–vacuum interface. The boundary condition expresses the relationship between the distribution functions of electrons departing from $f(k_x, \mathbf{k})$ and arriving at $f(-k_x, \mathbf{k})$ surface. In general, this relationship can be described in the integral form (see the review in Ref. 6), which automatically ensures the absence of a flux of particles across the surface of a sample:

$$f(k_x, \mathbf{k}) = f(-k_x, \mathbf{k}) - \int_{k' \leqslant k_F} \frac{d^2\mathbf{k}'}{(2\pi)^2} V(\mathbf{k}, \mathbf{k}') \times [f(-k_x, \mathbf{k}) - f(-k_x', \mathbf{k}')]. \quad (2)$$

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

$$k_x^2 + k^2 = k_x'^2 + k'^2 = k_F^2. \quad (3)$$

Here and below we assume, for the sake of simplicity, that the electron dispersion law is quadratic and isotropic; $\mathbf{k} = \{k_y, k_z\}$ is a two-dimensional wave vector. The equality (3) governs the dependence of the normal component k_x on $k = |\mathbf{k}|$ and $k_x'(k')$; $k_x(k) > 0$ and $k_x'(k') > 0$. The kernel of the collision integral $V(\mathbf{k}, \mathbf{k}')V(\mathbf{k}', \mathbf{k})$ was calculated by Fal'kovskiĭ[7] and in the Born approximation also by Okulov and Ustinov[8] who used the Kirchhoff approximation. In order to calculate $V(\mathbf{k}, \mathbf{k}')$ for an arbitrary value of the Rayleigh parameter, we must consider the general problem of the scattering of electrons by a rough surface.

Let us assume that the half-space occupied by the metal is bounded by a rough surface $x = \xi(\mathbf{r})$, where $\xi(\mathbf{r})$ is a random function of a two-dimensional radius vector $\mathbf{r} = \{y, z\}$. The average surface coincides with the coordinate plane $x = 0$ and the x axis is directed into the metal. A plane wave

$$\psi_{in}(x, \mathbf{r}) = k_x^{-1/2} \exp(-ik_x x + i\mathbf{kr}) \quad (4)$$

incident on the $x = \xi(\mathbf{r})$ boundary creates a scattered field $\psi_{sc}(x, \mathbf{r})$, which can be represented in the form

$$\psi_{sc}(x, \mathbf{r}) = \int_{-\infty}^{\infty} \frac{d^2\mathbf{q}}{q_x^{1/2}} S(\mathbf{q}, \mathbf{k}) \exp(iq_x x + i\mathbf{qr}), \qquad \operatorname{Im} q_x > 0. \quad (5)$$

The function $S(\mathbf{q}, \mathbf{k})$ is the surface-scattering amplitude. Its properties were considered in the review of Andreev[9] for the case of grazing incidence of electrons in metals with a complex Fermi surface. The general mathematical theory of the surface scattering matrix S was developed by Voronovich in Refs. 1 and 2.

The wave functions of an electron incident and reflected by the boundary of a metal can be expanded as a Fourier integral in terms of plane waves:

$$\Psi_{inc}(x, \mathbf{r}) = \int_{-\infty}^{\infty} \frac{d^2\mathbf{k}}{k_x^{1/2}} \varphi_-(k_x, \mathbf{k}) \exp(-ik_x x + i\mathbf{kr}), \quad (6)$$

$$\Psi_{refl}(x, \mathbf{r}) = \int_{-\infty}^{\infty} \frac{d^2\mathbf{k}}{k_x^{1/2}} \varphi_+(k_x, \mathbf{k}) \exp(ik_x x + i\mathbf{kr}). \quad (7)$$

On the other hand, it is quite obvious that the state of a reflected electron characterized by Eq. (7) can be expressed, using Eqs. (4)–(6), in terms of the scattering amplitude S:

$$\Psi_{refl}(x, \mathbf{r}) = \int_{-\infty}^{\infty} d^2\mathbf{k}\, \varphi_-(k_x, \mathbf{k}) \int_{-\infty}^{\infty} \frac{d^2\mathbf{q}}{q_x^{1/2}} S(\mathbf{q}, \mathbf{k}) \exp(iq_x x + i\mathbf{qr}). \quad (8)$$

We interchange the orders of integration in this expression and relabel the integration variables $\mathbf{k}$ and $\mathbf{q}$. Comparing the resultant expression with Eq. (7), we readily obtain the relationship between the Fourier coefficients φ_+ and φ_-:

$$\varphi_+(k_x, \mathbf{k}) = \int_{-\infty}^{\infty} d^2\mathbf{q}\, S(\mathbf{k}, \mathbf{q}) \varphi_-(q_x, \mathbf{q}). \quad (9)$$

The Fourier coefficients $\varphi_+(k_x, \mathbf{k})$ are the wave functions of an electron in the mixed $(x, \mathbf{k})$ representation at the average boundary of the metal in the $x = 0$ plane. The diagonal elements of the density matrix obtained in this approximation for $x = 0$ are $|\varphi_\pm(k_x, \mathbf{k})|^2$. Hence, it is clear that in the one-electron approximation the classical distribution function $f(\pm k_x, \mathbf{k})$ for the average (effective) boundary at $x = 0$ is the average of $|\varphi_\pm(k_x, \mathbf{k})|^2$ over the surface irregularities:

$$f(\pm k_x, \mathbf{k}) = \langle |\varphi_\pm(k_x, \mathbf{k})|^2 \rangle \theta(k_F^2 - k^2). \quad (10)$$

The angular brackets denote here the averaging of an ensem-

ble of realizations of the random function $\xi(\mathbf{r})$; $\theta(x)$ is the Heaviside theta function.

It follows from the definition (10) and Eq. (9) that the relationship between the distribution functions of the reflected and incident electrons can be expressed in terms of the second moment of the scattering amplitude S. In view of the statistical homogeneity of a random surface, we find that this moment is described by

$$\langle S(\mathbf{k}, \mathbf{q}) S^*(\mathbf{k}, \mathbf{q}') \rangle = (2\pi)^{-2} Q(\mathbf{k}, \mathbf{q}) \delta(\mathbf{q}-\mathbf{q}'). \quad (11)$$

Therefore, the required boundary condition can be described by

$$f(k_x, \mathbf{k}) = \int_{k' \leqslant k_F} \frac{d^2\mathbf{k}'}{(2\pi)^2} Q(\mathbf{k}, \mathbf{k}') f(-k_x', \mathbf{k}'). \quad (12)$$

It is obvious that the integral kernel $Q(\mathbf{k}, \mathbf{k}') = Q(\mathbf{k}', \mathbf{k})$ represents the probability density of a transition from a state $\mathbf{k}$ to a state $\mathbf{k}'$ as a result of collision of a particle with the surface. Since the boundary condition (12) can be satisfied identically, for an equilibrium distribution function, the probability density $Q(\mathbf{k}, \mathbf{k}')$ obeys the usual normalization condition:

$$\int_{k' \leqslant k_F} \frac{d^2\mathbf{k}'}{(2\pi)^2} Q(\mathbf{k}, \mathbf{k}') = 1. \quad (13)$$

The explicit form of the kernel $Q(\mathbf{k}, \mathbf{k}')$ depends on the nature of the scattered quasiparticles. They may be not only electrons, but—for example—also phonons. In the case of these two types of quasiparticle we find that different boundary conditions apply on the true (nonaverage) surface of a sample described by $x = \xi(\mathbf{r})$. In the case of electrons this is the Dirichlet condition for a wave function:

$$(\Psi_{\text{inc}} + \Psi_{\text{refl}})_{x=\xi(\mathbf{r})} = 0, \quad (14)$$

whereas for phonons in superfluid helium, it is the Neumann condition for the velocity potential:

$$\frac{\partial}{\partial n}(\Psi_{\text{inc}} + \Psi_{\text{refl}})_{x=\xi(\mathbf{r})} = 0, \quad (15)$$

where $\mathbf{n}$ is the normal to the surface $x = \xi(\mathbf{r})$. For this reason the explicit form of the scattering amplitude $S(\mathbf{k}, \mathbf{q})$ and, consequently, of the kernel $Q(\mathbf{k}, \mathbf{k}')$ for electrons is different from that for phonons. The problem of phonon scattering in superfluid helium by the irregularities of the walls of a capillary was solved in the Born approximation by Adamenko and Fuks.[10]

Therefore, the scattering of quasiparticles by static defects of a boundary reduces to finding the scattering amplitude $S(\mathbf{k}, \mathbf{q})$ and calculating the correlation function of Eq. (11). Since in our case the quasiparticles are electrons, we write down the scattering amplitude to second order in the parameter. According to Ref. 3, we have

$$S(\mathbf{k}, \mathbf{q}) = -\frac{(k_x q_x)^{1/2}}{k_x + q_x} \int_{-\infty}^{\infty} \frac{d^2\mathbf{r}}{(2\pi)^2} \exp[-i(k_x+q_x)\xi(\mathbf{r}) + i(\mathbf{q}-\mathbf{k})\mathbf{r}]$$
$$\times \left\{ 2 + i \int_{-\infty}^{\infty} \frac{d^2\mathbf{k}'}{(2\pi)^2} \xi(\mathbf{k}') \exp(i\mathbf{k}'\mathbf{r}) \right.$$
$$\left. \times [k_x(\mathbf{k}+\mathbf{k}') + k_x(\mathbf{k}-\mathbf{k}') - k_x - q_x] \right\}. \quad (16)$$

Here, $k_x(\mathbf{k} \pm \mathbf{k}') = [k_F^2 - (\mathbf{k} \pm \mathbf{k}')^2]^{1/2}$, $q_x = k_x(\mathbf{q}) = (k_F^2 - q^2)^{1/2}$, and

$$\xi(\mathbf{k}) = \int_{-\infty}^{\infty} d^2\mathbf{r} \xi(\mathbf{r}) \exp(-i\mathbf{k}\mathbf{r}).$$

We use the scattering amplitudes of Eq. (16) to form a bilinear combination of Eq. (11), and we shall subject it to averaging. Clearly, the averaging result depends on the law governing the distribution of the random functions $\xi(\mathbf{r})$. We shall assume that the distribution of fluctuations obeys the Gaussian law. This most frequently used distribution describes satisfactorily a random surface of a metal formed under the influence of a large number of independent factors. If the averaging is carried out in accordance with the rules of the Gaussian statistics, we obtain the following expression for the probability $Q(\mathbf{k}, \mathbf{k}')$:

$$Q(\mathbf{k}, \mathbf{k}') = \frac{4k_x k_x'}{(k_x+k_x')^2} \int_{-\infty}^{\infty} d^2\mathbf{r} \exp[i(\mathbf{k}'-\mathbf{k})\mathbf{r}$$
$$-\zeta^2(k_x+k_x')^2[1-\mathscr{W}(\mathbf{r})]]$$
$$\times \left\{ 1 + \zeta^2(k_x+k_x') \int \frac{d^2\mathbf{q}}{(2\pi)^2} W(q) (\exp(i\mathbf{q}\mathbf{r}) - 1] \right.$$
$$\left. \times [k_x(\mathbf{k}-\mathbf{q}) + k_x(\mathbf{k}'+\mathbf{q}) - k_x - k_x'] \right\}. \quad (17)$$

The integration with respect to $\mathbf{q}$ in Eq. (17) is carried out in domains where the quantities $k_x(\mathbf{k}+\mathbf{q})$ and $k_x(\mathbf{k}-\mathbf{q})$ are real. The rms height ζ of the surface irregularities and the correlation functions $\mathscr{W}(r)$ and $W(k)$ are defined as follows:

$$\langle \xi(\mathbf{r}) \xi(\mathbf{r}') \rangle = \zeta^2 \mathscr{W}(|\mathbf{r}-\mathbf{r}'|),$$
$$W(k) = \int_{-\infty}^{\infty} d^2\mathbf{r} \mathscr{W}(r) \exp(-i\mathbf{k}\mathbf{r}).$$

The binary correlation function $\mathscr{W}(r)$ varies over distances of the order of the average irregularity length L and its Fourier transform $W(k)$ on a scale of $2\pi/L$.

We apply the boundary condition in the form of Eq. (2) because it will be convenient both in our analysis and in applications. The kernels $Q(\mathbf{k}, \mathbf{k}')$ of Eq. (12) and $V(\mathbf{k}, \mathbf{k}')$ in Eq. (2) are related by

$$Q(\mathbf{k}, \mathbf{k}') = V(\mathbf{k}, \mathbf{k}') + \delta(\mathbf{k}-\mathbf{k}') \left[1 - \int_{q \leqslant k_F} \frac{d^2\mathbf{q}}{(2\pi)^2} V(\mathbf{k}, \mathbf{q}) \right]. \quad (18)$$

We can determine $V(\mathbf{k}, \mathbf{k}')$ if we represent the function $Q(\mathbf{k}, \mathbf{k}')$ of Eq. (17) in the form of a sum of smooth and circular (delta-function) terms. Dropping the cumbersome identity transformations, we give the final result for the function $V(\mathbf{k}, \mathbf{k}')$:

$$V(\mathbf{k}, \mathbf{k}') = -4\zeta^2 k_x k_x' \cdot 2\pi \int_0^{\infty} r\, dr \mathscr{W}'(r)$$
$$\times \frac{J_1(|\mathbf{k}-\mathbf{k}'|r)}{|\mathbf{k}-\mathbf{k}'|} \exp\{-\zeta^2(k_x+k_x')^2[1-\mathscr{W}(r)]\}. \quad (19)$$

Here, $J_1(x)$ is a Bessel function of the first order and a prime on the correlation function denotes a derivative with respect to r. Representation of the kernel $Q(\mathbf{k}, \mathbf{k}')$ in the form of Eq. (18) is possible only if it satisfies the normalization condition of Eq. (13). Otherwise, Eq. (18) has no solution.

The boundary condition of Eq. (2) together with the kernel of Eq. (19) is valid for any value of the Rayleigh parameter $k_x\zeta$. Its range of validity is limited only by the inequality (1).

3. ANALYSIS OF THE BOUNDARY CONDITION

1. We now investigate the boundary condition described by Eqs. (2) and (19) as a function of the Rayleigh parameter $k_x\zeta$ and determine how this condition reduces to the familiar conditions.[7,8]

In the Born approximation if

$$k_x\zeta \ll 1, \tag{20}$$

the exponential function in the integral of Eq. (19) can be assumed to be unity. The kernel $V(\mathbf{k}, \mathbf{k}')$ then becomes

$$V(\mathbf{k}, \mathbf{k}') = 4\zeta^2 k_x k_x' W(|\mathbf{k}-\mathbf{k}'|). \tag{21}$$

This is precisely the transition probability used in Ref. 7.

In the Kirchhoff approximation, when

$$k_x\zeta \gg 1, \tag{22}$$

the main contribution to the integral of Eq. (19) comes from the vicinity of the point $r = 0$ and this contribution must be calculated by the Laplace method. Then, the difference $1 - \mathscr{W}(r)$ is replaced with $r^2|\mathscr{W}''(0)|/2$ and we have $\mathscr{W}'(r) \approx -r|\mathscr{W}''(0)|$. Integration then gives

$$V(\mathbf{k}, \mathbf{k}') = \frac{8\pi k_x k_x'}{\zeta^2 (k_x + k_x')^4 |\mathscr{W}''(0)|} \times \exp\left[-\frac{|\mathbf{k}-\mathbf{k}'|^2}{2\zeta^2 (k_x + k_x')^2 |\mathscr{W}''(0)|} \right]. \tag{23}$$

The function $V(\mathbf{k}, \mathbf{k}')$ of Eq. (23), used in the boundary condition (2), is sharper than the distribution function $f(-k_x', \mathbf{k}')$. It follows that the collision integral in Eq. (2) can be obtained also in the Fokker–Planck approximation[11] by expanding it in terms of a small change in the momentum $\mathbf{k} - \mathbf{k}'$. Therefore, the boundary condition (2) assumes the following differential form:

$$f(k_x, \mathbf{k}) = f(-k_x, \mathbf{k}) + 2\zeta^2 |\mathscr{W}''(0)| (k_x^2 \nabla^2 - 2\mathbf{k}\nabla) f(-k_x, \mathbf{k}). \tag{24}$$

Here, ∇ and ∇^2 represent the two-dimensional forms of the gradient and Laplacian in the k space. The relationship (24) was first obtained for the limiting case of Eq. (22) in Ref. 8.

2. In general, the nature of the surface scattering of electrons is not governed by the Rayleigh parameter $k_x\zeta$, but by the ratio of the angular width ϕ of the scattering indicatrix (19) and the angle $\varphi \sim k_x/k_F$ of arrival of electrons at the boundary of a metal. In the boundary condition (2) these quantities determine, respectively, the scales of changes in the integral kernel $V(\mathbf{k}, \mathbf{k}')$ and in the distribution function $f(-k_x', \mathbf{k}')$. We now analyze Eqs. (2) and (19) as a function of the values of the parameter ϕ/φ.

We begin with the case of large-scale irregularities typical of metals, when the correlation radius L is much greater than the de Broglie electron wavelength $2\pi/k_F$:

$$k_F L \gg 1. \tag{25}$$

We can readily show that if the condition (25) is obeyed, the probability of the transition described by Eq. (19) and considered as a function of the difference $|\mathbf{k} - \mathbf{k}'|$ has a maximum at $\mathbf{k}' = \mathbf{k}$ whose width is of order $(1 + k_x\zeta)/L$. Such a change in the longitudinal wave vector $\mathbf{k}$ corresponds to the angular width of the scattering indicatrix

$$\phi \propto (1 + k_x\zeta)/k_x L. \tag{26}$$

We now consider the case of steep incidence of the electrons on a rough surface of a metal when $\gamma < \phi \ll \phi$, i.e.,

$$\zeta/L < (1 + k_x\zeta)/k_x L \ll k_x/k_F. \tag{27}$$

It follows from the inequality of Eq. (27) that in the steep-incidence case the indicatrix $V(\mathbf{k}, \mathbf{k}')$ becomes sharper in the integral (2). Therefore, the difference between the distribution functions can be expanded as a Taylor series in the small momentum transfer $\mathbf{k} - \mathbf{k}'$. It follows that in the situation described by Eqs. (25) and (27) the surface collision integral in Eq. (2) can be calculated in the Fokker–Planck approximation. Naturally, the kernel $V(\mathbf{k}, \mathbf{k}')$ can be described by a general expression (19) and not by the asymptote (23), which is valid only in the Kirchhoff approximation.

The differential boundary condition which is then obtained is exactly the same as that given by Eq. (24). This agreement confirms the validity of the earlier assumption that when electrons are scattered by a rough boundary, physically different situations differ not in the Rayleigh parameter $k_x\zeta$, but in the ratio of the characteristic arrival angle $\varphi \sim k_x/k_F$ to the width of the scattering indicatrix ϕ. In fact, the condition (27) for validity of Eq. (24) includes not only a wide range of the values of the Rayleigh parameter of Eq. (22), but also partly the range of the Born approximation of Eq. (20). In other words, the Fokker–Planck expansion for the kernel of Eq. (21) also gives the boundary condition of Eq. (24).

We next consider the case when electrons are incident at a smaller angle ($\gamma \ll \varphi \ll \phi$):

$$\zeta/L \ll k_x/k_F \ll (1 + k_x\zeta)/k_x L. \tag{28}$$

The distribution function $f(-k_x', \mathbf{k}')$ in the integral of Eq. (2) is sharper than the kernel $V(\mathbf{k}, \mathbf{k}')$. Therefore, the effective integration domain for the incoming term in Eq. (2) is considerably less than for the outgoing term, and we can ignore the incoming term. Therefore, the boundary condition (2) transforms to the algebraic condition of Fuchs[12] with the specularity parameter ρ dependent on the electron momentum and on the microscopic parameters of a rough boundary:

$$\rho = 1 - \int_{k' \leqslant k_F} \frac{d^2\mathbf{k}'}{(2\pi)^2} V(\mathbf{k}, \mathbf{k}'). \tag{29}$$

Since the inequalities of Eq. (28) may be satisfied only if $k_x\zeta \ll 1$, the transition probability $V(\mathbf{k}, \mathbf{k}')$ in Eq. (29) is governed by the Born approximation of Eq. (21).

The case of small-scale irregularities

$$k_F L \ll 1 \tag{30}$$

may be realized in semimetals and in metals with a complex Fermi surface for small groups of electrons with $k_F \ll 10^8$ cm^{-1}. In the case of samples characterized by small-scale ($k_F L \ll 1$) gently sloping ($\zeta/L \ll 1$) irregularities the Rayleigh parameter is always small ($k_x \zeta \ll 1$), and the transition probability $V(\mathbf{k}, \mathbf{k}')$ is governed by Eq. (21). The correlation function $W(|\mathbf{k}-\mathbf{k}'|)$ in the boundary condition (2) can then be regarded as constant throughout the domain of integration with respect to $\mathbf{k}'$ and equal to $W(0)$. The Born approximation of Eq. (21) is then valid also in the case when $k_F L \sim 1$.

It should be pointed out that the above analysis of the boundary condition of Eq. (2) with the kernel of Eq. (19) can be carried out from a unified standpoint if the angular width of the scattering indicatrix is described by the following interpolation expression:

$$\phi \propto (1+k_x\zeta)/(1+k_x L), \tag{31}$$

which is valid for any value of $k_x\zeta$ and $k_x L$.

3. A fundamental property of the boundary condition (2) with the integral kernel (19) is that, throughout the range of its validity given by Eq. (1), it represents the case of near-specular reflection of electrons from a rough surface of a metal. In fact, we can readily see that in all the cases under discussion the "diffuse" (integral) term in Eq. (2) is small compared with $f(-k_x, \mathbf{k})$. For example, if $\gamma < \phi \ll \varphi$, when the Fokker–Planck equation can be applied, the second term in Eq. (24) representing the degree of diffuseness is governed by a small parameter of the theory $(\gamma/\varphi)^2 \ll 1$. Hence, we reach a nonobvious conclusion that the diffuse reflection of electrons is possible only in the range of very small arrival angles when the condition (1) breaks down. Here ($\varphi < \gamma$), the shadow effect[5] increases the probability of scattering through large angles and this makes for diffuse scattering.

The shadow effect is governed not only by the parameter φ/γ, but also by the relationship between the average height of irregularities ζ and the size of a Fresnel zone $(L/k_F)^{1/2}$. If

$$\zeta^2 k_F/L \ll 1, \tag{32}$$

electrons "bend around" irregularities because of diffraction and reach the geometric shadow region.[13] The scattering of quasiparticles arriving at a boundary at angles $\varphi < \gamma$ is then described by the Born approximation and is consequently near-specular.

It therefore follows that the conditions

$$\zeta/L \ll 1, \ \zeta^2 k_F/L \ll 1 \tag{33}$$

ensure almost specular reflection of electrons for any arrival angle φ. The scattering can be diffuse if the slope of the irregularities is steep

$$\zeta/L \geqslant 1 \tag{34}$$

or when the following inequalities can be satisfied simultaneously:

$$k_x/k_F < \zeta/L \ll 1, \ L/\zeta^2 k_F \leqslant 1. \tag{35}$$

In this connection it is worth mentioning the experiments of Tsoĭ[14] and of Van Kempen *et al.*[4] on transverse focusing of electrons in a magnetic field. Near-specular reflection on a (001) face of silver was reported in Ref. 14. It was closer to specular than for a (011) face. A study of the structure of the faces of silver, carried out using a scanning tunnel microscope reported in Ref. 14, showed that the average slope ζ/L of irregularities on the (011) face was considerably greater than on the (001) face. The listed experimental observations can be explained in a natural manner using the theory proposed above.

4. The above conclusion that the diffuse reflection of electrons is possible in the case of extremely small arrival angles leads to an unexpected prediction of frequency and temperature dependences of the impedance Z of a metal under anomalous skin effect conditions.

The anomalous skin effect is observed in the following range of the incident wave frequencies ω:

$$\omega_n = \nu^3/\omega_{ir}^2 < \omega < \omega_{ir} = \omega_p (v_F/c), \tag{36}$$

where v_F, ν, and ω_p are the Fermi velocity, the frequency of bulk collisions, and the plasma frequency of a gas of conduction electrons; c is the velocity of light. The hf admittance of a metal is governed by the effective electrons with low incidence angles φ:

$$\varphi \sim \delta/|l_\omega| \ll 1, \tag{37}$$

$$\delta = (4c^2 v_F/3\pi\omega\omega_p^2)^{1/3}, \tag{38}$$

$$l_\omega = v_F/(\nu - i\omega). \tag{39}$$

It is obvious that by varying the wave frequency ω or the temperature T (i.e., the relaxation frequency ν) we can alter the arrival angle φ without disturbing the condition of anomalous behavior of the skin effect of Eq. (37). If such a change in φ results in a transition from the inequality (1) to the inequality (35), then the same sample may exhibit both specular and diffuse reflection of electrons. Since the impedance Z for the diffuse reflection case is 9/8 times greater than in the specular case, it follows that in the range of temperatures corresponding to such a transition the temperature dependence of the impedance should be smooth. The frequency dependence of the impedance however becomes nonmonotonic. Note that the dependence $Z(T)$ appears even in the lowest approximation in terms of the anomaly parameter δ/l_ω and not in the temperature corrections investigated earlier.[6,15,16]

We can determine the range of frequencies ω corresponding to the diffuse scattering of electrons if we bear in mind that the arrival angle of Eq. (37) has its minimum $\varphi = \varphi_{\min}$ at $\omega \sim \nu$. If $\varphi_{\min} > \zeta/L$, the reflection is near-specular throughout the full range of frequencies defined by Eq. (36) and the nonmonotonic frequency or temperature dependence does not appear. The last inequality means that

$$\omega_{ir}(\zeta/L)^{1/2} < \nu < \omega_{ir}. \tag{40}$$

The condition (40) is satisfied by a typical metal with $\omega_{ir} \sim 10^{13}\ s^{-1}$ and $\nu \sim 10^9\ s^{-1}$ if $\zeta/L < 10^{-3}$. This is a fairly stringent requirement on the quality of the surface treatment. If it is not satisfied, there is a frequency interval where the shadow effect is important. In fact, if the left-hand inequality in Eq. (40) is reversed, i.e., for

$$\nu < \omega_{ir}(\zeta/L)^{1/2} < \omega_{ir}, \tag{41}$$

the condition (1) breaks down at frequencies

$$\omega_n (L/\zeta)^3 < \omega < \omega_{ir} (\zeta/L)^{1/2}. \quad (42)$$

The shadow effect then increases the probability of the diffuse scattering of electrons. For example, for $\zeta/L \sim 10^{-2}$, $\nu \sim 10^9\ s^{-1}$, and $\omega_{ir} \sim 10^{13}\ s^{-1}$, then in the range of frequencies ω from 10^7 to $10^{10}\ s^{-1}$, the reflection is diffuse although at all other frequencies from ω_n to ω_{ir} the reflection is near-specular.

We can observe the transition from the specular to diffuse reflection most conveniently by considering the temperature rather than the frequency dependence. At sufficiently low temperatures when the condition (41) is satisfied, the reflection is diffuse. An increase in temperature increases the relaxation frequency ν and the angle of arrival φ. In the temperature range where $\nu = \nu^* \sim \omega_{ir} (\zeta/L)^{3/2}$, there is a change in the nature of the scattering of electrons from diffuse to specular and the impedance decreases by a factor of 9/8. A further increase in temperature does not alter the impedance considered in the lowest approximation as long as the anomalous skin effect condition (36) holds. Then, $Z(T)$ begins to rise in the range of the normal skin effect. This nonmonotonic behavior of $Z(T)$ should be observed for any frequency of a wave ω, provided it is less than ω_{ir}. However, the frequency $\omega = \nu^*$ is the most convenient for observations. At this frequency the temperature interval where the nature of the scattering changes is the narrowest.

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