About boundary conditions for kinetic equations in metal

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Abstract. Boundary conditions for kinetic equations describing the dynamics of electrons in the metal were analyzed. The boundary condition of the Fuchs and the boundary condition of Soffer were considered. The Andreev conditions for almost tangential moving electrons were taken into account. It is shown that the Soffer boundary condition does not satisfy this condition. The boundary condition was proposed that satisfies the Andreev condition. It is shown that this boundary condition passes in the limiting case into the mirror–diffuse Fuchs boundary condition.

1. Introduction
To describe the dynamics of electrons in the metal along with the kinetic equation one requires boundary conditions. These boundary conditions determine the nature of the interaction of electrons with the metal surface. Most often the mirror–diffuse Fuchs boundary condition are used. This condition implies that $q$–part of the electrons is reflected from the surface in the mirror manner. The remaining electrons are diffuse reflected. Then the electron distribution function $f$ on the surface changes as follows [1]— [3]

$$ f(v) = qf(v') + (1 - q)f_0(v), v' = v - 2n(nv). \quad (1) $$

Here $v$ – the electron velocity before the collision with surface, $v_0$ – the electron velocity after collision with the surface, $n$ – a unit normal to the surface. The function $f_0(v)$ – the equilibrium distribution function. For the degenerate electron gas in the metal it has the following form

$$ f_0(v) = \Theta(E_F - E), E = \frac{mv^2}{2}. $$

Here $E$ – electron energy, $E_F$– the Fermi energy, $\Theta(x)$ – the Heaviside step function. It is equal to zero when $x < 0$. In other cases, it is equal to unit.

2. Kinetic equation
In the Fuchs boundary conditions (1), the value of $q$ is considered constant. However, the coefficient of reflectivity $q$ should depend on the angle of incidence of electrons on the metal surface.

In the work [4], it is shown that the reflectivity coefficient $q = q(\theta)$ ($\theta$ – the angle of incidence of the electron on the border) tends to one when the angle of incidence $\theta$ tends to $\pi/2$. From this it follows that the reflectivity coefficient $q = q(\theta)$ at $\theta \to \pi/2$ can be represented as the following decomposition
Here $a_n$ — some coefficients depending on the properties of metal surface.

It was proposed the model describing the dependence of the reflectivity coefficient on the angle of incidence of electrons on metal surface [5]

$$q(\theta) = \exp\left[-\left(-4\pi G \cos \theta\right)^2\right], \quad G = \frac{h_s}{\lambda_F}. \tag{3}$$

In equation (3) value $h_s$ — the mean-squared height of the surface relief, $\lambda_F$ — the wavelength of an electron on the Fermi surface.

This dependence of the reflectivity coefficient on the incidence angle of electrons on the metal surface (3) has been used in several papers [6]– [8].

Let us consider the behavior of the reflectivity coefficient $q$ with almost tangential incidence of the electron onto the metal surface in the model of Soffer (3). Then $\theta \to \pi/2$ and $\cos \theta \to 0$. Therefore

$$q(\theta) \approx 1 - A (\cos \theta)^2. \tag{4}$$

Hence $q(\theta) \sim 1 - A (\cos \theta)^2$ in this limit.

This contradicts to the Andreev condition (2). In the Soffer model the reflectivity coefficient $q$ tends to unit too fast at $\theta \to \pi/2$.

Let us consider the model boundary conditions. These boundary conditions have to meet the Andreev condition (2). In addition they have under certain parameter values to go into Fuchs boundary conditions. And at certain angles of incidence of electrons on the metal surface with the appropriate parameters boundary conditions must reproduce the Soffer boundary conditions (3).

The following expression satisfies these conditions

$$q(\theta) = q_0 + (1 - q_0)\exp(-b_1 \cos \theta - b_2 \cos^2 \theta). \tag{5}$$

In this expression there are 3 parameters: $q_0, b_1, b_2$. These parameters are non-negative. Then, when $\theta \to \pi/2 (\cos \theta) \to 0$ the value $q(\theta) \to 1$.

In the linear approximation for $\cos \theta$ we have

$$q(\theta) = 1 - (1 - q_0)b_1 \cos \theta.$$

Therefore, there is the following relation with the expression (2)

$$a_1 = (1 - q_0)b_1.$$

The parameter $b_2$ is necessary to account for the Soffer boundary conditions [5], which can be implemented at intermediate values of the angle $\theta$.

If the parameters $b_1, b_2$ are large, then when the angle $\theta$ not too close to $\pi/2$, the value $q(\theta)$ is almost constant and close to $q_0$. Then the case of an ordinary mirror–diffuse boundary conditions [1] is implemented.

In the case $b_1 = 0$ and the angles $\theta$ close to $\pi/2$ we get

$$q(\theta) \approx 1 - b_2 (\cos \theta)^2.$$

This relation coincides with the Soffer result (4) if $b_2 = \left(4\pi G\right)^2$.

For metal

$$\cos \theta = \frac{|v_n|}{v_F}.$$

Here $v_n$ — component of electron velocity perpendicular to the surface, $v_F$ — the Fermi velocity. Then the expression (2) can be rewritten in the form
\[ q(\theta) = q_0 + (1 - q_0)\exp(-\beta_1 |v_z| - \beta_2 |v_z|^2). \]  

(6)

\[ \beta_1 = \frac{b_1}{v_F}, \beta_2 = \frac{b_2}{v_F}. \]

Fig. 1. The dependence of the reflectivity coefficient on the angle \( \theta \). Value \( q_0 = 0.5 \), and value \( b_1 = 1 \).

Fig. 2. The dependence of the reflectivity coefficient on the angle \( \theta \). Value \( q_0 = 0.5 \), and \( b_1 = 3 \). Curve 1 corresponds to the value of \( b_2 = 10 \). Curve 2 corresponds to the value of \( b_2 = 5 \). Curve 3 corresponds to the value of \( b_2 = 2 \). Curve 4 corresponds to the value of \( b_2 = 0 \).

From Fig. 1 and Fig. 2, we see that for large values of \( b_1 \) and \( b_2 \), the reflectivity coefficient \( q_0 \) for most angles of incidence remains constant. In this case the condition \( q = q_0 \) is satisfied. With the decrease of the coefficients \( b_1 \) and \( b_2 \) are deviations from the Fuchs boundary conditions (1) with constant reflectivity coefficient becomes evident. These deviations are particularly significant when the angle \( \theta \) close to \( \pi/2 \).

3. Conclusion
The paper considers a boundary condition to the kinetic equation for the electrons in the metal. This boundary condition is a generalization of the Fuchs and Soffer boundary conditions. In the limit cases it goes into these boundary conditions. In addition it satisfies the Andreev condition. The Fuchs and Soffer boundary conditions this condition not satisfy. The considered boundary condition can be used to describe the electron kinetics in thin films and wires. It is possible to use this boundary condition for describing the kinetics of electrons in small metal particles.

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