About boundary conditions for kinetic equations in metal

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

***Index Terms*—kinetic, boundary conditions, electrons, surface, mirror, diffuse**

I. 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 are 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]

$$f(\mathbf{v}) = qf(\mathbf{v}') + (1-q)f_0(v), \qquad \mathbf{v}' = \mathbf{v} - 2\mathbf{n}(\mathbf{n}\mathbf{v}). \quad (1)$$

Here $\mathbf{v}$ – the electron velocity before the collision with surface, $\mathbf{v}'$ – the electron velocity after collision with the surface, $\mathbf{n}$ – 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

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

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 one.

II. FORMULATION OF GENERALIZED BOUNDARY CONDITIONS

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 $q = q(\theta)$ (θ - the angle of incidence of the electron on the border) tends to one when the angle of incidence θ 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

$$q(\theta) = 1 - a_1\cos\theta - a_2\cos^2\theta - a_3\cos^3\theta + \cdots . \quad (2)$$

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]

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

In equation (3) value h_s — the mean-squared height of the surface relief, λ_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].

Consider the behavior of the reflectivity coefficient q with almost tangential fall of the electron on the metal surface in the model of Soffer (3). Then $\theta \to \pi/2$ and $\cos\theta \to 0$. Therefore

$$q(\theta) \simeq 1 - (4\pi G)^2(\cos\theta)^2. \quad (4)$$

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

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

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

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

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 θ.

If the parameters b_1, b_2 are large, then when the angle θ 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 θ close to $\pi/2$ we get

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

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

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

$$q(\theta) = q_0 + (1 - q_0) \exp(-\beta_1 |v_z| - \beta_2 |v_z|^2). \qquad (6)$$

$$\beta_1 = \frac{b_1}{v_F}, \quad \beta_2 = \frac{b_2}{v_F}.$$

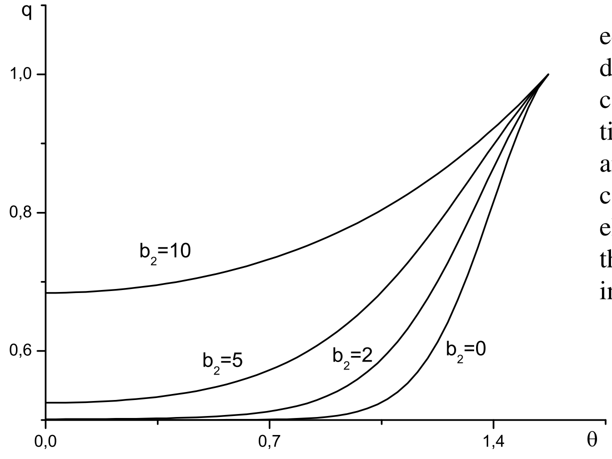

Fig. 1. The dependence of the reflectivity coefficient on the angle θ. Value $q_0 = 0.5$, and value $b_1 = 1$.

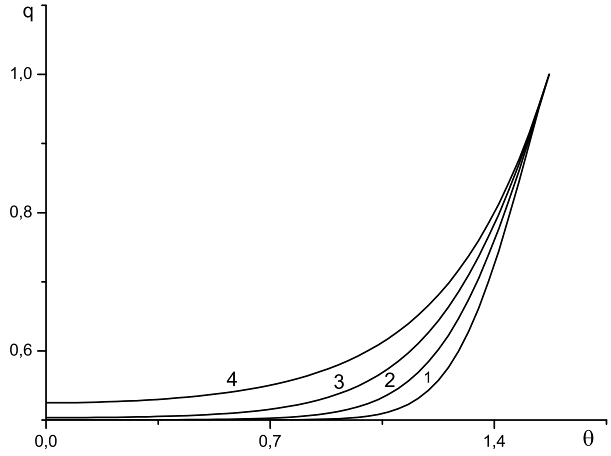

Fig. 2. The dependence of the reflectivity coefficient on the angle θ. Value $q_0 = 0.5$, and $b_1 = 3$. Curve 1 corresponds to the value of $b_2 = 10$. Curve 2 corresponds to the value of $b_2 = 5$. Curve 3 corresponds to the value of $b_2 = 2$. Curve 4 corresponds to the value of $b_2 = 0$.

From figures 1 and 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 θ close to $\pi/2$.

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 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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