Conductance of a tunnel point contact of noble metals in the presence of a single defect

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In paper (Avotina et al., Phys. Rev. B74, 085411 (2006)) the effect of Fermi surface anisotropy to the conductance of a tunnel point contact, in the vicinity of which a single point-like defect is situated, has been investigated theoretically. The oscillatory dependence of the conductance on the distance between the contact and the defect has been found for a general Fermi surface geometry. In this paper we apply the method developed in (Avotina et al., Phys. Rev. B74, 085411 (2006)) to the calculation of the conductance of noble metal contacts. An original algorithm, which enables the computation of the conductance for any parametrically given Fermi surface, is proposed. On this basis a pattern of the conductance oscillations, which can be observed by the method of scanning tunneling microscopy, is obtained for different orientations of the surface for the noble metals.

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The scanning tunneling microscope (STM) method enables to observe and investigate quantum interference phenomena concerned with electron scattering by single defects. One of them is Friedel-like oscillations of the differential tunneling conductance $G$ measured by STM around the defect. It is known that electrons of the surface states on the (111) surfaces of the noble metals Au, Ag, and Cu form a quasi-two-dimensional electron gas which is confined at the crystal surface. These electrons are scattered by surface defects, e.g. impurity atoms, adatoms, or step edges, and the STM conductance exhibits oscillatory patterns originating from an interference between the principal wave that is directly transmitted through the contact and the partial wave that is scattered by the contact and the defect [1–4]. The period of the conductance oscillations depends on a distance from the contact to the defect $r_0$ and double the Fermi wave vector $2k_F$. A similar dependence can result from the scattering of bulk electron states by subsurface defects [5–7]. It was found that the oscillatory pattern obtained by STM reflects the anisotropy of the Fermi surface (FS), i.e. the value of the vector $k_F$ depends on the direction in a plane of the sample surface, and surface Fermi contours can be determined by Fourier transform of the STM image [8–10]. Particularly, in Ref. 10 the contour related to the «neck» of the bulk FS that for Cu (111) and Au (111) surfaces had been observed.

In the papers [11–13] the effect of quantum interference of electron waves which are scattered by single defects below a metal surface to the conductance of a tunnel point-contact has been investigated theoretically. It has been shown [12] that the dependence of $G$ on an applied voltage measure $V$ can be used for the determination of defect positions below a metal surface. In Ref. 11 we have analyzed the conductance of a tunnel point-contact in the presence of a defect located inside the bulk for metals with arbitrary FS. In the quasiclassical approximation the conductance of the contact had been found. The general formula was illustrated for two non-spherical shapes for the FS: the ellipsoid and the corrugated cylinder (open surface). These relatively simple models of FS make it possible to get analytical expressions for the conductance.
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and to analyze the main manifestations of the FS anisotropy: «necks», inflection lines etc. In order to compare the theoretical results with experiment it is necessary to calculate the conductance for the real model of the FS of a specific metal. In this paper we present such calculations for noble metals.

We consider as a model for our system a nontransparent interface separating two metal half-spaces, in which there is an orifice (contact) of radius \( a << \lambda_F \) (\( \lambda_F \) is a characteristic Fermi wave length). The potential barrier in the plane of the contact is taken to be a delta function with a large amplitude \( U \) (the transmission coefficient of electron tunneling through the barrier is small, \( T \approx (\hbar v_F / U)^2 << 1, v_F \) is a Fermi velocity). At the distance \( r_0 > \lambda_F \) from the contact a point-like defect, which is described by a short range potential, is placed. The interaction of electrons with the defect is taken into account in the framework of perturbation theory with the constant of this interaction \( g \). We also assume the applied bias \( \epsilon V \) is much smaller than Fermi energy, \( \epsilon_F \). The conductance of the contact is calculated in linear approximation in the transmission coefficient \( T \), the constant \( g \) and the voltage \( \epsilon V \) by the method developed in Refs. 12, 14. Under the listed assumptions a general formula for the conductance derived in Ref. 11:

\[
G = G_0 \left( 1 - \frac{1}{\pi} \sum_{n,s} \text{Re} \Lambda_{ss}^{as} (r_0, \epsilon_F) \text{Im} \Lambda_{ss}^{as} (r_0, \epsilon_F) \right) \tag{1}
\]

Here \( G_0 \sim T \) is the conductance of the tunnel point contact without defect, \( \tilde{g} \approx g m^2 v_F / \hbar^3 \) is a dimensionless constant of electron-impurity interaction (\( m^* \) is the effective electron mass). The function \( \Lambda_{ss}^{as} (r, \epsilon_F) \) defines the asymptote of the wave function \( \psi(r) \sim \sqrt{\det \Lambda(r)} \) of the electrons transmitted through the contact at large distances \( r > > \lambda_F \) from the contact. For points in momentum space for which the Gaussian curvature \( K(\epsilon, p_\perp) \) of the FS \( \alpha(p_\perp, p_z) = \epsilon_F \) \( (z \) is directed along the contact axis, \( p_\perp \) and \( p_z \) are components of the momentum tangential and perpendicular to the interface) is not equal to zero, the function \( \Lambda_{ss}^{as} (r, \epsilon_F) \) is given by

\[
\Lambda_{ss}^{as} (r, \epsilon_F) = \frac{\cos \vartheta}{2 \pi r \hbar \sqrt{\det \Lambda(r)}} \exp \left[ i \Gamma + \frac{\pi}{4} \text{sgn} \left( \frac{\partial^2 p_z^{(+)}}{\partial p_z^2} \right) (1 + \text{sgn} K) \right] \tag{2}
\]

where \( \Gamma(p_\perp, r) \) is the phase accumulated over the path travelled by the electron between the contact and the point \( r \),

\[
\Gamma(p_\perp, r) = \frac{1}{\hbar} (p_\perp \rho + p_z^{(+)})(p_\perp)z, \tag{3}
\]

\( p_z^{(+)}(\epsilon_F, p_z) \) is the root of the equation \( \alpha(p_\perp, p_z^{(+)}) = \epsilon_F \) corresponding to a wave with a \( z \)-component of the velocity \( v_z^{(+)}(\epsilon_F, p_z) > 0 \), and \( \cos \vartheta(r) = z/r \), \( \vartheta \) is the angle between the vector \( r \) and the \( z \) axis. The momenta \( p_{\perp, s} = p_{s, \perp, \perp}^{(a)} \) \( (s = 1, 2, \ldots) \) are defined by the equation,

\[
\frac{\partial \vartheta}{\partial p_s} = 0. \tag{4}
\]

Originally, \( p_{\perp, s} = p_{s, \perp, \perp}^{(a)} \) are the stationary phase points of the integral wave function [11]. These projections of the momentum correspond to the velocities \( \chi(\epsilon, p_{s, \perp, \perp}^{(a)}) \) \( |r \), i.e., at large distances from the contact the electron wave function for a certain direction \( r \) is defined by those points on the FS for which the electron group velocity is parallel to \( r \) [11, 15]. If the curvature of the FS changes sign, Eq. (4) has more than one solution \( (s = 1, 2, \ldots) \). It may also occur that Eq. (4) does not have any solution for given directions of the vector \( r \), and the electrons cannot propagate along these directions [16].

At the stationary phase points the curvature \( K(\epsilon, p_\perp) \) can be written as

\[
K_0(\epsilon, n) = \frac{1}{|\epsilon|} \sum_{l,k} A_{ik} n_l n_k \tag{5}
\]

where \( A_{ik} = \frac{\partial \det(m^{-1})}{\partial m_{ik}} \) is the algebraic adjunct of the element \( m^{-1}(p) \)

\[
\frac{\partial^2 \epsilon}{\partial p_s^2} \tag{6}
\]

of the inverse mass matrix \( m^{-1} \) [17]; \( n_l \) are components of the unit vector \( n = r/r \).

For those points at which \( K_0 = 0 \) the amplitude of the electron wave function in a direction of zero Gaussian curvature is larger than for other directions. This results in an enhanced current flow near the cone surface defined by the condition \( K_0 = 0 \) [15]. If the FS is open, there are directions along which the electrons cannot move at all. These properties of the wave function manifest itself in an oscillatory part of the conductance (1):

1. The amplitude of oscillations is maximal if the direction from the contact to the defect corresponds to the electron velocity belonging to an inflection line.
2. There are no oscillations of \( G \) if this direction belong to cones, in which the electron motion is forbidden.

Further calculations requires the information about the FS, \( \alpha(p) = \epsilon_F \). We use the parameterization of the FS of the noble metals copper, silver and gold from [18].
The orientation of the Fermi surface relative to the contact axis for three principal lattice orientations.

Fig. 1. The main contributions to the conductance oscillations caused by a defect at \( r_0 \) come from the points on the Fermi surface where the normal vector (velocity vector) points in the same direction as the vector \( \mathbf{r}_0 \).
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amplitude conductance oscillations have already been reported in experiments on Ag and Cu (111) surfaces [6].

From Figs. 3–5 it can be seen that the interference pattern of the conductance oscillations, in particular the size and appearance of «dead» regions, depend on the depth of the defect. These characteristics of the part of the conductance related to the scattering by the defect contains the information about the position of the defect. For all orientations of the metal surface the defect position in the plane of the surface corresponds to a center of symmetry. The depth can be found in the following way: the orientation of the «neck» axes defines the axes of the cones, in which there are no scattered electrons. Vertexes of the cones coincide with the defect. If the contact is situated at a point which belongs to a sectional plane of the cones by a surface plane, the conductance of the contact is equal to its value without the defect (we called these «dead» regions). A rough estimation of the defect depth can be obtained if we use the approximation of a cone of revolution with an opening angle $2\gamma$. For example, in Fig. 5 the radius $R$ of the central «dead» region is defined by the equality $R = z_0 \cot \gamma (\gamma \approx 30^\circ)$ [6]. Using a fitting of experimental results with theoretical calculations in the framework our method enables one to find the depth of the defect below metal surface more exactly.

Thus, we have demonstrated the possibility of calculations of anisotropic conductance oscillation caused by electron scattering by the defect in noble metals. The developed algorithm of calculations can be used for any parametrically given FS. We have shown that the analysis of interference patterns makes it possible to find the position of the defect below metal surface.

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