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

Ye.S. Avotina[1,2], Yu.A. Kolesnichenko[1,2], S.B. Roobol[2], and J.M. van Ruitenbeek[2]

[1]*B. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine*
47 Lenin Ave., Kharkov 61103, Ukraine
E-mail: kolesnichenko@ilt.kharkov.ua

[2]*Kamerlingh Onnes Laboratorium, Universiteit Leiden, Postbus 9504, 2300 Leiden, The Netherlands*

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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.

PACS: **73.23.–b** Electronic transport in mesoscopic systems;
72.10.Fk Scattering by point defects, dislocations, surfaces, and other imperfections.

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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 $\mathbf{k}_F$ 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 countour 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

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 $a << \lambda_F$ (λ_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 eV is much smaller than Fermi energy, ε_F. The conductance of the contact is calculated in linear approximation in the transmission coefficient T, the constant g and the voltage V by the method developed in Refs. 12,14. Under the listed assumptions a general formula for the conductance derived in Ref. 11:

$$G = G_0\left(1 - \tilde{g}\sum_{s,s'} \mathrm{Re}\,\Lambda_s^{as}(\mathbf{r}_0,\varepsilon_F)\,\mathrm{Im}\,\Lambda_{s'}^{as}(\mathbf{r}_0,\varepsilon_F)\right). \quad (1)$$

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 $\Lambda_s^{as}(\mathbf{r},\varepsilon)$ defines the asymptote of the wave function $\psi(\mathbf{r}) \sim \sqrt{T}\Lambda^{as}(\mathbf{r})$ 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 $K(\varepsilon, \mathbf{p}_t)$ of the FS $\varepsilon(\mathbf{p}_t, p_z) = \varepsilon_F$ (z is directed along the contact axis, $\mathbf{p}_t$ and p_z are components of the momentum tangential and perpendicular to the interface) is not equal to zero, the function $\Lambda_s^{as}(\mathbf{r},\varepsilon_F)$ is given by

$$\Lambda_s^{as}(\mathbf{r},\varepsilon_F) = \frac{\cos\vartheta}{2\pi\hbar r\sqrt{|K|}} \times$$

$$\times \exp\left[i\Gamma + i\frac{\pi}{4}\mathrm{sgn}\left(\frac{\partial^2 p_z^{(+)}}{\partial p_x^2}\right)(1+\mathrm{sgn}\,K)\right]_{\mathbf{p}_t = \mathbf{p}_{t,s}^{(\mathrm{st})}}, \quad (2)$$

where $\Gamma(\mathbf{p}_t, \mathbf{r})$ is the phase accumulated over the path travelled by the electron between the contact and the point $\mathbf{r}$,

$$\Gamma(\mathbf{p}_t, \mathbf{r}) = \frac{1}{\hbar}(\mathbf{p}_t\rho + p_z^{(+)}(\mathbf{p}_t)z), \quad (3)$$

$p_z^{(+)}(\varepsilon_F, \mathbf{p}_t)$ is the root of the equation $\varepsilon(\mathbf{p}_t, p_z^{(+)}) = \varepsilon_F$ corresponding to a wave with a z-component of the velocity $v_z^{(+)}(\varepsilon_F, \mathbf{p}_t) > 0$, and $\cos\vartheta(\mathbf{r}) = z/r$, ϑ is the angle between the vector $\mathbf{r}$ and the z axis. The momenta $\mathbf{p}_t = \mathbf{p}_{t,s}^{(\mathrm{st})}$ ($s = 1,2...$) are defined by the equation,

$$\left.\frac{\partial\Gamma}{\partial\mathbf{p}_t}\right|_{\mathbf{p}_t = \mathbf{p}_{t,s}^{(\mathrm{st})}} = 0. \quad (4)$$

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

At the stationary phase points the curvature $K(\varepsilon, \mathbf{p})$ can be written as

$$K_0(\varepsilon, \mathbf{n}) = \left[\frac{1}{|\mathbf{v}|^2}\sum_{i,k=x,y,z} A_{ik} n_i n_k\right]_{\mathbf{p}_t = \mathbf{p}_t^{(\mathrm{st})}}, \quad (5)$$

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

$$m_{ik}^{-1}(\mathbf{p}) = \frac{\partial^2\varepsilon}{\partial p_i \partial p_k} \quad (6)$$

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

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, $\varepsilon(\mathbf{p}) = \varepsilon_F$. We use the parameterization of the FS of the noble metals copper, silver and gold from [18]

$$\varepsilon(\mathbf{p}) = \alpha\left[-3 + \cos\frac{p_x a}{2\hbar}\cos\frac{p_y a}{2\hbar} + \cos\frac{p_y a}{2\hbar}\cos\frac{p_z a}{2\hbar} + \right.$$
$$\left. + \cos\frac{p_z a}{2\hbar}\cos\frac{p_x a}{2\hbar} + r\left(-3 + \cos\frac{p_x a}{\hbar} + \cos\frac{p_y a}{\hbar} + \cos\frac{p_z a}{\hbar}\right)\right]. \quad (7)$$

This parameterization is accurate up to 99%. The value of the constants are $r = 0.0995$, and $\varepsilon/\alpha = 3.63$, and a is different for each metal. For copper, silver and gold a = 0.361, a = 0.408 and a = 0.407 nm, respectively. The Fermi energy of copper is 7.00 eV, for silver 5.49 eV and for gold it is 5.53 eV.

The FS (7) has the BCC symmetry. It basically looks like a sphere with 8 «necks» positioned at the 8 vertices of a cube (Fig. 1). The central part of the surface «belly» has a positive curvature $K > 0$ while the ends near the Brillouin zone boundary («necks») have negative curvature. The size of the «necks» and the curvature of the spherical areas are slightly different for each noble metal. In the regions of «necks» there are the inflection lines, at which the curvature $K = 0$.

In Eq. (7) for the FS, the x, y and z directions correspond to a [100] direction, and the xy interface plane is therefore a (100) crystal plane. To align the xy plane with a (110) plane, the FS is rotated by $\pi/4$ along the x or y axis. For the (111) orientation, the total rotation consists of a rotation of $\pi/4$ along the z-axis, followed by a rotation of arcsin $(1/\sqrt{3})$ along the x or y axis.

A direct way to find solutions $\mathbf{p}_t = \mathbf{p}_{t,s}^{(\mathrm{st})}$ of Eq. (4) numerically for a certain position of the defect $\mathbf{r}_0$ and calculate $\Lambda_s^{as}(\mathbf{r}_0, \varepsilon_F)$ (2) is not most suitable. Instead, the result that $\mathbf{p}_t = \mathbf{p}_{t,s}^{(\mathrm{st})}$ corresponds to the direction of the electron velocity along the direction from the contact to the defect can be used. We start with a point $\mathbf{p}$ on the FS, calculate the value of $\Lambda_s^{as}(\mathbf{r}, \varepsilon_F)$ for every point $\mathbf{r} \| \mathbf{v} = \partial\varepsilon(\mathbf{p})/\partial\mathbf{p}$ in the real space, and then repeat this for all points on the FS. Next, it is easy to perform the summation over all points on the FS, in which $\mathbf{r} \| \mathbf{v}$ to obtain the conductance. This idea is shown schematically in Fig. 1.

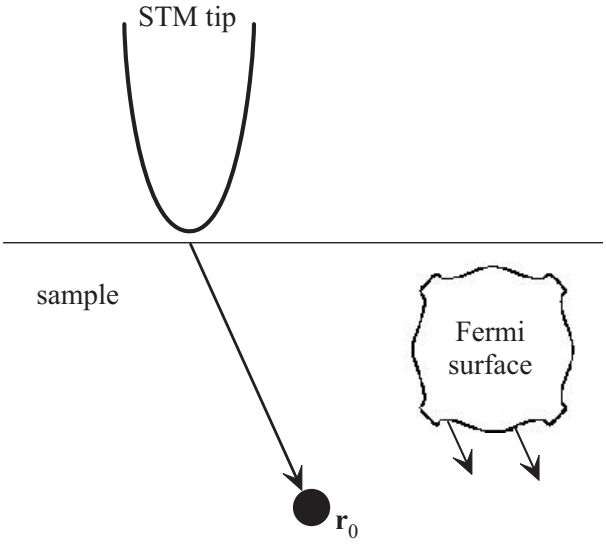

Fig. 1. The main contributions to the conductance oscillations caused by a defect at $\mathbf{r}_0$ come from the points on the Fermi surface where the normal vector (velocity vector) points in the same direction as the vector $\mathbf{r}_0$.

Strictly speaking, the asymptotic Eq. (1) is correct at $a << \lambda_F$, $r_0 >> \lambda_F$. However, as it was shown in Ref. 11 from a comparison of the exact result for the ellipsoidal FS with asymptotic expression (1), Eq. (1) describes the conductance qualitatively correctly for $a < \lambda_F$ and distances r_0 of a few λ_F. The other point is that at the inflection lines, which define the classically inaccessible regions, the curvature $K = 0$. As it was shown in Ref. 11, for such directions of the vector $\mathbf{r}_0$ the amplitude of the conductance oscillations increases remains finite. Below we restrict ourselves to the condition $K \neq 0$ and do not approach the inflection lines to a distance for which the second term in the Eq. (1) becomes of the order of unity.

We present the result of computations for three different crystallographic orientations (Fig. 2). The conductance as a function of the contact position for a defect in a noble metal at various depths are plotted in Figs. 3–5 for the (100), (110) and (111) lattice orientations respectively. For each of the lattice orientations, the graphs have the symmetries of that particular orientation of the FS. In all figures «dead» regions, in which there are no conductance oscillations, can be seen. These regions originate from the «necks» of the FS and their edges are defined by the inflection lines. In our plots the edges are abrupt. In reality there is a smooth change from a maximum to a zero of amplitude of the oscillations in the «dead» regions. This change cannot be described by Eq. (1), and a numerical solution of the Schrödinger equation with energy-momentum relation (7) must be used. However, the problem becomes much more complicated, while it does not give any additional physical information. The rings of high

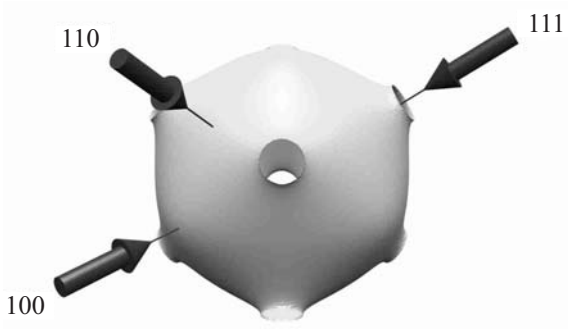

Fig. 2. The orientation of the Fermi surface relative to the contact axis for three principal lattice orientations.

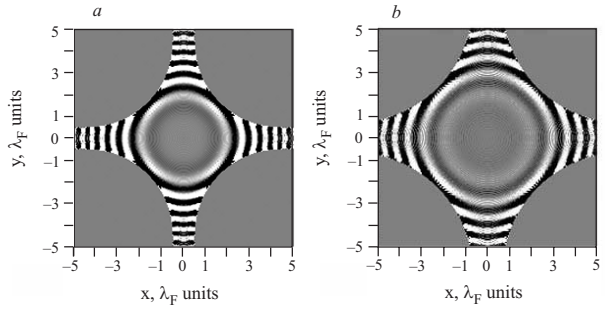

Fig. 3. Conductance G as a function of the contact position for a defect at the origin at depths 5 λ_F (*a*) and 7 λ_F (*b*) for a (100) interface plane. The x and y directions both correspond to $\langle 100 \rangle$ directions. The conductance is plotted in gray scale, where the color of the «dead» regions corresponds to the conductance value in absence the defect $G = G_0$, positive addition to G is white and negative is black.

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 2γ. For example, in Fig. 5 the radius R of the central «dead» region is defined by the equality

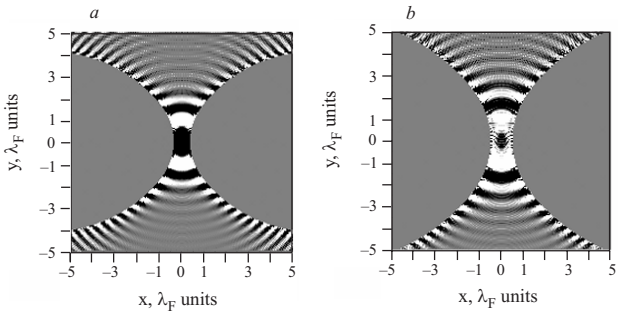

Fig. 4. Same as Fig. 3, but for a (110) interface plane. The x and y directions correspond to [001] and $[1\,\bar{1}\,0]$ directions respectively.

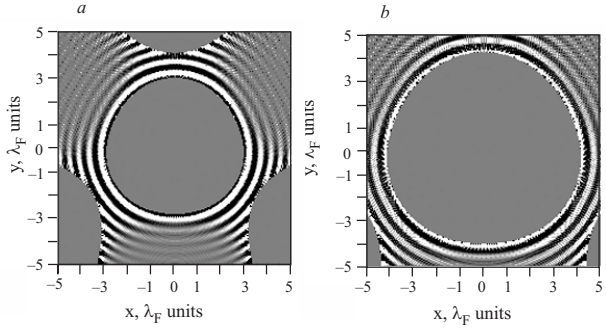

Fig. 5. Same as Fig. 3, but for a (111) interface plane. The x and y directions correspond to $[11\bar{2}]$ and $[1\,\bar{1}\,0]$ directions respectively.

$R = z_0 \cot\gamma$ ($\gamma \approx 30°$) [6]. Using a fiting 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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1. M.F. Crommie, C.P. Lutz, and D.M. Eigler, *Science* **262**, 218 (1993).
2. O.Yu. Kolesnychenko, R. de Kort, M.I. Katsnelson, A.I. Lichtenstein, and H. van Kempen, *Nature* **415**, 507 (2002).
3. N. Knorr, H. Brune, M. Epple, A. Hirstein. M.A. Schneider, and K. Kern, *Phys. Rev*. **65**, 115420 (2002).
4. L.Bürgi, N. Knorr, H. Brune, M.A. Schneider, and K. Kern, *Appl. Phys*. **A75**, 141 (2002).
5. M. Schmid, W. Hebenstreit, P. Varga, and S. Crampin, *Phys. Rev. Lett*. **76**, 2298 (1996).
6. N. Quaas, *Ph.D. Thesis*, Göttingen University (2003).
7. N. Quaas, M. Wenderoth, A. Weismann, R.G. Ulbrich, and K. Schönhammer, *Phys. Rev*. **B69**, 201103(R) (2004).
8. P.T. Sprunger, L. Petersen, E.W. Plummer, E. Lagsgaard, and F. Besenbacher, *Science* **275**, 1764 (1997).
9. Ph. Hofmann, B.G. Briner, M. Doering, H.-P. Rust, E.W. Plummer, and A.M. Bradshaw, *Phys. Rev. Lett*. **79**, 265 (1997).
10. L. Petersen, P. Laitenberger, E. Laegsgaard, and F. Besenbacher, *Phys. Rev*. **B58**, 7361 (1998).
11. Ye.S. Avotina, Yu. A. Kolesnichenko, A.F. Otte, and J.M. Ruitenbeek, *Phys. Rev*. **B74**, 085411 (2006).
12. Ye.S. Avotina, Yu.A. Kolesnichenko, A.N. Omelyanchouk, A.F. Otte, and J.M. Ruitenbeek, *Phys. Rev*. **B71**, 115430 (2005).
13. Ye.S. Avotina, Yu.A. Kolesnichenko, A.F. Otte, and J.M. Ruitenbeek, *Phys. Rev*. **B75**, 125411 (2007).

14. I.O. Kulik, Yu.N. Mitsai, and A.N. Omelyanchouk, *Zh. Exp. Teor. Fiz*. **63**, 1051 (1974).
15. A.M. Kosevich, *Fiz. Nizk. Temp*. **11**, 1106 (1985) [*Sov. J. Low Temp. Phys.* **11**, 611 (1985)].
16. I.M. Lifshits, M.Ya. Azbel', and M.I. Kaganov, *Electron Theory of Metals*, New York, Colsultants Bureau (1973).
17. G. Korn and T. Korn, *Mathematical Handbook*, McGraw-Hill Company (1968).
18. Arthur P. Cracknell, *The Fermi Surfaces of Metals: a Description of the Fermi Surfaces of the Metallic Elements*, Taylor and Francis, London (1971).