Journal of Physics: Conference Series **150** (2009) 022045 doi:10.1088/1742-6596/150/2/022045

The signature of a single subsurface defect in the conductance of a tunnel point-contact

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

[1] B.I. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 47, Lenin Ave., 61103, Kharkov,Ukraine.

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

E-mail: kolesnichenko@ilt.kharkov.ua

Abstract. The conductance of a tunnel point-contact in an STM-like geometry having a single defect placed below the surface is investigated theoretically. The effect of quantum interference of electron waves, which are scattered by the contact and the defect, has been taken into account. It is shown that this effect leads to oscillations of the conductance as a function of applied voltage and position of the defect. We demonstrate that the amplitude and period of the conductance oscillations are determined by the local geometry of the Fermi surface. The influence of a quantizing magnetic field has been considered. We predict that the conductance exhibits specific magneto-quantum oscillations, the amplitude and period of which depend on the distance between the contact and the defect. It is shown that multiple electron scattering by the magnetic impurity and the metal surface plays a decisive role in the point-contact conductance at voltages near the Kondo resonance. We find that the shape of the Kondo anomaly depends on the position of the defect.

Electron scattering by a single defect results in a local perturbation of the density of states, which oscillates with the distance to the defect (Friedel's oscillations), is anisotropic as a consequence of the scattering anisotropy in metals having a complicated Fermi surface, and carries further interesting properties. These properties of electron scattering by defects have been known and have been theoretically investigated many years ago. But for many years they could be observed only as indirect manifestations in the kinetic characteristics of macroscopic samples, in which the contribution of the electron scattering usually is averaged over large numbers of defects and over the momentum of the electrons. The development of Scanning Tunneling Microscopy (STM) makes it possible to investigate the variation in the local density of electron states near the metal surface at the atomic scale. One may consider a defect as a test probe, and by placing it in a pure conductor and investigating its influence on the local conducting properties it provides information on the characteristics of the host conductor. For these reasons there is an interest in theoretical investigations of the conductance of tunnel contacts of small size, in the vicinity of which a single defect is placed in the bulk of the metal. Such defects may be vacancies or foreign atoms. In this paper we present a series of theoretical results, which illustrate the possibilities and perspectives of investigations of electron interaction with single defects by means of STM experiments.

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 $a < \lambda_{\mathrm{F}}$, where λ_{F} is the characteristic

Fermi wave length. The potential barrier in the plane of the contact is taken to be a delta function with a large amplitude, i.e., the transmission coefficient of electron tunnelling through the barrier is assumed to be small, $T \ll 1$. At a distance $r_0 \gg \lambda_{\mathrm{F}}$ from the contact a point-like defect is placed, which is described by a short range potential. The interaction of electrons with the defect is taken into account in the framework of perturbation theory, with g the constant of this interaction. We also assume the applied bias eV is much smaller than the 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 Ref. [1].

The presence of an elastic scattering center located inside the bulk, either in the vicinity of the tunnel contact in an STM configuration, or in one of the banks of a ballistic point contact, has been shown to cause oscillatory fluctuations in the conductance of the junction. For small contact radii these oscillations result solely from interference of electron waves that are directly transmitted on the one hand, and electrons that are both backscattered by the defect and again reflected by the contact, on the other. This effect can be employed experimentally for three dimensional mapping of subsurface impurities. For a model of free electrons the oscillatory part of the conductance $G^{osc}(V)$ can be expressed by

$$G^{osc}(V) \propto g\frac{z_0^2\lambda_F^2}{r_0^4}\sin 2\widetilde{k}_F r_0, \quad \widetilde{k}_F r_0 \gg 1; \tag{1}$$

where $\widetilde{k}_F = \sqrt{k_F^2 + 2meV/\hbar^2}$ is the wave vector of electrons that are passing through the orifice after acceleration by the applied voltage and z_0 is the depth of the defect under the surface; $r_0 = \sqrt{\rho_0^2 + z_0^2}$; ρ_0 is the coordinate of the defect in the plane of the surface. The actual experiment would consist of sensitively measuring $\frac{dI}{dV}(V)$ curves on a tight grid of ρ coordinates. The lateral positions of defects could then be identified as the centers of radially symmetric patterns in this signal. Next, the depth of an impurity should be derived from the period of the oscillation in the $\frac{dI}{dV}(V)$ curve at $\rho_{\mathbf{0}}$.

In the majority of conductors, with the exception of the alkali metals, the anisotropy of the electronic structure will have to be taken into account. For example, in the case of Au(111) the ‘necks’ in the Fermi surface (FS) should cause a defect to be invisible when probed exactly from above.

An expression for the oscillatory part of the conductance, G^{osc}, valid for an arbitrary FS, has been derived in Ref. [2]:

$$G^{osc} \propto g\sum_{s,s'} Re\Lambda_s(\mathbf{r}_0)\, Im\Lambda_{s'}(\mathbf{r}_0)\,; \tag{2}$$

$$\Lambda_s(\mathbf{r}) = \frac{\cos\vartheta}{2\pi\hbar r\sqrt{|K|}}\exp\left[\frac{i}{\hbar}\mathbf{p}_{0s}\mathbf{r} \pm i\frac{\pi}{4}\left(1 + sgnK\left(\mathbf{p}_{0s}\right)\right)\right], \tag{3}$$

where ϑ is the angle between the vector $\mathbf{r}$ and the z axis. Momenta $\mathbf{p}_{0s}$ are defined as having velocities $\mathbf{v}(\mathbf{p}_{0s}) \parallel \mathbf{r}_0$. If the curvature $K(\mathbf{p})$ of the FS changes sign there is more than one FS point $\mathbf{p}_{0s}$ $(s = 1, 2...)$. Contrary to the case of a spherical FS [1] in general the center of the conductance oscillation pattern does not need to coincide with the actual position of the defect. It may also occur that there is no velocity $\mathbf{v}(\mathbf{p}_{0s})$ for a given direction of the vector $\mathbf{r}$, and the electrons cannot propagate along these directions. For such positions of the contact $G^{osc} = 0$. The edges of such 'dead' regions on the metal surface sharply define the position of the defect. In the paper we formulate optimal conditions for the determination of defect positions in metals with closed and open Fermi surfaces.

In a quantizing magnetic field H directed along the contact axis the conductance of a tunnel point contact exhibits magneto-quantum oscillations, the amplitude and period of which depend on the distance between the contact and the defect. The oscillating with H part of the conductance $G^{osc}(H)$ for a free electron model is given by [3],

$$G^{osc}(H) \propto g \left(Im \sum_{n'=0}^{n_{\max}(\varepsilon_{\mathrm{F}})} \chi(n', \mathbf{r}_0) Re \sum_{n''=0}^{\infty} \chi(n'', \mathbf{r}_0) \right).$$

Here,

$$\chi(n, \mathbf{r}_0) = \exp\left(-\frac{\xi}{2}\right) L_n(\xi) \exp\left(\frac{i}{\hbar} p_{z,n} z_0\right), \tag{4}$$

$L_n(\xi)$ are Laguerre polynomials, $\xi = \rho^2/2a_H^2$, a_H the quantum magnetic length, $p_{z,n} = \sqrt{2m^*(\varepsilon_{\mathrm{F}} - \varepsilon_n)}$, ε_n are Landau levels in the magnetic field; $n_{\max}(\varepsilon_{\mathrm{F}})$ is the maximum value of the quantum number n for which $\varepsilon_n < \varepsilon_{\mathrm{F}}$.The non-monotonic dependence of the conductance $G^{osc}(H)$ results from the superposition of two types of oscillations: (a) A short period oscillation arising from electron focusing by the field H and (b) a long period oscillation of Aharonov-Bohm-type originating from the magnetic flux passing through the area enclosed by the electron trajectories from contact to defect and vice versa.

We have also studied the influence of multiple electron scattering by a single defect on the current through a tunnel point-contact [4]. In the approximation of s-wave scattering by the defect a general expression for the conductance $G(V, \mathbf{r}_0)$ has been found. The results obtained have been analyzed for the model s-wave phase shift describing the Kondo scattering by a magnetic impurity. It is shown that taking multiple scattering into account is most essential near voltage values corresponding to the Kondo resonance condition. It is found that the the shape as well as the sign of the Kondo anomaly depends on the position of the defect. This dependence results from quantum interference of partial waves directly transmitted through the contact with the partial wave scattered by the defect and reflected by the interface. We have shown that for certain positions of the contact relative to the magnetic defect the zero bias anomaly may have a 'Fano-like' shape. Such a shape of this anomaly is not related to the many-body Fano-resonance but it originates from the interference of single particle electron waves scattered by the defect.

[1] Avotina Ye.S., Kolesnichenko Yu.A., Omelyanchouk A.N., Otte A.F. and van Ruitenbeek J.M., 2005, *Phys. Rev. B*, **71**, 115430.
[2] Avotina Ye.S., Kolesnichenko Yu.A., Otte A.F. and van Ruitenbeek J.M., 2006, *Phys. Rev. B*, **74**, 085411.
[3] Avotina Ye.S., Kolesnichenko Yu.A., Otte A.F. and van Ruitenbeek J.M., 2007, *Phys. Rev. B*, **75**, 125411.
[4] Avotina Ye.S., Kolesnichenko Yu.A., and van Ruitenbeek J.M., 2008, *J. Phys.: Condens. Matter*, **20**, 115208.