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Aharonov-Bohm type oscillations in the system of two tunnel point-contacts in the presence of single scatterer: determination of the depth of the buried impurity

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Abstract. The conductance of a system containing two tunnel point-contacts and a single subsurface scatterer in the presence of a magnetic field is investigated theoretically. A general formula for the dependence of the conductance on the distance between contacts, the defect position, and the magnetic field is obtained. It is shown that in the presence of a magnetic field the conductance undergoes Aharonov-Bohm type oscillations. We find a simple relation between the period of the oscillations and the depth of the subsurface impurity. On the basis of this fact a new and easy method of determination the depth of the buried impurity is proposed.

Subsurface defects, as well as adatoms and steps on the metal surface, result in the appearance of Friedel-like oscillations in the STM differential conductance $G = dI/dV$ - a nonmonotonic dependence of G with the distance between the STM tip and the defect r_0. The study of this dependence can be used for the detection of buried defects and for investigation of their characteristics. Methods for determining defect positions below a metal surface using a single tip STM have been proposed before: this can be achieved using the period of oscillation of the conductance as a function of bias or by exploiting the interference pattern of conductance as a function of position, $G(r_0)$, which is very pronounced for open directions of Fermi surface (for a review see [1]).

With the further development of scanning tunneling microscopy (STM) it has become clear that a single STM-probe is often not enough for obtaining information on the detailed characteristics of the surface under investigation. A logical development of the one-tip approach is a dual-tip experimental setup, which can provide us with richer information than conventional single-probe STM. Despite the apparent technical complexity of the dual-tip STM (DT STM) in comparison with standard STM several groups have demonstrated successful solutions for such refinement of the STM-technology [2, 3, 4, 5].

The idea of using multiple tunneling contacts for determining the depth and location of impurities under a metal or semiconductor surface has been expressed earlier in Ref. [6]. The

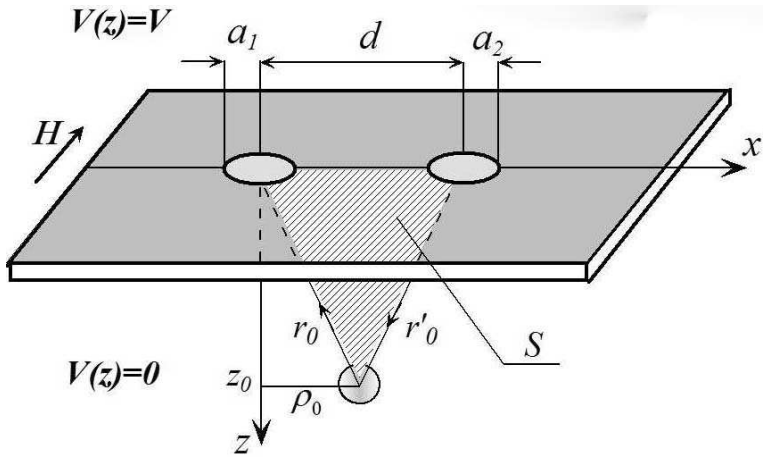

Figure 1.

paper by Niu *et al.*, Ref. [6], proposes a method for determining the desired depth by measuring the trans-conductance between two tips of the DT STM.

In the present paper we consider another scheme of DT STM experiment [7], in which the bias is applied between the two tips and the sample, i.e. the current flows from two contacts into the sample. We propose to determine a depth of the defect below conductor surface by measuring the oscillatory dependence of the DT STM conductance on the strength of a magnetic field **H** applied parallel to the conductor surface. These oscillations result from the quantization of the magnetic flux $\Phi = \mathbf{HS}$ through the area formed by the electron trajectories from the contacts to the defect and the line connecting the contacts (Fig.1). If $r_0 \ll r_H = \hbar c k_{\mathrm{F}}/eH$ (k_{F} is the Fermi wave vector), the electron trajectories and the line connecting the contacts form a triangle, and from its area S the defect depth can be found easily.

As a model of DT STM we consider two metal half-spaces separated by infinitely thin nonconducting interface at $z = 0$, which incorporates two small orifices (contacts) allowing for electron tunneling (see Fig.1). The origin of coordinates $\mathbf{r} = 0$ is chosen in the center of the first contact. The x axis is directed along the line connecting the contacts. To describe the potential barrier in the plane $z = 0$ we use the function [8]

$$U(\mathbf{r}) = U_0 f(\rho)\,\delta(z)\,. \tag{1}$$

where $\delta(z)$ is the Dirac delta function, ρ is a two-dimensional vector in the plane of the interface. The function $f(\rho)$ provides a path for electron tunelling only through two small areas with characteristic radii a_1 and a_2, as shown in Fig.1. In the vicinity of the contacts a single defect is placed, described by a short-range potential $D(\mathbf{r})$.

The electron wave function $\psi(\mathbf{r})$ in the presence of a magnetic field satisfies the Schrödinger equation

$$\left[\frac{\hbar^2}{2m^*}\left(\hat{\mathbf{k}} - \frac{e}{c\hbar}\mathbf{A}(\mathbf{r})\right)^2 + U(\mathbf{r}) + D(\mathbf{r})\right]\psi(\mathbf{r}) = \varepsilon\psi(\mathbf{r})\,, \tag{2}$$

and boundary conditions of continuity and of the jump of its derivative at $z = 0$. Here $\hat{\mathbf{k}} = -i\nabla$, $A(\mathbf{r})$ is the vector potential of the magnetic field, m^* is the electron effective mass, and ε is the electron energy.

If the Larmor radius of the electron trajectory r_H is much larger then the distances between the contacts and the defect we can neglect the effects of Landau quantization and bending of the trajectory, which has been analyzed in Ref.[9]. The wave function $\psi(\mathbf{r})$ for the system

considered here at $H = 0$ was obtained previously, in first approximation in the small parameter $1/U_0$, in Ref.[10]

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \frac{2m^*}{\hbar^2} T(k)\, G_0^+(\mathbf{r}, \mathbf{r}_0)\, \psi_0(\mathbf{r}_0), \tag{3}$$

where $G^+(\mathbf{r}, \mathbf{r}_0)$ is the retarded Green's function of a free electron in the half-space $z > 0$, $\mathbf{r}_0$ is the position of the center of the scattering potential $D(\mathbf{r})$, and $T(k)$ is the scattering matrix, which for this short-range scatterer can be expressed by means of an s-wave scattering phase shift δ_0 [11]

$$T(k) = \frac{-\pi\hbar^2 \left(e^{2i\delta_0} - 1\right)}{m^* ik \left(1 + \frac{1}{4ikz_0}\left(e^{2i\delta_0} - 1\right) e^{2ikz_0}\right)}. \tag{4}$$

In the limit $ka_{1,2} \ll 1$ (i.e. for tunnel point-contacts) the wave function of the system without scatterer is given by [10]

$$\psi_0(\mathbf{r}) = \frac{\hbar^2 k_z}{2m^* U_0}\left[(ka_1)^2 \frac{z}{r} h_1^{(1)}(kr) + (ka_2)^2 \frac{z}{r'} h_1^{(1)}(kr') e^{i\varkappa\mathbf{d}}\right], \tag{5}$$

where $\mathbf{k} = (\varkappa, k_z)$ is the electron wave vector, $k = |\mathbf{k}|$, $h_1^{(1)}(kr)$ is the spherical Bessel function of the third kind, $r' = |\mathbf{r} - \mathbf{d}|$, the vector $\mathbf{d}$ connects the two contacts, and $r, r' \gg a$.

The electron wave function under the influence of a vector potential $\mathbf{A}(\mathbf{r})$ acquires an additional phase

$$\psi(\mathbf{r}) \longrightarrow \psi(\mathbf{r}) \exp\left(\frac{ie}{c\hbar}\int_0^{\mathbf{r}} \mathbf{A}(\mathbf{r}')\, d\mathbf{r}'\right). \tag{6}$$

For the calculation of the conductance G we use the following approach: The probability density flow is found by using the wave function $\psi(\mathbf{r})$ (6) of electrons that tunnel through the potential barrier in the plane of the orifices. The total electric current I through the system is calculated by integration over electron momenta and over a surface overlapping the contacts. Here we will consider the case of zero temperature and a small applied voltage V (Ohm's low approximation). Under these assumptions the conductance G can be written as

$$G = \frac{e^2\hbar}{m^*}\nu(\varepsilon_{\mathrm{F}}) \int\limits_{S_{\mathrm{F}}, \nu_z > 0} d\Omega_{\mathbf{p}} \int_S d\Omega r^2 \mathrm{Im}\left[\psi^*(\mathbf{r}) \frac{\partial\psi(\mathbf{r})}{\partial r}\right]. \tag{7}$$

In Eq.(7) $\nu(\varepsilon_{\mathrm{F}})$ is the electron density of states at the Fermi surface $\varepsilon = \varepsilon_{\mathrm{F}}$, $d\Omega$ and $d\Omega_{\mathbf{p}}$ are solid angles in the real and momentum spaces, respectively. As the surface for space integration we choose a half-sphere of radius r larger than the distance between the contacts d, centered at the first contact, $r = 0$, and covering the contacts in the half-space $z > 0$. The integration over directions of the momentum on the Fermi surface S_{F} is carried out for electrons tunneling with a positive projection v_z of the electron velocity on the contact axis z. As consequence of current conservation the integral over $d\Omega$ does not depend on the choice of radius r.

Substituting the wave function (6) into Eq. (7) we can find the conductance of the system. The general formula for the conductance can be simplified for large distance between the contacts and the defect ($r_0 \gg 1/k_{\mathrm{F}}$,d) and a weak scattering potential, $\delta_0 \ll 1$. Under these assumptions to first order in δ_0 the oscillatory part of the conductance is proportional to,

$$\triangle G_{osc}(r_0, d, H) \sim \frac{\delta_0 z_0^2}{k_{\mathrm{F}}^2 (r_0 r_0')^2} \times \tag{8}$$
$$\left[\cos(k_{\mathrm{F}} r_0) \sin\left(k_{\mathrm{F}} r_0' - \frac{\pi\Phi}{\Phi_0}\right) + \cos(k_{\mathrm{F}} r_0') \sin\left(k_{\mathrm{F}} r_0 - \frac{\pi\Phi}{\Phi_0}\right)\right],$$

where $\Phi_0 = \pi c\hbar/e$ is the flux quantum, $k_{\rm F}$ is the Fermi wave vector, and z_0 is the depth of the defect. This formula shows that the conductance oscillates with a period that depends on the flux Φ through the triangle formed by the two tips and the defect (see the shaded area in Fig.1).

When the period of the oscillations is known, the depth z_0 can be determined using the following procedure: In the most convenient geometry of the experiment the contacts should be placed such that the vectors $\mathbf{r}_0$, $\mathbf{r}'_0$ and the normal to the sample surface are situated in the same plane, i.e. the vectors **H** and **S** are parallel. For our illustration in Fig.1 this means that the coordinate ρ_0 of the defect in the plane xy is found on the line connecting the tips. In this case the relation between the period of oscillations ΔH and the depth z_0 is very simple

$$z_0 = \frac{4\Phi_0}{d \triangle H} \tag{9}$$

Note that observation of the conductance oscillations (8) requires a sufficiently strong magnetic field. Currently in low-temperature STM magnetic fields up to 15T are reachable [12]. For example, in order to observe a quarter period $\triangle H$ for $z_0 = d = 20$ nm it is necessary to apply a field of $H = 5T$. For typical metals, for which $\lambda_{\rm F} \sim 0.5$ nm, at a distance between the contacts and the defect as large as $r_0 \gtrsim 10$ nm the amplitude of the conductance oscillations becomes very small $G_{osc} \sim G_0(\lambda_{\rm F}/r_0)^2 \sim (10^{-3} \div 10^{-4})G_0$, with G_0 the conductance of the system of two tunnel point-contacts without the impurity nearby. Therefore more suitable systems for the application of the proposed method of determination of the defect position below the surface are semiconductors, or semimetals (Bi, Sb and their ordered alloys) where the Fermi wave length $\lambda_{\rm F} \sim 10$ nm. Also, a large amplitude $G_{osc} \sim (10^{-2} \div 10^{-3})G_0$ could be expected in the metals of the first group, the Fermi surface of which has small pockets with effective mass $m^* \simeq 10^{-2} \div 10^{-3} m_0$ (m_0 is the mass of a free electron). In all cases a low-temperature STM should be used to avoid electron-phonon scattering on the electron trajectory.

Thus, in this paper we have investigated theoretically the conductance of a system consisting of two closely separated tunnel point contacts in the vicinity of which a point defect is situated, to which a magnetic field is **H** applied. For the case of a magnetic field parallel to the surface of the sample the depth of the subsurface impurity can be easily found from the period of Aharonov-Bohm type oscillations of conductance, which arise in this case.

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