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The signature of subsurface Kondo impurities in the local tunnel current

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 Avenue, 61103, Kharkov, Ukraine
[2] Kamerlingh Onnes Laboratorium, Universiteit Leiden, Postbus 9504, 2300 Leiden, The Netherlands

E-mail: kolesnichenko@ilt.kharkov.ua

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Abstract

The conductance of a tunnel point contact in a scanning tunneling microscope-like geometry having a single defect placed below the surface is investigated theoretically. The effect of multiple electron scattering by the defect after reflections by the metal surface is taken into account. In the approximation of s-wave scattering the dependence of the conductance on the applied voltage and the position of the defect is obtained. The results are illustrated for a model s-wave phase shift describing Kondo resonance scattering. We demonstrate that multiple electron scattering by the magnetic impurity plays a decisive role in the point contact conductance at voltages near the Kondo resonance. We find that the sign and shape of the Kondo anomaly depends on the position of the defect.

1. Introduction

Various surface defects have been observed and investigated by scanning tunneling microscopy (STM) [1–4]. The interference of the surface electron waves results in an oscillatory dependence of the tunneling conductance measured as a function of the separation between the STM tip and the defect. Remarkable manifestations of quantum interference were observed in artificial structures built from single atoms on a clean metal surface, the so-called quantum corrals [5]. Magnetic adatoms on non-magnetic host metal surfaces are of special interest as they produce a characteristic many-body resonance structure in the differential conductance near zero voltage bias attributed to the Kondo effect [8, 6, 7, 9]. The surface electron waves contain information of the magnetic impurity and by focusing the waves it has been possible to create a mirage image of the impurity [10]. The shape of the resonance in the differential conductance, $\mathrm{d}I/\mathrm{d}V$, is usually asymmetric and is described by a Fano line shape [11–14].

In principle STM spectroscopy should also provide access to information on the structure of the metal *below* the surface. This possibility is based on the influence on the conductance caused by quantum interference of electron waves that are scattered by defects and reflected back by the contact. This effect was explored by Schmidt and co-workers [15] for the investigation of subsurface bubbles of implanted gas in Al. The observation of interference patterns due to electron scattering by Co impurities in the interior of a Cu sample was reported by Quaas *et al* [16]. Theoretically, the influence of single defects in the bulk of a metal on the quantum conductance of tunnel point contact has been discussed in [17–19]. In these papers it has been shown that the location of defects below the surface can be identified from the interference pattern in constant-current STM images combined with the information obtained from the dependence of the conductance on the applied voltage. In the previous work of [17–19] the scattering of electrons with a defect has been taken into account in the framework of perturbation theory. Such an approximation is valid as long as the strength of the electron–impurity scattering interaction is small. In the case of a magnetic defect at low temperatures ($T \ll T_K$, where T_K is the Kondo temperature) the Kondo resonance results in a dramatic enhancement of the effective electron–impurity interaction [20] and the perturbation method becomes inapplicable.

In this paper we present the quantum conductance G of the tunnel point contact in the vicinity of which a single point-like defect is situated, for arbitrary values of the scattering potential. We express the conductance by means of an s-wave scattering phase shift δ_0. The results describe the influence on the conductance of multiple scattering of the electrons by

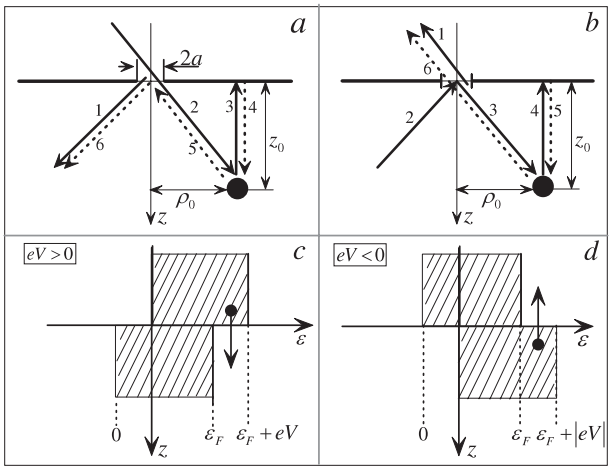

Figure 1. ((*a*), (*b*)) Model of the contact and ((*c*), (*d*)) illustration of the occupied energy bands in the two metal half-spaces for both signs of the applied bias eV. In panels (*a*), (*b*) the defect is placed at the point $\mathbf{r}_0 = (\rho_0, z_0)$. Electron trajectories are shown schematically. Note that we take the z-axis pointing downward.

a single defect. Multiple scattering needs to be included even for a single defect because of electron reflection by the metal surface. This results in the appearance of harmonics in the dependence of G on the applied voltage and on the distance between the contact and the defect. We apply the analysis of the non-monotonic voltage dependence of the conductance specifically for the interesting problem of Kondo scattering, using an appropriate phase shift [21]. To our knowledge, the observation of subsurface Kondo impurities has not yet been reported in experiments, and the present analysis may guide future experimental investigations.

2. Model and basic equations

In our model of the system we represent the contact by an orifice of radius a centered at the location of the 'STM tip', $\mathbf{r} = 0$. The orifice provides a tunneling window in the otherwise impenetrable infinitely thin interface at $z = 0$ between two metal half-spaces (figure 1). The potential barrier at the plane of the interface, $z = 0$, is taken to be described by a delta function, $U(\mathbf{r}) = U_0 f(\rho)\delta(z)$, where ρ is the length of the radius vector ρ in the plane $z = 0$. The function $f(\rho) \to \infty$ at all points of the plane except in the contact, where $f(\rho) = 1$. At the point $\mathbf{r}_0$ a defect described by the potential $D(|\mathbf{r} - \mathbf{r}_0|)$ is placed.

We consider an almost ballistic configuration (the electrons are elastically scattered by the single defect only) and neglect electron–phonon scattering assuming the electron mean free path to be much larger than the distance between the contact and the defect. In [22] the authors reported the observation of conductance oscillations for a voltage range up to 1.5 eV at a temperature of 4.2 K. Large bias voltages can be applied to small tunnel junctions created by STM or break-junction methods without significant heating of the electrodes. Because of the high resistance of the contact the current density remains small. Below we restrict our plots to the range $eV < \varepsilon_F$.

For the host metal we will consider a free electron model with an electron effective mass m^* and a dispersion relation $\varepsilon_\mathbf{k} = \hbar^2 k^2/2m^*$, where $\mathbf{k}$, and $\varepsilon_\mathbf{k}$ are the electron wavevector and electron energy, respectively. The electron wavefunction $\psi_\mathbf{k}$ satisfies the Schrödinger equation

$$\frac{\hbar^2}{2m^*}\nabla^2\psi_\mathbf{k}(\mathbf{r}) + [\varepsilon_\mathbf{k} - U(\mathbf{r}) - V(\mathbf{r})]\,\psi_\mathbf{k}(\mathbf{r}) = D(|\mathbf{r} - \mathbf{r}_0|)\psi_\mathbf{k}(\mathbf{r}), \tag{1}$$

where $V(\mathbf{r})$ is the applied electrostatic potential. The function $\psi_\mathbf{k}(\rho, z)$ satisfies boundary conditions of continuity and of the jump of its derivative at the boundary $z = 0$. We will assume that the transmission amplitude of electrons through the barrier in the orifice is small,

$$t(k) \approx \hbar^2 k/im^* U_0; \qquad |t| \ll 1. \tag{2}$$

For small transparency t the voltage drop due to the applied bias is entirely localized at the barrier. The electric potential can be described by a step function, $V(z) = V\,\Theta(-z)$. As a result, the occupied energy bands in the half-spaces $z > 0$ and $z < 0$ are shifted by eV. We take the zero of energy, $\varepsilon = 0$, to coincide with the bottom of the lower of the two bands, i.e. $\varepsilon = 0$ lies at the bottom of the band in the half-space $z > 0$ when $eV > 0$ and at the bottom of the band in the half-space $z < 0$ for $eV < 0$. At zero temperature electrons tunnel to the lower half-space (figures 1 (c), (d)) when $eV > 0$, and for $eV < 0$ electrons can tunnel only to available states in the upper half-space.

As shown in [23, 17] equation (1) can be solved for the arbitrary form of the function $f(\rho)$ in the limit $|t| \to 0$. To a first approximation in the small parameter $|t| \ll 1$ (2) the wavefunction $\psi_\mathbf{k}(\mathbf{r})$ can be written as

$$\psi_\mathbf{k}(\mathbf{r}) = \psi_{\mathbf{k}0}(\mathbf{r}) + \psi_{\mathbf{k}1}(\mathbf{r}), \tag{3}$$

where $\psi_{\mathbf{k}1}(\mathbf{r}) \sim 1/U_0$. This latter part of the wavefunction (3) describes the electron tunneling through the barrier and determines the electrical current. The first term in equation (3) is the solution of the Schrödinger equation for the metallic half-spaces without the contact. It satisfies the boundary condition $\psi_{\mathbf{k}0}(\rho, 0) = 0$ at the interface.

For $|t| \ll 1$ the boundary condition for the jump of the derivative of the total wavefunction is reduced to [23]

$$\mp\frac{\partial\psi^{(\mp)}_{\tilde{\mathbf{k}}0}}{\partial z}\bigg|_{z=\mp 0} = \frac{2m^*}{\hbar^2}U_0 f(\rho)\psi^{(\pm)}_{\mathbf{k}1}(\rho, 0), \tag{4}$$

where $\psi^{(\pm)}_{\mathbf{k}s}(s = 0, 1)$ are the wavefunctions for $z \gtrless 0$, $\tilde{\mathbf{k}}$ is the electron wavevector for electrons arriving in one half-space from the other half-space through the orifice, ($|\tilde{\mathbf{k}}| = \sqrt{k^2 - 2m^*|eV|/\hbar^2}$).

Thus, the function $\psi_{\mathbf{k}1}(\mathbf{r})$ can be expressed by means of the solution $\psi_{\mathbf{k}0}(\mathbf{r})$. By using the Fourier transform of the wavefunction (3) we find

$$\psi^{(\pm)}_{\mathbf{k}1}(\mathbf{r}) = \mp\frac{\hbar^2}{2m^*U_0}\int_{-\infty}^{\infty} d\kappa' e^{i\kappa'\rho + ik'_z|z|}\frac{\partial\psi^{(\mp)}_{\tilde{\mathbf{k}}0}}{\partial z}\bigg|_{z=\mp 0} \times\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} d\rho' \frac{e^{i\kappa'\rho'}}{f(\rho)}, \tag{5}$$

where $k'_z = \sqrt{k^2 - \kappa'^2}$. The electron wavefunction, $\psi_{\mathbf{k}}(\mathbf{r})$, which takes into account the scattering by the defect, can be expressed by means of the retarded Green function $G_0^+(\mathbf{r}', \mathbf{r}; \varepsilon)$ of the homogeneous equation (1) at $D = 0$ and $U \to \infty$. To first approximation in the transmission amplitude t (2) the integral equation for $\psi_{\mathbf{k}s}(\mathbf{r})$ is given by

$$\psi_{\mathbf{k}s}(\mathbf{r}) = \psi_{\mathbf{k}s}^{(0)}(\mathbf{r}) + \frac{2m^*}{\hbar^2}\int \mathrm{d}\mathbf{r}' D\left(\left|\mathbf{r}' - \mathbf{r}_0\right|\right) G_0^+\left(\mathbf{r}, \mathbf{r}'; \varepsilon\right) \psi_{\mathbf{k}s}(\mathbf{r}'), \tag{6}$$

where

$$G_0^+\left(\mathbf{r}, \mathbf{r}'; \varepsilon\right) = -\frac{\mathrm{i}k}{4\pi}\{h_0^{(1)}(k|\mathbf{r} - \mathbf{r}'|) - h_0^{(1)}(k|\mathbf{r} - \tilde{\mathbf{r}}'|)\}, \tag{7}$$

$\tilde{\mathbf{r}}' = (\rho', -z')$. In equation (7) and below $h_l^{(1)}(x)$ are the spherical Hankel functions. The first term in the braces is the Green function for free electrons in the infinite space and the second one takes into account the specular electron reflection from the interface. The functions $\psi_{\mathbf{k}s}^{(0)}(\mathbf{r})$ are the wavefunctions to zeroth and first order in t in the absence of the defect ($D = 0$). The electron wavefunction in the metal half-spaces is

$$\psi_{\mathbf{k}0}^{(0)}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\kappa\rho}(\mathrm{e}^{\mathrm{i}k_z|z|} - \mathrm{e}^{-\mathrm{i}k_z|z|}), \tag{8}$$

where κ and k_z are the components of the vector $\mathbf{k}$ parallel and perpendicular to the interface. The wavefunction $\psi_{\mathbf{k}1}^{(0)}(\mathbf{r})$ of the electrons that are transmitted through the contact has been obtained in [23]. In order to simplify further calculations we consider a point contact, taking the limit $a \to 0$. The solution $\psi_{\mathbf{k}1}^{(0)}(\mathbf{r})$ in this limit is given in [18] for any arbitrary anisotropic quadratic electron dispersion law $\varepsilon_{\mathbf{k}}$. For an isotropic band $\varepsilon_{\mathbf{k}} = \hbar^2k^2/2m^*$ this takes the form

$$\psi_{\mathbf{k}1}^{(0)}(\mathbf{r}) = t\left(\tilde{k}_z\right)\frac{\mathrm{i}\,(ka)^2\cos\theta}{2}h_1^{(1)}(kr). \tag{9}$$

Here, (r, θ, φ) are the spherical coordinates of the vector $\mathbf{r}$, with θ the angle between the vector $\mathbf{r}$ and the contact axis. $\tilde{k}_z$ is the z-component of the vector $\tilde{\mathbf{k}}$. The plane wave (8) is transformed into a spherical p-wave $h_1^{(1)}(kr)$ (9) after scattering by the point contact.

This model allows us to solve the three-dimensional Schrödinger equation in the limit of small transparency of the barrier and find the analytical formulas for the conductance. Our method is similar to the widely employed tunneling Hamiltonian approach, where in the limit of small transparency of the barrier the distribution functions of electrons in the electrodes can be taken to be in equilibrium (Fermi functions) with chemical potentials shifted by the bias eV. For a barrier of finite width the electric field distribution changes which influences the nonlinear dependence of the conductance. This dependence becomes very important if the bias is comparable with the work function of the metal. For any three-dimensional models of the potential barrier the dependence $G(V)$ may be calculated only numerically. In our paper we did not make it our aim to investigate the intrinsic conductance of the tunnel junction $G_0(V)$. The purpose of the work is to investigate the oscillatory and resonance additions to the conductance $G_0(V)$ in the presence of a defect in the bulk of the metal, where the distribution functions are in equilibrium (in leading approximation in the barrier transparency). We believe that the part of the conductance related to the defect, which will be obtained in following sections, is correct if the bias eV is less than the Fermi energy ε_{F}.

3. The scattered wavefunction in the s-wave approximation

Let $D(|\mathbf{r} - \mathbf{r}_0|)$ be a spherically symmetric scattering potential which is finite at the point $\mathbf{r} = \mathbf{r}_0$ and tends to zero at a distance $r_D \ll r_0$ that is of the order of the Fermi wavelength λ_{F}. As is well known, s-wave scattering is dominant for scattering by a short range potential [24]. In order to express the wavefunction (6) using the s-wave phase shift δ_0 we use the 'sharpness' of the function $D(|\mathbf{r}' - \mathbf{r}_0|)$, which essentially differs from zero only in a small region of the radius r_D near the point $\mathbf{r}' = \mathbf{r}_0$. The main contribution to the integral in equation (6) comes from this region and the 'smooth' functions $\psi_{\mathbf{k}s}(\mathbf{r}')$ and $h_0^{(1)}(k|\mathbf{r} - \tilde{\mathbf{r}}'|)$ can be taken outside the integral at the point $\mathbf{r}' = \mathbf{r}_0$. For $|\mathbf{r} - \mathbf{r}_0| \gg r_D$ the solution of equation (6) takes the form [18]

$$\psi_{\mathbf{k}s}(\mathbf{r}) \approx \psi_{\mathbf{k}s}^{(0)}(\mathbf{r}) + \frac{2m^*}{\hbar^2}T(k)\psi_{\mathbf{k}s}^{(0)}(\mathbf{r}_0)\, G_0^+(\mathbf{r}, \mathbf{r}_0; \varepsilon), \tag{10}$$

where

$$T(k) = \frac{g}{1 + \frac{m^*\mathrm{i}k}{2\pi\hbar^2}\left[Y(k) - gh_0^{(1)}(2kz_0)\right]}, \tag{11}$$

$$Y(k) = \int \mathrm{d}\mathbf{r}' D\left(r'\right) h_0^{(1)}\left(kr'\right), \qquad g = \int \mathrm{d}\mathbf{r}' D\left(r'\right). \tag{12}$$

Let us compare the wavefunction (10) with the formal solution $\psi_{\mathbf{k}}^{\mathrm{sc}}(\mathbf{r})$ of the scattering problem for the spherically symmetrical potential $D(|\mathbf{r} - \mathbf{r}_0|)$ in infinite space:

$$\psi_{\mathbf{k}}^{\mathrm{sc}}(\mathbf{r}) \approx \psi_{\mathbf{k}}^{\mathrm{in}}(\mathbf{r}) - \frac{\mathrm{i}m^*k}{2\pi\hbar^2}T_0(k)\psi_{\mathbf{k}}^{\mathrm{in}}(\mathbf{r}_0)\, h_0^{(1)}(k\,|\mathbf{r}_0 - \mathbf{r}|), \tag{13}$$

where $\psi_{\mathbf{k}}^{\mathrm{in}}$ and $\psi_{\mathbf{k}}^{\mathrm{sc}}$ are incident and scattered waves, and

$$T_0(k) = \frac{g}{1 + \frac{m^*\mathrm{i}k}{2\pi\hbar^2}Y(k)}, \tag{14}$$

is the T matrix. Taking into account the relation between T_0 and the s-wave phase shift $\delta_0(k)$

$$-\frac{m^*}{2\pi\hbar^2}T_0 = \frac{1}{k}\mathrm{e}^{\mathrm{i}\delta_0}\sin\delta_0, \tag{15}$$

we rewrite equation (11) in the form

$$T(k) = -\frac{\pi\hbar^2}{m^*\mathrm{i}k}\frac{\mathrm{e}^{2\mathrm{i}\delta_0} - 1}{1 + \frac{1}{2}\left(\mathrm{e}^{2\mathrm{i}\delta_0} - 1\right)h_0^{(1)}(2kz_0)}. \tag{16}$$

Note that the effective T-matrix (16) is an oscillatory function of the distance z_0 between the defect and the interface that results from repeated electron scattering by the defect after its reflections from the interface.

For a calculation of the current we should know the wavefunctions of the electrons transmitted through the contact, from one half-space to the other. For $z > 0$ and $eV > 0$ (i.e. for electron tunneling into the half-space in which the defect is situated) we find

$$\psi^{(+)}_{\mathbf{k}1}(\mathbf{r}) = \psi^{(0)}_{\mathbf{k}1}(\mathbf{r}) - \frac{m^* \mathrm{i}k}{2\pi\hbar^2} T(k)\psi^{(0)}_{\mathbf{k}1}(\mathbf{r}_0) \times \{h^{(1)}_0(k\,|\mathbf{r}-\mathbf{r}_0|) - h^{(1)}_0\left(k\,|\mathbf{r}-\tilde{\mathbf{r}}_0|\right)\}. \tag{17}$$

For $z < 0$ and $eV < 0$ (i.e. for electron tunneling from the half-space in which the defect is situated) the $\psi^{(-)}_{\mathbf{k}1}(\mathbf{r})$ is written as

$$\psi^{(-)}_{\mathbf{k}1}(\mathbf{r}) = \psi^{(0)}_{\mathbf{k}1}(\mathbf{r}) + \frac{\mathrm{i}m^* k^3 a^2 z z_0}{\hbar^2 r r_0} \times T(\tilde{k})t(\tilde{k})\psi^{(0)}_{\tilde{\mathbf{k}}0}(\mathbf{r}_0)h^{(1)}_1(kr)h^{(1)}_1(\tilde{k}r_0). \tag{18}$$

Here $\psi^{(0)}_{\mathbf{k}0,1}(\mathbf{r})$ and $T(k)$ are given by equations (8), (9) and (16). The wavefunctions (17) and (18) have a completely different form: in the lower half-space the wavefunction (17) is the superposition of the transmitted p wave $\psi^{(0)}_{\mathbf{k}1} \sim h^{(1)}_1(kr)$, (9), and two s waves, one of which, $h^{(1)}_0(k|\mathbf{r}-\mathbf{r}_0|)$, is the wave scattered by the defect while the other $h^{(1)}_0(k|\mathbf{r}-\tilde{\mathbf{r}}_0|)$ is the scattered wave, which undergoes reflection from the interface at $z = 0$ (the wave moving from the 'image' defect placed in the mirror point $\tilde{\mathbf{r}}_0$, $|\mathbf{r}_0 - \tilde{\mathbf{r}}_0| = 2z_0$). In the upper half-space there is only the p wave $\psi^{(-)}_{\mathbf{k}1} \sim h^{(1)}_1(kr)$, the amplitude of which depends on the scattering on the defect because the wave incident with the contact is not a plane wave in this case.

4. Total current and conductance

The tunneling current $I(V) = I^{(+)}(V) - I^{(-)}(V)$ is the difference between two currents flowing through the contact in opposite directions. Each of them can be evaluated by means of the probability current density integrated over a half-sphere of arbitrary radius r, centered at the point contact $r = 0$ and covering the contact from the appropriate side, and integrating over all directions of the electron wavevector. In this case the integrated probability current density $J^{(\pm)}_k(V)$ is written as

$$J^{(\pm)}_k(V) = -\frac{r^2\hbar}{m^*}\int \mathrm{d}\Omega\,\Theta(\pm z)\int \mathrm{d}\Omega_{\mathbf{k}}\Theta(\pm k_z) \times \mathrm{Im}\left(\psi^{(\pm)}_{\mathbf{k}1}(\mathbf{r})\frac{\partial\psi^{(\pm)*}_{\mathbf{k}1}(\mathbf{r})}{\partial r}\right), \tag{19}$$

where $\mathrm{d}\Omega$ and $\mathrm{d}\Omega_{\mathbf{k}}$ are elements of solid angle in the real and momentum spaces, respectively. The total current through the contact is

$$I(V) = \frac{2e}{(2\pi)^3}\int_0^\infty \mathrm{d}k\,k^2\big[J^{(+)}_k(V)\,f_{\mathrm{F}}(\varepsilon_{\mathbf{k}}-eV)\,(1-f_{\mathrm{F}}(\varepsilon_{\mathbf{k}})) - J^{(-)}_k(V)\,f_{\mathrm{F}}(\varepsilon_{\mathbf{k}})(1-f_{\mathrm{F}}(\varepsilon_{\mathbf{k}}-eV))\big], \tag{20}$$

where $f_{\mathrm{F}}(\varepsilon_{\mathbf{k}})$ is the Fermi function. At zero temperature only one of the terms in square brackets in equation (20) differs from zero, i.e. only in one of the half-spaces are states available for tunneling, depending on the sign of the bias. Using the wavefunctions (17) and (18), after integration through equation (19) the electrical current $I^{(\pm)}(V)$ at $|eV| < \varepsilon_{\mathrm{F}}$ and $T = 0$ takes the form

$$I^{(\pm)}(V) = \frac{e\hbar a^4}{36\pi m^*}\int_{k_{\mathrm{F}}}^{\sqrt{k_{\mathrm{F}}^2+2m^*|eV|/\hbar^2}} \mathrm{d}k\,k^5|t(\tilde{k})|^2(1+\Phi(k^{(\pm)})), \tag{21}$$

where the integration is carried out over the absolute value of the wavevector k within the interval $|eV|$ of allowed energies. We define $k^{(+)} = k$, $k^{(-)} = \tilde{k} = \sqrt{k^2 - 2m^*|eV|/\hbar^2}$, where k_{F} is the Fermi wavevector,

$$\Phi(k) = D^{-1}\sin\delta_0\frac{z_0^2}{r_0^2}\big[12 j_1(kr_0)(-y_1(kr_0)\cos\delta_0 + \{j_1(kr_0)(j_0(2kz_0)-1) + y_0(2kz_0)\,y_1(kr_0)\}\sin\delta_0) + 6(1-j_0(2kz_0))(kr_0)^{-4}\left(1+(kr_0)^2\right)\sin\delta_0\big], \tag{22}$$

and

$$D = 1 + 2\sin\delta_0 \times\left[\left(\frac{1}{2(2kz_0)^2} - j_0(2kz_0)\right)\sin\delta_0 - y_0(2kz_0)\cos\delta_0\right], \tag{23}$$

and $j_l(x)$ and $y_l(x)$ are the spherical Bessel functions. From equation (21) it follows that the current–voltage dependence need not be symmetric in voltage in the presence of a defect.

The differential conductance $G = \mathrm{d}I/\mathrm{d}V$ for $|eV| < \varepsilon_{\mathrm{F}}$ and for $eV > 0$ is given by

$$G(V) = G_0\left[q(V)\left(1+\Phi(\tilde{k}_{\mathrm{F}})\right) - \frac{2}{k_{\mathrm{F}}^4}\int_{k_{\mathrm{F}}}^{\tilde{k}_{\mathrm{F}}}\mathrm{d}k\,k^5\Phi(k)\right], \tag{24}$$

and for $eV < 0$,

$$G(V) = G_0\left[q(V) + \frac{\tilde{k}_{\mathrm{F}}^2}{k_{\mathrm{F}}^2}\Phi(\tilde{k}_{\mathrm{F}}) - \frac{4}{k_{\mathrm{F}}^4}\int_{k_{\mathrm{F}}}^{\tilde{k}_{\mathrm{F}}}\mathrm{d}k\,k^3\tilde{k}^2\Phi(k)\right]. \tag{25}$$

Here $\tilde{k}_{\mathrm{F}} = \sqrt{k_{\mathrm{F}}^2 + 2m^*eV/\hbar^2}$ and

$$q(V) = 1 + \frac{2m^*|eV|}{\hbar^2k_{\mathrm{F}}^2} - \frac{1}{3}\left(\frac{2m^*|eV|}{\hbar^2k_{\mathrm{F}}^2}\right)^3. \tag{26}$$

$$G_0 = |t(k_{\mathrm{F}})|^2\frac{e^2(k_{\mathrm{F}}a)^4}{36\pi\hbar} \tag{27}$$

is the conductance of the tunnel point contact in the absence of a defect in the limit $V \to 0$. At low voltage the conductance can be expressed as an expansion in the parameter $1/(k_{\mathrm{F}}z_0) < 1$,

$$G(0) = G_0\left\{1 + 12\frac{z_0^2}{r_0^2}\frac{1}{(k_{\mathrm{F}}r_0)^2}\sum_{n=1}^{\infty}(-1)^n\frac{\sin^n\delta_0}{(2k_{\mathrm{F}}z_0)^{n-1}} \times\left[\frac{1}{2}\left(1-\frac{1}{(k_{\mathrm{F}}r_0)^2}\right)\sin(2k_{\mathrm{F}}(r_0+(n-1)z_0)+n\delta_0) + \frac{1}{k_{\mathrm{F}}r_0}\cos(2k_{\mathrm{F}}(r_0+(n-1)z_0)+n\delta_0)\right]\right\}. \tag{28}$$

The second term in equation (28) corresponds to the sum over n events of scattering by the defect and $n-1$ reflections by the surface. If we keep only the term for $n = 1$ equation (28) is consistent with the results obtained from perturbation theory previously [17–19].

5. Discussion and application to Kondo scattering

The expansion (28) of the conductance G demonstrates that as a result of multiple scattering the conductance G_0, equation (27), of the tunnel point contact becomes modified with oscillatory contributions ΔG_n, which at $1/(k_F z_0) \ll 1$ and $z_0 \simeq r_0$ are of order

$$\Delta G_n \sim \frac{1}{(k_F r_0)^{n+1}} \sin\left(2k_F\left(r_0 + (n-1)z_0\right) + n\delta_0\right), \quad (29)$$

where $n = 1, 2, \ldots$ is the number of scattering events on the defect placed at a distance r_0 from the contact (and at a distance z_0 from the interface), and $(n-1)$ is the number of reflections by the interface. The argument of the sine function in equation (29) corresponds to the phase that the electron accumulates while moving along a semiclassical trajectory. In figures 1 (a) and (b) such trajectories are illustrated for the case of scattering twice by the defect and one specular reflection by the interface. For $eV > 0$ (figure 1(a)) this trajectory consists of a segment (labeled 2) passing through the contact and arriving at the defect, two line segments (3 and 4) connecting the defect and the interface (these segments are perpendicular to the interface because only along such a trajectory can the electron return to the defect and undergo the second scattering), and the part (5) from the defect to the contact. After specular reflection from the contact this wave interferes with the partial wave (1) that is directly transmitted through the contact.

When $eV < 0$ (figure 1(b)) a wave incident with the contact (trajectory 2) is partially reflected from the contact. The electron moving along the trajectory 3 from the contact to the defect is partially scattered towards the interface (line segments 4) where it undergoes specular reflection from the interface (5) and comes back to the defect, from which it returns to the contact via trajectory 6. Tunneling through the contact, this partial wave interferes with the partial wave that is directly transmitted (1) in the half-space $z < 0$. At each scattering on the defect the electron acquires an additional phase shift δ_0. The phase shift $\Delta\phi$ between the two interfering partial waves for an electron with wavevector $\mathbf{k}$ is $\Delta\phi = 2kr_0 + 2kz_0 + 2\delta_0$. Because the maximum value of the electron wavevector depends on the applied voltage the conductance oscillates as a function of eV.

The differential conductance, as the derivative of the current, distinguishes a bound of the energy interval, which depends on the bias eV, i.e. for $eV > 0$ the period of oscillations is defined by the energy $\varepsilon_F + eV$ and for $eV < 0$, by the energy $\varepsilon_F - |eV|$.

However, the current–voltage characteristic is not symmetric relative to the point $V = 0$. This asymmetry results from the dependencies of the phase shift $\delta_0(\tilde{k}_F)$ and the absolute value of the wavevector $\tilde{k}_F = \sqrt{k_F^2 + 2m^* eV/\hbar^2}$ on the sign of eV. The physical origin of this asymmetry is that the scattering depends on the electron energy in the lower half-space, which is different for different directions of the current.

The dependence $\delta_0(k)$ on k is defined by the form of the scattering potential $U(r)$. To illustrate the results obtained for an s-wave phase shift we use the following model function [5, 21]:

$$\delta_0(k) = \delta_{0K} + \delta_{0D} = \left[\frac{\pi}{2} - \tan^{-1}\left(\frac{\varepsilon_k - \varepsilon_K}{T_K}\right)\right] - kr_D. \quad (30)$$

The first term in equation (30) describes the resonant scattering on a Kondo impurity level ε_K (T_K is the Kondo temperature). For $\varepsilon_k \to \varepsilon_K$ the effective electron scattering cross section acquires a maximum value corresponding to the Kondo phase shift $\delta_{0K} = \pi/2$ [20]. For a non-magnetic impurity this term is absent. The second term takes into account the usual potential scattering. For simplicity we use the s-wave phase shift for a hard sphere potential of radius r_D ($k_F r_D < 1$). Inelastic scattering by the magnetic defect can be taken into account in the scattering formalism by introducing an imaginary part of the phase (30).

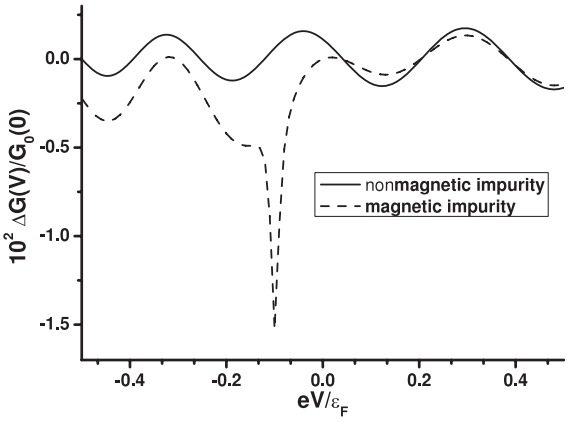

Figure 2. Voltage bias dependences of the normalized conductance corrections $\Delta G(V)/G_0$ for a magnetic and a non-magnetic impurity calculated from equations (24) and (25). We have used the parameters $\varepsilon_K = 0.9\varepsilon_F$, $k_B T_K = 0.01\varepsilon_F$, $r_D = 0.1\lambda_F/2\pi$, $\rho_0 = 0$, and $z_0 = 20\lambda_F/2\pi$.

Figure 2 shows the dependences of the corrections to the normalized conductance $\Delta G(V)/G_0 = (G(V) - G_0(V))/G_0$ resulting from the scattering by a defect placed on the contact axis for a magnetic and a non-magnetic impurity. The figure illustrates the appearance of a Kondo anomaly in the conductance seen as an extremum in the differential conductance, $G(V)$, near the bias eV_K corresponding to the resonance condition $\varepsilon_F + eV_K - \varepsilon_K = 0$. The plots show a slowly increasing background on top of the oscillating $\Delta G(V)$ dependence. The background arises from the integral terms in equations (24), (25), which take into account the contribution of all available states within interval $|eV|$. The monotonic part in $\Delta G(V)$ is more pronounced in the case of Kondo scattering, which gives a large contribution to this part at any voltage.

It is interesting to observe that the sign of the Kondo anomaly depends on the distance between the contact and the defect r_0. This distance in combination with the value of the wavevector $\tilde{k}_F$ determines the period of oscillation of $\Delta G(V)$, which is indeed a non-monotonic function of $\tilde{k}_F r_0$. If the bias eV_K coincides with a maximum in the oscillatory part of conductance the sign of the Kondo anomaly is positive and,

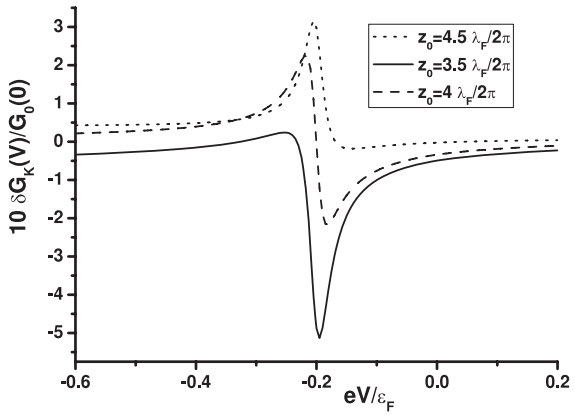

Figure 3. Difference $\delta G_K(V)/G_0$ between the voltage dependences of the conductance for a magnetic and for a non-magnetic impurity. We have used the parameters $\varepsilon_K = 0.9\varepsilon_F$, $k_B T_K = 0.01\varepsilon_F$, and $r_D = 0.1\lambda_F/2\pi$.

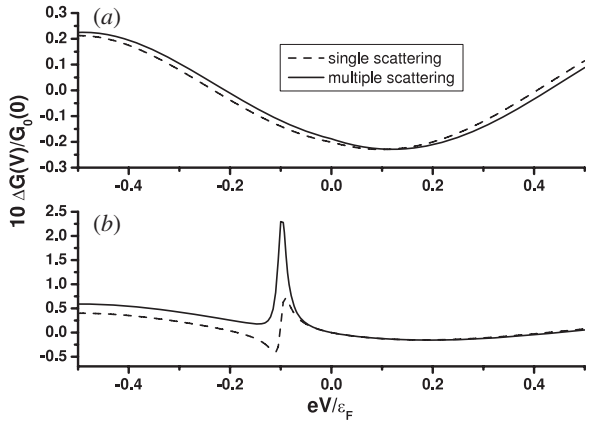

Figure 4. Comparison of the oscillatory parts of the conductance $\Delta G(V)/G_0$ calculated by using equations (24) and (25) (full curves) and by means of results obtained in the framework of perturbation in the electron–impurity interaction (dashed curves); (*a*) non-magnetic defect; (*b*) magnetic defect. We have used the parameters $\varepsilon_K = 0.9\varepsilon_F$, $k_B T_K = 0.01\varepsilon_F$, $r_D = 0.1\lambda_F/2\pi$, $\rho_0 = 0$, and $z_0 = 5\lambda_F/2\pi$.

vice versa, the negative sign of the Kondo anomaly is found at a minimum in the periodic variation of ΔG.

In figure 3 we present the difference $\delta G_K(V)/G_0 = (\Delta G_m - \Delta G_n)/G_0$ between voltage dependences for a magnetic ΔG_m and a non-magnetic ΔG_n impurity, having the same potential scattering strength. The plots in figure 3 show the evolution of the shape of the Kondo anomaly for several values of the distance between the contact and the impurity, placed on the contact axis. The change of distance changes the periodicity of the normal scattering oscillations which is illustrated to lead to a changing of sign in the Kondo signal. A similar dependence of the differential conductance with the distance between an STM tip and an adatom on the surface of a metal has been obtained theoretically in [13, 25] in the terms of the Anderson impurity Hamiltonian [26]. Note that we obtained the Fano-like shape of the Kondo resonance in the framework of a single-electron approximation while in [13, 25] the many-body effects were taken into account.

Figure 4 illustrates the importance of multiple scattering for this problem. It shows the oscillatory parts of the conductance $\Delta G(V)/G_0$ calculated by using equations (24) and (25) in comparison to results obtained in the framework of perturbation in the electron–impurity interaction [17, 18], i.e. neglecting multiple electron scattering. While for the non-magnetic impurity (figure 4(*a*)) the difference between two curves is small it is seen that for a magnetic impurity (figure 4(*b*) the perturbation method does not describe the conductance correctly in a region of the Kondo resonance. For non-magnetic impurities multiple scattering has a negligible effect due to the smallness of contributions of the multiple scattering paths described by the parameter $(k_F z_0)^{-1}$, which is no longer true near the Kondo resonance, where the increasing of the scattering amplitude is the dominant effect.

6. Conclusion

We have studied the influence of multiple electron scattering by a single defect on the current through a tunnel point contact. In the approximation of s-wave scattering by the defect a general expression for the conductance G has been found ((24), (25)). The results obtained have been analyzed for the model s-wave phase shift (30) describing the Kondo scattering by a magnetic impurity. We demonstrated that taking multiple scattering into account is most essential near voltage values corresponding to the Kondo resonance condition $\varepsilon_F + eV = \varepsilon_K$. It is found that 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. The phase shift between the two waves produces the oscillations of the conductance. A maximum in the regular oscillation of G leads to a positive sign of the Kondo anomaly at that position, while a minimum produces a negative sign. These results may be exploited in future experiments for detecting and investigating the Kondo effect of individual impurities in the bulk of a host metal.

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