Line Shape in the Mirage Experiment

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Abstract

Using a many-body theory, we calculate the change in differential conductance \(\Delta dI/dV\) after adding an impurity either on a clean surface or inside an elliptic quantum corral. Using the same set of parameters for both cases, the qualitative features of the voltage dependence of \(\Delta dI/dV\) observed in recent experiments, are reproduced.

Introduction

In recent experiments a Co atom (acting as a magnetic impurity) was placed at one focus of an elliptic corral, and a depression in the differential conductance \(dI/dV\) as a function of voltage (a signature of the Kondo effect) was observed not only at this focus, but also at the other one. The space dependence of \(\Delta dI/dV\) (\(dI/dV\) after subtracting the corresponding result for the empty corral) reflects mainly the density of the eigenstate of two-dimensional free electrons confined in the corral which lies at the Fermi energy. This space dependence has been reproduced by several theories. The voltage dependence is more subtle and requires in principle a many-body calculation of the Kondo resonance. However, most theories treat the interactions in a phenomenological way. Many-body effects were included either by perturbation theory or by numerical diagonalization in a restricted subspace. Unfortunately, since the separation of the relevant eigenstates of the corral (those with a sizeable hybridization with the impurity) is larger than the Kondo temperature, these numerical results cannot reproduce the observed line shape.

Here we extend our previous approach to the clean surface and take into account the direct tunneling between the tip and the impurity, in order to compare the line shape of \(\Delta dI/dV\) for an impurity inside the corral or on a clean surface.

The model

The simplest description of the problem includes a non-degenerate highly correlated impurity state and the surface states near the Fermi energy \(\varepsilon_F\). For the clean Cu(111) surface, the latter are uncoupled from bulk states for wave vectors inside the neck of the Fermi surface. Band structure calculations indicate that these states have a weight larger than 60% in the first layer. The remaining weight is mainly due to other surface states at different energies. Taking a standard \(r^{-7/2}\) distance dependence between \(sp\) and \(d\) electrons, and considering that the impurity atom enters in the three-fold coordinated position at the surface, one obtains that the hybridization of the impurity with the surface layer is nearly 17 times larger than that with the second layer. Since the density of \(sp\) states at the first layer is also larger, this information suggests that the direct hybridization of the impurity with bulk states can be neglected. Taking into account that the distance between Cu atoms is smaller than the Fermi wave length \(2\pi/k_F \sim 30\text{Å}\), the hybridization of the impurity with a surface state \(j\) can be approximated as \(V\lambda\phi_j(R_i)\), where \(R_i\) is a two-dimensional vector 1) Corresponding author; Phone: +54 2944 445170, Fax: +54 2944 445299, e-mail: aligia@cab.cnea.gov.ar
denoting the position of the impurity, \( \varphi_j(r) \) is the wave function of state \( j \) normalized as
\[
\int |\varphi_j(r)|^2 d^3r = 1, \quad \lambda \text{ is a length scale which we take as the square root of the surface per Cu atom} \quad (\lambda = 2.38 \text{ Å}).
\]
and \( V \) is an energy which would represent the hopping between one atom of the surface and the impurity in a tight-binding description. For the clean surface, \( j \) labels the allowed wave vectors of extended Bloch states in a large area with periodic boundary conditions, while for the mirage experiment, the \( \varphi_j(r) \) are localized inside the corral.

The above considerations lead to the following Anderson model:
\[
H = \sum_{j,\sigma} \varepsilon_j c_{j,\sigma}^\dagger c_{j,\sigma} + E_d \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma} + U d_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow} + V \lambda \sum_{j,\sigma} [\varphi_j(R_c) d_{\sigma}^\dagger c_{j,\sigma} + \text{H.c.}].
\]  

Here \( c_{j,\sigma}^\dagger \) and \( d_{\sigma}^\dagger \) create an electron on the \( j^{th} \) conduction eigenstate and the impurity respectively.

**Approximations and relevant equations**  
At sufficiently low temperatures, the differential conductance \( dI/dV \) when the probing tip is at position \( r \), is proportional to the density of the mixed state \( f_\sigma(r) = \lambda \sum_j \varphi_j(r) c_{j,\sigma} + q d_{\sigma} \).
\[
\frac{dI(V)}{dV} \sim \rho_f(\epsilon_F + eV) = -\frac{1}{\pi} \text{Im} G_j(\epsilon_F + eV),
\]
where \( G_j(\omega) = \langle \langle f_\sigma; f_{\sigma}^\dagger \rangle \rangle_\omega \) is the Green function of \( f_\sigma(r) \) and \( q \) is the ratio between tunneling matrix elements between impurity and tip and between impurity and surface. It is different from zero only for \( r \) very near \( R_c \). The change in \( dI/dV \) after adding the impurity is proportional to the corresponding change in \( \rho_j \). From the equations of motion:
\[
\Delta G_j(r, \omega) = (VG_j^0(r, R_c, \omega) + q)(VG_j^0(R_c, r, \omega) + q)G_d(\omega),
\]
where \( G_d(\omega) = \langle \langle d_{\sigma}; d_{\sigma}^\dagger \rangle \rangle_\omega \) is the impurity Green function and \( G_j^0 \) is the conduction electron Green function for \( V = 0 \):
\[
G_j^0(r, r, \omega) = \sum_j \frac{\lambda^2 \varphi_j^*(r) \varphi_j(r')}{\omega + i\delta - \varepsilon_j},
\]  
where \( \delta \) is a positive infinitesimal. For the clean surface, the eigenvalues \( \varepsilon_j \) form a continuum of constant density of states \( \rho_0 = 0.045 \text{ states/(eV site)} \), using an effective mass 0.38 times the electron mass \( m_e \). For a hard wall elliptic corral, the \( \varepsilon_j \) are discrete. For a finite confinement potential, the eigenstates inside the corral become resonances and the spectrum is continuous again. However, from results borrowed mainly from nuclear physics, we know that \( G_j^0 \) inside the corral can be expressed as a discrete sum of complex poles \( \frac{1}{\omega + i\delta - \varepsilon_j} \). Thus, the form of \( G_j^0 \) for the hard wall corral is retained, but \( \delta \) becomes finite. Here we retain the values of \( \varepsilon_j \) and \( \varphi_j(r) \) of the hard wall corral calculated before \( 2 \) up to an energy of 1 eV above \( \epsilon_F \). This approximation is justified by comparison with the Green function which results for a scattering potential consisting of delta functions regularly spaced at the boundary of the ellipse \( \lambda \). For all continuum states around a resonance, the wave function inside the corral is essentially the same, differing only outside the corral. In addition, with an effective mass 0.378 \( m_e \), the hard wall results for \( \varepsilon_j \) around \( \epsilon_F \) reproduce the experimental results. For simplicity, we take \( \delta \) independent of \( j \).
The impurity Green function is given by:

\[ G_{d}^{-1}(\omega) = \omega - \tilde{E}_d - V^2 G_{c}^0(R_i, R_i, \omega) - \Sigma(\omega), \]

where in our approach, \( \tilde{E}_d \) is a renormalized \( d \) level, and \( \Sigma(\omega) \) is the self energy calculated in second order in \( U \). Because of the limitations of the perturbative approach, we have chosen a moderate value of \( U = 1 \) eV, and \( \tilde{E}_d \simeq \epsilon_F \) (near the symmetric case). We have taken \( V = 0.64 \) eV, to lead to a half width at half maximum near \( T_K = 4 \) meV for the spectral density \( \rho_d(\omega) \) of the impurity on a clean surface. The resulting impurity resonant level width is \( \Delta \simeq 58 \) meV. For this value of \( U/\Delta \), the position of the peak is not adequately given by perturbation theory. Then we used independent values of \( \tilde{E}_d \) for the impurity on the clean surface or inside the corral, to control this position. The other parameters of the model are the same in both situations. The width \( \delta \) is the only free parameter to control the line shape for the impurity inside the corral.

**Results** In Fig. 1 (a), we show \( \Delta \rho_f \), proportional to \( \Delta dI/dV \), at the impurity position for the clean surface and several values of \( q \). The result for \( q = 0 \) is symmetrical and proportional to \( \rho_d(\omega) \). The experimental \( \Delta dI/dV \) is larger for positive sample bias, corresponding to positive energy \( \omega \). This asymmetry can be achieved increasing \( q \). However, the experimental
line shape shows a relative maximum also at negative $\omega$, in contrast to our result. This feature seems difficult to explain. Except for this fact, the observed line shape is qualitatively reproduced for $\delta$ between 0.03 and 0.04.

In Fig. 1 (b), (c) and (d) we show $\Delta \rho_f$ for an elliptical corral with eccentricity $e = 1/2$, and semimajor axis $a = 71.3$ Å, with an impurity placed at the left focus, for several values of $\delta$ and $q$, and for both foci. If $\delta < T_K$, the Kondo resonance at $\epsilon_F$ is absent. Instead, both $\rho_d$ and $\rho_f$ present two narrow peaks at both sides of the Fermi energy. In the absence of the impurity, $\rho_f$ has a peak at $\epsilon_F$ which corresponds to the state 42 ($\epsilon_F = \epsilon_{42}$). As a consequence, the difference $\Delta \rho_f$ present two narrow peaks above zero and a depression with negative $\Delta \rho_f$ (see Fig. 1 (b)). For $\delta \gg T_K$ (Fig. 1 (c) and (d)), a Kondo resonance quite similar to that of the clean surface is formed. However, due to the asymmetry of the amplitude of the wave functions of the corral above and below $\epsilon_F$ at the impurity site, the line shape is asymmetric for $q = 0$, being higher at negative energies. This asymmetry is opposite to the experimentally observed in the case of the clean surface. Thus, while a positive value of $q$ renders the line shape asymmetric for a clean surface, it restores a rather symmetric line shape in the case of the corral, as experimentally observed.

As $\delta$ increases, the magnitude of the depression observed at the empty focus decreases. This is due to an increasing negative interference of the corral state 42, which is even under interchange of both foci, with other odd states, whose weight at $\epsilon_F$ increase with $\delta$. For $\delta \sim 40$ meV, the main aspects of the observed space and voltage dependence of $\Delta dI/dV$ are reproduced.

**Conclusion** An Anderson model in which the magnetic impurity is hybridized with surface states, which are extended in the case of a clean surface or resonances in presence of a quantum corral, is able to reproduce the qualitative features of the observed change in the voltage dependence of the differential conductance $\Delta dI/dV$ (in particular its asymmetry) in both cases. This requires a small direct tunneling between the impurity and probing tip, when the tip is above the impurity. The rather symmetric line shape observed above the impurity at the focus in the quantum corral is the result of the compensation of two effects which alone would produce an asymmetry in opposite directions: the direct tunneling between the impurity and tip, and the particular electronic structure of the resonances inside the corral, above and below the Fermi energy. Work to study the line shape in other physical situations, for example for a mirage out of focus, is in progress.

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