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Observation of two impurity Kondo effect in Scanning Tunneling Spectroscopy

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Abstract. We derive a formula for the differential conductance measured in Scanning Tunneling Spectroscopy for two magnetic atoms absorbed on metal surface. We find that the shape of the differential conductance spectra varies with the distance between the two atoms. This change indicates the variation in effective range of the Kondo effect and the RKKY interaction effect.

1. Introduction
A magnetic dimer adsorbed on a nonmagnetic metal surface is a classic system in which two impurity Kondo effect is expected to lead to a significant change in the corresponding surface electron state. In such systems, Scanning Tunneling Spectroscopy (STS) is a powerful tool for detecting the Yosida-Kondo peak, a hallmark of Kondo effect [1–3]. Especially in the case of a magnetic dimer, through the STS spectrum, the real space observation of two impurity Kondo effect is possible. In a recent experiment, the observed change in the shape of the differential conductance (dI/dV) is attributed to the RKKY interaction [4]. In this study, to gain a more detailed insight into the origin of the shape variation of the STS spectra, we derive the formula for the dI/dV (V) for varying the distances between adatoms.

2. Model and Method
We consider a magnetic dimer on a nonmagnetic metal surface as shown in Fig. 1. In this study, we set the coordinate with its origin at the contact point between magnetic atom1 and metal surfaces and we set the STM tip directly above atom1. The distance between atom1 and atom2 is a [Å]. We modeled this system with the following Hamiltonian,

\[ H = H_{A2} + H_{tip} + H_{mix} \]

\[ = \sum_{i, \sigma} E_d d^\dagger_{i \sigma} d_{i \sigma} + \sum_{k, \sigma} E_k c^\dagger_{k \sigma} c_{k \sigma} + \sum_{i} (V_{kdi} c^\dagger_{k \sigma} d_{i \sigma} + h.c.) + \sum_{i} U n_{i \uparrow} n_{i \downarrow} \]

\[ + \sum_{l, \sigma} (E_l - \mu) c^\dagger_{l \sigma} c_{l \sigma} + \sum_{l i} (T_{pld} c^\dagger_{l \sigma} d_{i \sigma} + h.c.) + \sum_{l k \sigma} (W_{plk} c^\dagger_{l \sigma} c_{k \sigma} + h.c.). \]  

(1)

Here \( d^\dagger_{i \sigma}, c^\dagger_{k \sigma} \) and \( c_{l \sigma} \) are the creation operators with spin \( \sigma \) for \( d \) electron on adatoms, conduction electrons on metal surface, and electrons on tip, respectively. \( i=1,2 \) is the index of the adatoms.
Figure 1. STS observation of magnetic dimer on nonmagnetic metal surface. Distances are given in Ångströms

$k$ is the corresponding wavenumber of metal surface electrons, and $l$ is the eigenstate index of the tip. $T_{pdi}$ is the tunneling matrix element between tip and adatom, $W_{pk}$ is the tunneling matrix element between tip and surface, and $V_{d2}$ is the tunneling matrix element between adatom and surface. $µ$ is the chemical potential of tip, adjusted to the bias voltage. We approximate the coefficients in the Hamiltonian (1) as follows,

$$V_{d1} = V_0, \quad V_{d2} = V_0 \exp(-i\kappa \alpha)$$
$$W_{kp} = W_0 \exp(-(z_p - R_s)/\lambda) \exp(-i(kr_p)) \quad T_{pdi} = T_0 \frac{\psi_{di}(r_p - R_s)}{\psi_{di}(R_1 + R_2)}.$$  (2)

Here, $\psi_{di}$ is the $d$ electron orbital of adatom $i$. $W_0$ and $T_0$ is the values of the tunneling matrix elements when the tip contacted to the surface or adatoms, respectively. Using non-equilibrium Green’s function(NEGF) method [3, 5], the current from the STM tip to the surface can be described as

$$J = \frac{2e}{h} \sum_\sigma \int d\omega (f_k - f_p) \left\{ 2\pi T_0^2 \Phi_{d1}^2 + \Phi_{d2}^2 \rho_p \Im G_{11\sigma}^r + 4\pi T_0 \Phi_{d1} \Phi_{d2} \rho_p \Im G_{12\sigma}^r - 2\pi^2 \rho_p \rho_p W_0^2 e^{-2(z_p - R_s)/\lambda} \right.$$  
$$- 4\pi T_0 (\Phi_{d1} J_{vw}(r_1) + \Phi_{d2} J_{vw}(r_2) - \rho_p R G_{11\sigma}^r - 2\pi T_0 (\Phi_{d1} J_{vw}(r_2) + \Phi_{d2} J_{vw}(r_1)) \rho_p R G_{12\sigma}^r) \right\}.$$  (3)

$f_k$ and $f_p$ are the Fermi distribution function for the surface and tip, respectively. And,

$$\Phi_i = \frac{\psi_i(r_p - R_s)}{\psi_i(R_1 + R_2)}, \quad J_{vw}(r) = \pi \rho_p J_0(k_F r) V_0 W_0 \exp(-(z_p - R_s)/\lambda).$$  (4)

$\lambda$ is the decay constant of surface wave function and $J_0$ is the 0th order Bessel function. We calculated the differential conductance based on this formula. To derive the necessary Green’s function, we adopt the Numerical Renormalization Group (NRG) technique [6].

3. Results and Discussions
We show the calculation results for the differential conductance in Fig. 2. In the NRG calculation, for the sake of simplicity, we set the band width of surface electron to 1.0 eV and we approximate the energy dispersion of the surface electron state as that of two dimensional free electrons. In the two dimensional free electrons, when we set the Fermi energy as 0 eV, the dispersion of the energy and wavelength is $E = \frac{\hbar^2 k^2}{2m_e} - D$ and $k_F \sim 0.5123 \sqrt{m_s/m_e}$. Here $m_s$ is the effective mass of conduction band electrons and $m_e$ is the elementary electronic mass. We set the effective mass as 0.5$m_e$. So the Fermi wavenumber $k_F$ is $\sim 0.3623 \AA^{-1}$. In setting the parameters and wavefunction of adatoms, we reffered to the case of Co/Cu(111) [3] as a typical Kondo system. We set the Coloumb interaction $U = 0.3eV$, $\pi \rho_p V_0^2 = 0.041eV$ so as to reproduce the experimentally measured Kondo temperature, 50K [3]. As shown in Fig. 2, the peak structure near Fermi level varies in shape, especially in the peak width, changing with the
distance between adatoms. We consider of the origin of this deformation of the peak structure from the energy flow diagram obtained from NRG calculation.

In the NRG calculation for Green’s function, we transform the Hamiltonian of the magnetic dimer and the metal surface following [8, 9], and using the logarithmic discretization for conduction electron band [9] and Lanczos based method [7], the Hamiltonian can be rewritten in a suitable form for NRG calculation as follows,

\[
H_{A2} = \sum_{n, \sigma} E_{n, \sigma} f_n^{\dagger} f_n + \sum_{n, \sigma} (t_{n, \sigma} f_{n+1, \sigma} + H.c.) + \sum_{p, \sigma} \epsilon_p n_p + U \sum_{p, \sigma} n_{dp} n_{dp} + \sqrt{2D} \sum_{p, \sigma} (\gamma f_{dp}^{\dagger} d_p + H.c.).
\]  

(5)

Here \( f_{n, \sigma} \), \( d_{\sigma} \) are derived from the canonical transformation of the operators for conduction bands and adatoms, respectively. With this transformation, the Hamiltonian reduces to the two impurity form with parity \( (p = \pm) \) connected to each tight-binding chain constructed from \( f_{n, \sigma} \) operators. So we can consider that there are 2 channels with indices \( \pm \) connected to the 2 impurities. When the conduction band is that for a two dimensional free electron,

\[
f_0 = \int_{-D}^{D} \sqrt{\gamma_\pm} c_\pm / \sqrt{\gamma_\pm} d\epsilon, \quad \gamma_\pm = \frac{1 \pm J_0(k \sigma)}{2}, \quad \gamma_0 = \int_{-D}^{D} \gamma_\pm(\epsilon) d\epsilon, \quad \Gamma = \pi \rho V_0^2.
\]  

(6)

We define two physical quantities, total charge \( Q \) and total parity \( P \) as,

\[
Q = \sum_{\sigma} (n_{d, \sigma} - 1) + \sum_{\sigma} (n_{f, \sigma} - 1)
\]

\[
P = \sum_{\sigma} (n_{d, \sigma} - 1) + \sum_{\sigma} (n_{f, \sigma} - 1) - \sum_{\sigma} (n_{d, -\sigma} - 1) - \sum_{\sigma} (n_{f, -\sigma} - 1).
\]  

(7)

(8)

Q, total spin \( S \), and \( P \) are commutative with the Hamiltonian (5). So we characterized the state using \((Q, S, P)\). Eq.5 can be diagonalized iteratively. We show its low lying scaled eigenvalue in odd iteration in Fig. 3. As shown in Fig. 3, there are 4 state \((Q, S, P)\)=(-1 1 1), (1 1 -1), (-1 1 -1) and (1 1 -1) converging to the ground state. \((Q, S, P)\)=(-1 1 1) and (1 1 -1) states correspond to one hole excitation and one particle excitation in -channel, respectively. \((Q, S, P)\)=(-1 1 -1) and (1 1 -1) states are in +channel. The number of iteration needed to converge to the ground state depends on the parity of the channel including excitation. This means that the corresponding effective Kondo temperatures in each channel are different. The change in effective Kondo
temperature with magnetic interaction was also shown in earlier studies for two impurity Kondo Hamiltonian and suggested the relationship with RKKY interaction between adatoms [10]. The strength of the RKKY interaction, $I_{RKKY}$ is approximated by

$$I_{RKKY} \sim \frac{2mJS^2k_F^4}{(2\pi)^2} \frac{2k_Fa \cos(2k_Fa) - \sin(2k_Fa)}{(2k_Fa)^4}, \quad (J = 8V^2/U)$$

and varies in its sign and value with the product of distance between adatoms and Fermi wavenumber [11]. From the energy flow diagram, we conclude that for the $a=3.0\text{Å}$ case, corresponding to the existing strong ferromagnetic interaction case and the ferromagnetic RKKY interaction is dominant in almost all temperature regions except near 0K. Regarding the other three cases, the RKKY interaction between adatoms is weak. The RKKY interaction is ferromagnetic in $a=5.0\text{Å}$ and $a=7.0\text{Å}$ case, and anti-ferromagnetic in $a=10.0\text{Å}$ case. In these three cases, the Kondo exchange is dominant and the RKKY interaction play a minor role, just changing the Kondo temperature slightly. To summarize, a change in the peak width of differential conductance reflects a change in the effective Kondo temperature originating from the competitions between the Kondo exchange and the RKKY interaction, and we may estimate directly the strength of the RKKY interaction in surface magnetic dimer through the STS spectra.

4. Summary
We derived a formula for the differential conductance measured in STS for two magnetic atoms absorbed on metal surface. We found that the shape of the differential conductance spectra varies with the distance between the two atoms. From the energy flow chart of NRG calculation, we conclude that this change reflects the change of the effective Kondo temperature originating from the competition between the Kondo exchange and the RKKY interaction effect. These results suggest the possibility of direct estimation of the strength of RKKY interaction in surface magnetic dimer through the STS spectra.
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