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# Local Electronic Structure and Fano Interference in Tunneling into a Kondo Hole System

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Motivated by recent success of local electron tunneling into heavy fermion materials, we study the local electronic structure around a single Kondo hole in an Anderson lattice model and the Fano interference pattern relevant to STM experiments. Within the Gutzwiller method, we find that an intragap bound state exists in the heavy Fermi liquid regime. The energy position of the intragap bound state is dependent on the on-site potential scattering strength in the conduction and  $f$ -orbital channels. Within the same method, we derive a new  $dI/dV$  formulation, which includes explicitly the renormalization effect due to the  $f$ -electron correlation. It is found that the Fano interference gives asymmetric coherent peaks separated by the hybridization gap. The intragap peak structure has a Lorentzian shape, and the corresponding  $dI/dV$  intensity depends on the energy location of the bound state.

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*Introduction.* The intermetallic heavy fermion compounds based on either rare earth elements or on actinides [1–3] exhibit many unusual properties like heavy Fermi liquid (HFL), magnetic ordering, quantum phase transitions and associated non-Fermi liquid, as well as unconventional superconductivity [4]. In these materials, there are two types of electrons: delocalized conduction electrons ( $c$ -electrons), which derive from outer atomic orbitals, and strongly localized  $f$ -electrons that singly occupy inner orbitals. It is well accepted that the interplay between the  $c$ - $f$  hybridization and the screened on-site Coulomb repulsion is the key to the above-mentioned anomalous properties. However, the precise nature of the coherent Kondo state responsible for the formation of HFLs remains hotly debated [5–8]. Recent success of scanning tunneling microscopy (STM) experiments on heavy fermion materials [9–11] opens a new avenue toward understanding of these remarkable properties. Interest in the problem was also stimulated by the possibility to reveal the nature of electronic correlation effects by impurities and defects in heavy fermion materials as in unconventional superconductors including cuprates [12] and iron pnictides [13–15] or selenides [16].

Theoretical challenge in the interpretation of differential tunneling conductance as measured by STM in heavy-fermion lattice systems and around a single magnetic impurities or, more generally, disordered Kondo lattice systems, requires a proper treatment of electron correlation effects and quantum interference between the electrons tunneling from the STM tip into the conduction band and into the magnetic  $f$ -electron states. In the single Kondo impurity case, the line shape of  $dI/dV$  has been described reasonably well with a phenomenological form, as first discussed by Fano [17]. A microscopic understanding of this Fano line shape was recently provided [18, 19] in the single Kondo impurity case. In addition, the essence of a similar line shape observed on a clean crystal surface [9, 10], which has the lattice translational symmetry, can be captured within a similar microscopic

approach [18–21]. However, there is still a significant question about the role of correlation effect in the Fano interference. In one scenario [18], the passage of an electron from the STM tip is accompanied by a simultaneous spin flip of the localized moments via cotunneling mechanism. When the local spin operator is represented in terms of pseudofermions, this cotunneling term is equivalent to an effective tunneling in the pseudofermion channel renormalized by a local boson condensation order parameter inherent to the Kondo lattice itself [18]. In another scenario within the same Kondo lattice model [19], the renormalization factor is absent in the  $dI/dV$  formula. For both the single Kondo impurity problem and the Kondo lattice model, since the renormalization factor can be absorbed into the bare tunneling amplitude, this difference will not cause qualitative difference in analysis of STM data. However, for a Kondo hole or a more general disordered Kondo lattice problem, a logically consistent  $dI/dV$  formulation is important. In connection with the STM measurements, the latter type of problems just began to attract more focused interest because the inhomogeneity may provide important insight into the complex electronic structure of heavy fermion materials.

The Kondo hole problem was previously studied within an Anderson lattice model, where the  $f$ -electron self-energy for the pristine system was obtained from the second-order perturbation in Hubbard repulsion [22]. In the Kondo insulator (KI) regime, in which a hybridization gap is open at the Fermi energy, it was shown from the  $f$ -electron local density of states [22] that the Kondo hole introduced an intragap bound state. However, a very recent study of a single Kondo hole problem within the Kondo lattice model indicated that the existence of the intragap bound state depends on the nature of defects in the HFL regime [23]. This discrepancy suggests further theoretical studies are needed. In addition, existing studies [22, 23] are limited to local density of states and an analysis of Fano interference in the Kondo hole problem is still lacking. In this Letter, we study the local electronic

structure around a single Kondo hole in an Anderson lattice model as well as the Fano interference pattern relevant to STM experiments. Within the Gutzwiller method, we are able to demonstrate that the intragap bound state exists regardless of whether the system is in the HFL or KI regime. The energy position of the intragap bound state is dependent on the on-site potential scattering strength in the conduction and  $f$ -orbital channels. The same Gutzwiller method enables us to include explicitly the renormalization effect due to the  $f$ -electron correlation into the  $dI/dV$  formulation, which is conceptually consistent with the cotunneling mechanism [18]. It is found that the Fano interference does give rise to an asymmetric coherent peaks separated by the hybridization gap, while it tunes the intragap peak structure dependent on the energy location of the bound state, as shown in  $dI/dV$ .

*Kondo hole model and Gutzwiller formalism.* Our Hamiltonian for the single Kondo hole system is written as

$$\begin{aligned}
H = & - \sum_{ij,\sigma} (t_{ij}^c + \mu\delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i,\sigma} [V_{cf} c_{i\sigma}^\dagger f_{i\sigma} + \text{H.c.}] \\
& + \sum_{i,\sigma} (\epsilon_f - \mu) f_{i\sigma}^\dagger f_{i\sigma} + \sum_i U_f n_{i\uparrow}^f n_{i\downarrow}^f \\
& + \sum_{\sigma} \epsilon_c^I c_{I\sigma}^\dagger c_{I\sigma} + \sum_{\sigma} (\epsilon_f^I - \epsilon_f) f_{I\sigma}^\dagger f_{I\sigma} - U_f n_{I\uparrow}^f n_{I\downarrow}^f \\
& + \sum_{\sigma} [(V_{cf}^I - V_{cf}) c_{I\sigma}^\dagger f_{I\sigma} + \text{H.c.}]. \quad (1)
\end{aligned}$$

Here the operators  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) create (annihilate) a conduction electron at site  $\mathbf{r}_i$  with spin projection  $\sigma$  while the operators  $f_{i\sigma}^\dagger$  ( $f_{i\sigma}$ ) create (annihilate) a  $f$ -level electron at site  $\mathbf{r}_i$  with spin projection  $\sigma$ . The number operators for  $c$  and  $f$  orbitals with spin  $\sigma$  are given by  $n_{i\sigma}^c = c_{i\sigma}^\dagger c_{i\sigma}$  and  $n_{i\sigma}^f = f_{i\sigma}^\dagger f_{i\sigma}$ , respectively. The quantity  $t_{ij}^c$  is the hopping integral of the conduction electrons, and  $\epsilon_f$  is the local  $f$ -orbital energy level on the magnetic atoms. The hybridization between the conduction and  $f$ -orbital on the magnetic atoms is represented by  $V_{cf}$  and the  $f$ -electrons on the magnetic atoms experience the Coulomb repulsion of strength  $U$ . The first two lines on the right-hand side of Eq. (1) constitute the standard Anderson lattice model; while the last two lines represent the effect of a doped nonmagnetic atom, which without loss of generality is located at the origin  $\mathbf{r}_I = (0, 0)$ . The  $f$ -orbital energy level on the singly doped nonmagnetic atom is given by  $\epsilon_f^I$ . In the Kondo hole problem,  $\epsilon_f^I$  will be adjusted to ensure there is no  $f$ -electron occupation on the missing  $f$ -character center and as such the effect of on-site Coulomb repulsion can be negligible in the study of low energy electronic structure. In addition, the Kondo hole will also give rise to a potential scattering potential  $\epsilon_c^I$  and a possible change of local hybridization  $V_{cf}^I$ . These three parameters make the description of a Kondo hole more realistic, demonstrating the flexibility of the Anderson lattice Hamiltonian. For simplicity, the effect of local hybridization change is neglected by assuming  $V_{cf}^I = V_{cf}$  in the present work.

Due to the presence of onsite Hubbard interaction  $U$  between the  $f$ -electrons on the magnetic atoms in Eq. (1), the

above problem is strongly correlated. This strong correlation effect can be accounted for by reducing the statistical weight of double occupation in the Gutzwiller projected wavefunction approach [24], and the projection can be carried out semi-analytically within the Gutzwiller approximation [25–27]. In the present problem, the lattice translation symmetry is broken due to the Kondo hole, we use a spatially unrestricted Gutzwiller approximation (SUGA) [28–32] to translate the original Hamiltonian Eq. (1) into the following renormalized mean-field Hamiltonian:

$$\begin{aligned}
H_{\text{eff}} = & - \sum_{ij,\sigma} (t_{ij}^c + \mu\delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i \neq I, \sigma} [V_{cf} g_{i\sigma} c_{i\sigma}^\dagger \tilde{f}_{i\sigma} + \text{H.c.}] \\
& + \sum_{i \neq I, \sigma} (\epsilon_f + \lambda_{i\sigma} - \mu) \tilde{f}_{i\sigma}^\dagger \tilde{f}_{i\sigma} + \sum_{i \neq I} U_f d_i + \sum_{\sigma} \epsilon_c^I c_{I\sigma}^\dagger c_{I\sigma} \\
& + \sum_{\sigma} (\epsilon_f^I - \mu) \tilde{f}_{I\sigma}^\dagger \tilde{f}_{I\sigma} + \sum_{\sigma} [V_{cf}^I c_{I\sigma}^\dagger \tilde{f}_{I\sigma} + \text{H.c.}], \quad (2)
\end{aligned}$$

where  $\lambda_{i\sigma}$  and  $d_i$  are the Lagrange multiplier and the double occupation at site  $i$ . We have used  $\tilde{f}_{i\sigma}^\dagger$  ( $\tilde{f}_{i\sigma}$ ) to denote the quasiparticle field operators to differentiate from the truly  $f$ -electron operators in Eq. (1). The local  $c$ - $f$  hybridization has been renormalized by a factor of  $g_{i\sigma}$ , which is given by

$$g_{i\sigma} = \left[ \frac{(\bar{n}_{i\sigma}^{\tilde{f}} - d_i)(1 - \bar{n}_{i\sigma}^{\tilde{f}} + d_i)}{\bar{n}_{i\sigma}^{\tilde{f}}(1 - \bar{n}_{i\sigma}^{\tilde{f}})} \right]^{1/2} + \left[ \frac{d_i(\bar{n}_{i\sigma}^{\tilde{f}} - d_i)}{\bar{n}_{i\sigma}^{\tilde{f}}(1 - \bar{n}_{i\sigma}^{\tilde{f}})} \right]^{1/2}, \quad (3)$$

with  $\bar{n}_{i\sigma}^{\tilde{f}}$  being the expectation value of the spin- $\sigma$  density operator  $n_{i\sigma}^{\tilde{f}} = \tilde{f}_{i\sigma}^\dagger \tilde{f}_{i\sigma}$  and  $\bar{n}_i^{\tilde{f}} = \sum_{\sigma} \bar{n}_{i\sigma}^{\tilde{f}}$ . Minimization of the expectation value of  $H_{\text{eff}}$  leads to the following self-consistency conditions for  $\lambda_{i\sigma}$  and  $d_i$ :

$$\lambda_{i\sigma} = V_{cf} \frac{\partial g_{i\sigma}}{\partial \bar{n}_{i\sigma}^{\tilde{f}}} (\langle c_{i\sigma}^\dagger \tilde{f}_{i\sigma} \rangle + \text{c.c.}), \quad (4a)$$

$$-U = V_{cf} \sum_{\sigma} \frac{\partial g_{i\sigma}}{\partial d_i} (\langle c_{i\sigma}^\dagger \tilde{f}_{i\sigma} \rangle + \text{c.c.}), \quad (4b)$$

for  $i \neq I$ . Equation (2) can be cast into the Anderson-Bogoliubov-de Gennes (Anderson-BdG) equations [33]

$$\sum_j \begin{pmatrix} h_{ij}^c & \Delta_{ij} \\ \Delta_{ji}^* & h_{ij}^{\tilde{f}} \end{pmatrix} \begin{pmatrix} u_{j\sigma}^n \\ v_{j\sigma}^n \end{pmatrix} = E_n \begin{pmatrix} u_{i\sigma}^n \\ v_{i\sigma}^n \end{pmatrix}, \quad (5)$$

subject to the constraints given by Eq. (4). Here  $h_{ij}^c = -t_{ij}^c - \mu\delta_{ij} + \epsilon_c^I \delta_{iI} \delta_{ij}$ ,  $\Delta_{ij} = V_{cf} [g_i(1 - \delta_{iI}) + \delta_{iI}] \delta_{ij}$ , and  $h_{ij}^{\tilde{f}} = [(\epsilon_f + \lambda_i)(1 - \delta_{iI}) + \epsilon_f^I \delta_{iI} - \mu] \delta_{ij}$ . Since most of heavy-fermion systems have a layered structure, in which the dominant effects occur in the planes containing  $f$ -electron atoms, we solve this set of equations self-consistently via exact diagonalization on a two-dimensional square lattice. After the self-consistency is achieved, one can then calculate the projected local density of states (LDOS) as defined by:

$$(\rho_i^c, \rho_i^{c\tilde{f}}, \rho_i^{\tilde{f}}) = -2 \sum_n (|u_i^n|^2, u_i^n v_i^n, |v_i^n|^2) \frac{\partial f_{FD}(E - E_n)}{\partial E}, \quad (6)$$

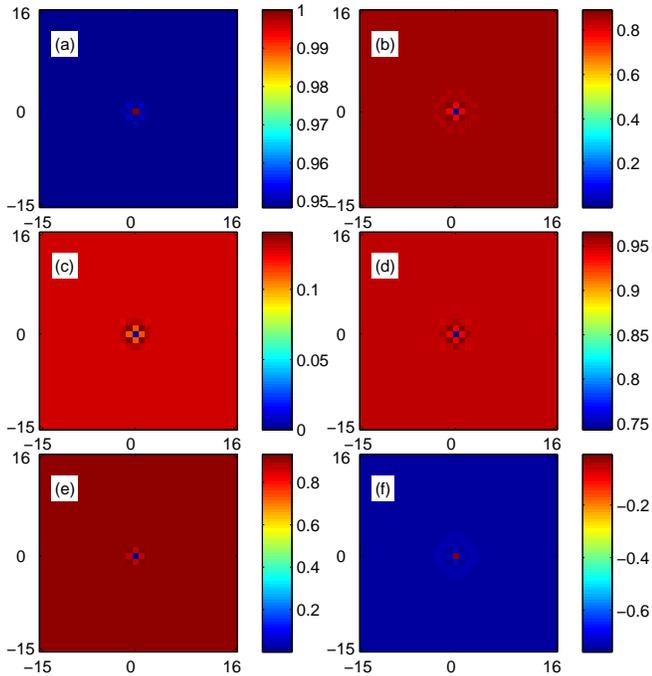


FIG. 1. (Color online) Solution to the Kondo hole problem in the heavy Fermi liquid regime for  $\mu = -0.4$ . Contour plots of the Gutzwiller factor  $g_i$  (a), the Lagrange multiplier  $\lambda_i$ , the double occupation  $d_i$  (c), the  $c$ -electron density  $\bar{n}_i^c$  (d),  $f$ -electron density  $\bar{n}_i^f$  (e), and the hybridization density  $\bar{n}_i^{cf}$  (f). The parameter values  $\epsilon_f^I = 100$  and  $\epsilon_c^I = 0$ . The values of other parameters are given in the main text.

where the Fermi-Dirac distribution function  $f_{FD}(E) = [\exp(E/k_B T) + 1]^{-1}$ . Here we have used the fact that the eigenfunctions are real and the system has a two-fold spin degeneracy in the non-magnetic state, for which quantities like  $\bar{n}_{i\sigma}^f$ ,  $g_{i\sigma}$ , and  $\lambda_{i\sigma}$  become spin-independent. Throughout this work, the quasiparticle energy is measured with respect to the Fermi energy and the energy unit  $t^c = 1$  is chosen.

*Local electronic structure around the Kondo hole.* In our numerical calculations, we take the following values of parameters for the pristine system: The on-site Coulomb interaction on  $f$ -electrons  $U = 2$ , the bare hybridization  $V_{cf} = 1$ , and the local  $f$ -level is taken to be  $\epsilon_f = -1$ . The temperature is fixed at  $T = 0.01$ . We solve the Anderson-BdG equations on a  $32 \times 32$  square lattice (by assuming a periodic boundary condition) to determine the self-consistency parameters  $g_i$  and  $\lambda_i$  while calculate the LDOS by using the supercell technique [34] ( $8 \times 8$  supercells are used). The chemical potential is varied so that the pristine system can be tuned into the HFL or KI regime. To describe the Kondo hole, we have fixed the value of  $\epsilon_f^I$  to be positive. This choice is consistent with the experimental realization of Kondo holes by substituting a Ce ion in a stoichiometric Ce compound by a La atom or a U ion in a U-heavy-fermion system by a Th atom, where the  $f$ -level is unoccupied by electrons on these impurity atoms.

Figure 1 shows the spatial variation of the self-consistently

determined Gutzwiller factor  $g_i$  (panel (a)), Lagrange multiplier  $\lambda_i$  (panel (b)), the double occupation  $d_i$ , as well as partial charge density  $\bar{n}_i^c$  (panel (d)),  $\bar{n}_i^f$  (panel (e)), and  $\bar{n}_i^{cf}$  (panel (f)) around the Kondo hole in the HFL regime with  $\mu = -0.4$ . Here  $\epsilon_f^I = 100$  and  $\epsilon_c^I = 0$ . The change of all these quantities happens around the Kondo hole. The short length scale of the change is consistent with the coherence length as estimated by  $\xi = \hbar \langle v_F \rangle / \pi g V_{cf}$ , where  $\langle v_F \rangle$  and  $g$  are the averaged Fermi velocity and the Gutzwiller renormalization factor for the pristine system. With the given set of parameter values, we estimate  $\hbar \langle v_F \rangle = 4.89$ , and  $g = 0.95$  from the self-consistent iterations, which leads to  $\xi$  being about 1.64 lattice constants. The anisotropy of the spatial change follows the underlying lattice, which is similar to that expected for a superconducting order parameter around a unitary non-magnetic impurity in a short-coherence  $s$ -wave superconductor. With the chosen parameter, it is found that the Kondo hole is negatively charged in the conduction band, by which we mean the conduction electron density on the Kondo hole is smaller than the value for the underlying pristine system. To get a positively charged Kondo hole in the conduction band, an attractive potential scattering  $\epsilon_c^I$  must be introduced.

In Fig. 2, we show the local partial and hybrid DOS in the HFL regime but with various values of  $\epsilon_f^I$  and  $\epsilon_c^I$  [The profile of self-consistency quantities around the Kondo hole remains similar to those shown in Fig. 1 and not shown here]. In the

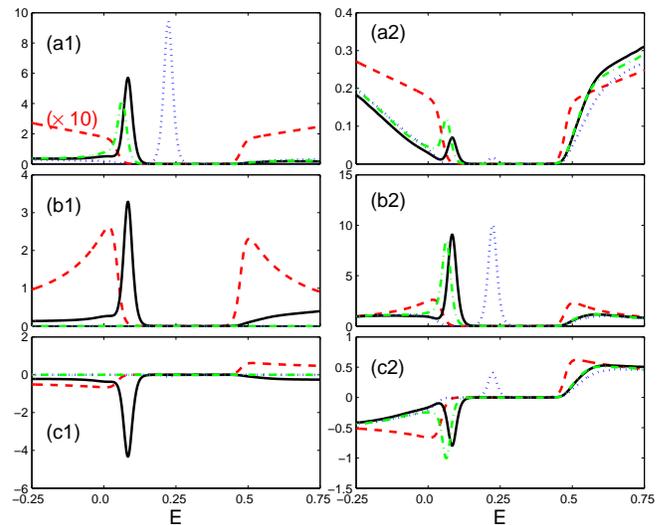


FIG. 2. (Color online) Local density of states, in the HFL regime, on the Kondo hole site (left column) and on its nearest neighboring site (right column). Panels with label (aX), (bX), and (cX) correspond to the conduction band and  $f$ -quasiparticle, and hybrid density of states, respectively. The red-dashed line is for the pristine case; the black-solid and blue-dotted lines for  $\epsilon_f^I = 1.0$  and  $100$  with  $\epsilon_c^I = 0$  fixed, the green-dashdotted line for  $\epsilon_f^I = 100$  while  $\epsilon_c^I = -1.0$ . The coherent peaks for the pristine system are located at  $E = 0.016$  and  $0.504$ . The bound state peak due to the presence of Kondo hole is located at  $E = -0.082$  and  $0.224$  for  $\epsilon_f^I = 1$  and  $100$  with  $\epsilon_c^I = 0$  fixed, and at  $E = 0.064$  for  $\epsilon_f^I = 100$  but  $\epsilon_c^I = -1.0$ .

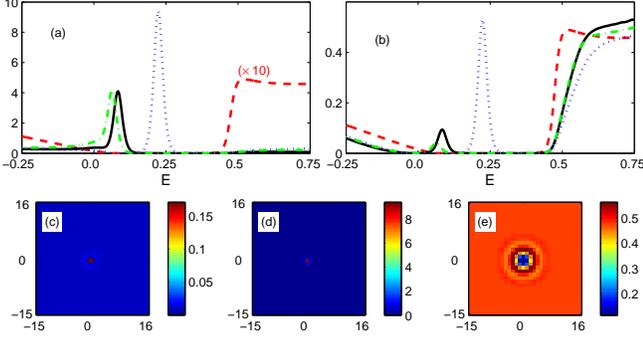


FIG. 3. (Color online)  $dI/dV$ , in the heavy Fermi liquid regime, as a function of energy on the Kondo hole (a) and its nearest neighboring site (b) corresponding to Fig. 2, as well as the  $dI/dV$  spatial map with selected energies  $E = 0.016$  (c),  $0.224$  (d), and  $0.504$  (e). These energies correspond to the coherent peak position ( $E = 0.16$  and  $0.504$ ) and the intra-gap peak position ( $E = 0.224$ ) for  $\epsilon_f^I = 0$  and  $\epsilon_c^I = 0$ .

absence of Kondo hole, the LDOS is spatially independent, but both the local partial and hybrid DOS is asymmetric with respect to the chemical potential ( $E = 0$ ). The DOS intensity is peaked at the coherent gap edge (see the red-dashed line in the figure) and is finite at the Fermi energy, indicating the electron states are in the HFL regime. In the presence of Kondo hole, when  $\epsilon_f^I$  is increased, an intragap bound state is formed with the energy position moved toward the center of the gap. With increased  $\epsilon_f^I$ , the DOS intensity on the  $f$ -channel vanishes directly on the Kondo hole site while becomes stronger on the site nearest neighboring to the Kondo hole. However, the corresponding DOS in the conduction band has an opposite trend. Furthermore, an attractive potential scattering on the conduction channel will further tune the bound state peak away from the gap center. It is also interesting to note that the hybrid DOS exhibits negative-sign peak for the intragap state for weak to intermediate values of  $\epsilon_f^I$  and  $\epsilon_c^I$ . Our result agrees with the STM observation of an electronic bound state at thorium atoms, when they are substituted for U atoms in  $\text{URu}_2\text{Si}_2$  [35].

*Fano interference pattern around the Kondo hole.* To model the STM electron tunneling, for which a schematic picture can be found in Fig. 1 of Ref. 18, we introduce the tunneling Hamiltonian between the STM tip and the sample at a specified measure site “ $i$ ”:  $H_T = \sum_{\sigma} V_{tc} \{c_{t\sigma}^{\dagger} [c_{i\sigma} + (V_{tf}/V_{tc})f_{i\sigma}] + \text{H.c.}\}$ , where  $V_{tc}$  and  $V_{tf}$  are the amplitudes for tunneling into conduction and  $f$ -electron states. Within the Gutzwiller approach to account for the  $f$ -electron correlation, tunneling amplitude  $V_{tf}$  will be renormalized by the local Gutzwiller factor  $g_i$ , that is,  $V_{tf} \rightarrow g_i V_{tf}$ , which leads to, in the weak-tunneling limit, the zero-temperature differential tunneling conductance [36]:

$$\frac{dI}{dV} = \frac{2e^2\pi N_0 V_{tc}^2}{\hbar} [\rho_i^c(E) + 2r g_i \rho_i^{c\bar{f}}(E) + r^2 g_i^2 \rho_i^{\bar{f}}(E)], \quad (7)$$

where  $r = V_{tf}/V_{tc}$ . Here we have assumed the tip density of

states to be independent of energy and approximated its value at the Fermi energy  $N_0$ , which is on the order of magnitude of the inverse band width of the tip. Equation (7) indicates that the renormalization due to the  $f$ -electron correlation effect in the heavy fermion materials must be taken into account explicitly in the tunneling conductance formula. This formula is logically consistent with the cotunneling mechanism [18], and must be used in theoretical approaches based on an auxiliary field theory.

As is shown in Fig. 2, the hybrid DOS is not positively definite, the line shape of  $dI/dV$  is determined not only by whether the electronic structure for the pristine system has the particle-hole symmetry but also by the relative strength of tunneling amplitude of conduction band and  $f$ -electron channel. Figure 3 shows the energy dependence of  $dI/dV$  on the Kondo hole (panel (a)) and its nearest-neighboring site (panel (b)), as well as its spatial dependence at selected energies (panels (c)-(e)), in the HFL regime with  $r = 0.2$ . We used the zero-temperature formula (Eq. (7)), for  $T = 0.01$  as a very low temperature solely for technical reasons. As can be seen from Fig. 3(a)-(b), the Fano interference makes the  $dI/dV$  characteristic strongly asymmetric, with the continuum part of  $dI/dV$  intensity at negative energies much smaller than at positive energies. The Fano interference also leads to different  $dI/dV$  intensity maps at the two gap edges (see Fig. 3(c) and (e)) with a ripple-like structure easily visible at the positive energy side. However, the peak structure due to the intragap bound state formed around the Kondo hole is robust against the Fano interference. On the Kondo hole site, the overall  $dI/dV$  characteristic is similar to that of LDOS on the conduction band; while its nearest neighboring site, the characteristic is sensitive to the detailed parameter values of  $\epsilon_f^I$  and  $\epsilon_c^I$ . In addition, the spatial imaging of  $dI/dV$  characteristic (Fig. 3(d)) suggests the Kondo hole induced intragap states are localized states.

*Conclusion.* We have studied the local electronic structure around a single Kondo hole in an Anderson lattice model and the Fano interference pattern relevant to STM experiments. Within the Gutzwiller method, we have obtained the existence of the intragap bound state induced around the Kondo hole in the HFL regime. The energy position of the intragap bound state is dependent on the on-site potential scattering strength in the conduction and  $f$ -orbital channels. Within the same method, we have also derived a new  $dI/dV$  formulation, which includes explicitly the renormalization effect due to the  $f$ -electron correlation. It has been found that the Fano interference gives rise to highly asymmetric coherent peak structure separated by the hybridization gap. The intragap peak structure has a Lorentzian shape. The corresponding  $dI/dV$  intensity depends on the energy location of the bound state and the location of the STM measuring point. We have also addressed the Kondo hole problem in the Kondo insulator regime with  $\mu = 0$  (not shown). The major finding for the HFL regime still holds except for the fact that the electronic states are fully gapped at the Fermi energy, and the Kondo hole becomes positively charged for  $\epsilon_c^I = 0$ .

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