Electron Cotunneling into a Kondo Lattice

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Motivated by recent experimental interest in tunneling into heavy-electron materials, we present a theory for electron tunneling into a Kondo lattice. The passage of an electron into a Kondo lattice is accompanied by a simultaneous spin flip of the localized moments via cotunneling mechanism. We compute the tunneling current with the large-N mean field theory. In the absence of disorder, differential tunneling conductance exhibits two peaks separated by the hybridization gap. Disorder effects lead to the smearing of the gap resulting in a Fano line shape.

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Major developments in scanning tunneling electron spectroscopy (STEM) over the last decade, particularly as a probe of cuprate superconductors [1–4], suggest that this tool will find increasing utility as an atomic-scale probe of many-body phenomena in new classes of materials. One area of particular promise lies in the application of STEM to heavy-fermion materials.

Heavy-fermion compounds contain a dense lattice of localized magnetic moments interacting with a sea of conduction electrons to form a "Kondo lattice" [5,6]. These materials exhibit a diversity of many-body behaviors, including anisotropic superconductivity, Kondo insulating behavior, and quantum criticality. Motivated by recent tunneling experiments on f-electron materials [7–9], in this Letter we develop a theory for tunneling into a coherent Kondo lattice.

How do electrons tunnel into a Kondo lattice, where the main degrees of freedom are local moments? Since direct tunneling into localized magnetic orbitals is blocked by Coulomb interactions, the naive expectation is that the electrons can only tunnel into the surrounding conduction sea. In 1960s Anderson and Appelbaum [10–12] recognized that magnetic ions actively participate in the tunneling process via a "cotunneling mechanism" [13,14] in which the passage of a tip electron into the conduction sea occurs cooperatively with a spin-flip of localized moments (Fig. 1). The manifestation of cotunneling in the tunneling conductance of quantum dots and magnetic atoms adsorbed on surfaces is well established experimentally [13–16]. Here we examine the effect of these processes on tunneling into a coherent band of excitations of a Kondo lattice, deriving a new expression for the tunneling current into a Kondo lattice in terms of the Green's function of composite cotunneling operators. Using the large-N approximation, we show how cotunneling processes open a direct tunneling channel between the tip and the composite quasiparticle states of the Kondo lattice. Once coherence develops, cotunneling and direct tunneling processes interfere, giving rise to distinctive two-peak structures in tunneling spectra.

We begin by writing down the Kondo lattice Hamiltonian in the presence of a tunneling probe, which takes the form $\hat{H} = \hat{H}_{\rm KL} + \hat{H}_{\rm tip} + \hat{H}_T$, where

$$\hat{H}_{\rm KL} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J \sum_j \vec{S}_f(j) \cdot (c^\dagger_{j\alpha} \vec{\sigma}_{\alpha\beta} c_{j\beta}) \quad (1)$$

is the unperturbed Kondo lattice Hamiltonian, $c_{j\sigma} = (1/\sqrt{V}) \sum_{\mathbf{k}} c_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{R}_j}$ creates a conduction electron and $\vec{S}_f(j)$ is the spin operator of a localized f electron at site j, respectively. The term $\hat{H}_{\rm tip} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} p^\dagger_{\mathbf{k}\sigma} p_{\mathbf{k}\sigma}$ describes the electrons in the tip. A crucial new feature of this model lies in the composite character of the tunneling Hamiltonian. When the tip lies in the vicinity of site 0, the tunneling Hamiltonian is given by

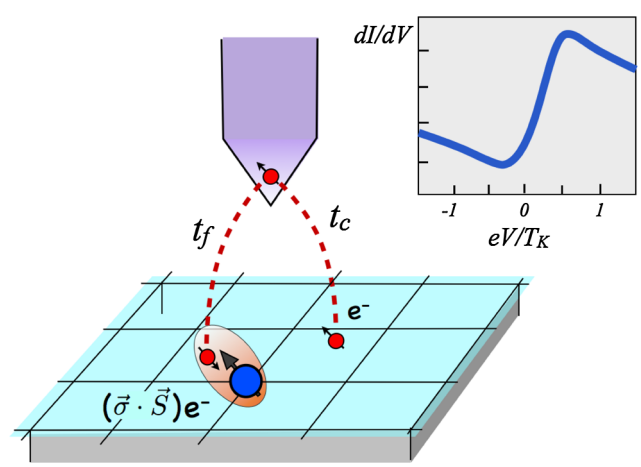

FIG. 1 (color online). Electron tunneling into a heavy-fermion material involves two parallel processes: direct tunneling with amplitude t_c into the conduction sea, and cotunneling with amplitude t_f into a composite combination of the conduction electron and local magnetic f moments. These composite states are expected to develop coherence below the Kondo temperature T_K. Inset shows a typical differential conductance curve observed for tunneling into a single Kondo ion.

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$$\hat{H}_T = p_{0\alpha}^\dagger \psi_{0\alpha} + \text{H.c.}, \tag{2}$$

where

$$\psi_{0\alpha} = t_c c_{0\alpha} + \tilde{t}_f[\vec{\sigma}_{\alpha\beta} \cdot \vec{S}_f(0)]c_{0\beta} \tag{3}$$

contains a direct tunneling term of amplitude t_c and a cotunneling term of amplitude t_f. From the equations of motion, the tunneling current operator is

$$\hat{I} = e\dot{N}_c = \frac{ie}{\hbar}\sum_\alpha(\psi_{0\alpha}^\dagger p_{0\alpha} - \text{H.c.}), \tag{4}$$

where $N_c = \sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$ is the number operator of the conduction electrons. From the form of $\hat{I}$ and $\hat{H}_T$, we see that the passage of an electron from the tip into the lattice is accompanied by a spin flip of a local moment. In this way, one-particle states in the tip are coupled to the composite fields which define heavy-electron quasiparticles.

The Hamiltonian (2) is a Kondo lattice generalization of the Anderson-Appelbaum tunneling Hamiltonian [11,12], first introduced to explain zero-bias anomalies associated with tunneling between two metallic leads via a single localized moment. Similar models have subsequently been used to describe tunneling through a quantum dot [14]. The cotunneling component of H_T can be understood as a result of mixing between states in the tunneling tip and the localized orbitals of the Kondo lattice. This process distorts the symmetry of the Wannier states that hybridize with the localized moments, partially delocalizing them into the tip. A derivation of the cotunneling terms can be done by carrying out a Schrieffer-Wolff transformation on the Anderson model describing the lattice and the tip [12,14,17]. In the Anderson model, the localized f electrons hybridize with the conduction electrons. When a tip is introduced above site 0 of the lattice, tunneling between the f state and the probe electrons modifies the hybridization according to $\hat{H}_h \to (Vc_{0\sigma}^\dagger + t_f p_{0\sigma}^\dagger)f_{0\sigma} + \text{H.c.}$, where t_f is the amplitude to tunnel directly from an f state to the probe, so that the tip modifies the orbital hybridizing with the f state:

$$c_{0\sigma} \to c_{0\sigma} + \frac{t_f}{V}p_{0\sigma}. \tag{5}$$

After a Schrieffer-Wolff transformation is carried out, which reduces the Anderson model to a Kondo model, this same replacement must be made to the Kondo interaction at site 0 in the unperturbed Kondo lattice model. To leading (linear) order in t_f/V, the result of this procedure is the quoted result in (3), where $\tilde{t}_f = Jt_f/V$.

Next, we compute the tunneling current. One of the questions that immediately arises, is whether the differential conductance can be analyzed in a conventional way when cotunneling terms are present. We now show that even though $\hat{I}$ contains a composite operator, the weakness of the tunneling matrix elements still permits us to expand the current to leading order in the tunneling matrix elements, thereby rewriting it in terms of the full many-body Green's functions of the bulk. To carry out this procedure, we write steady-state tunneling current as [18]

$$I(eV) \equiv \langle\hat{I}\rangle = \frac{e}{h}\,\text{Re}\int\frac{d\omega}{2\pi}G_{p\psi}^K(\omega), \tag{6}$$

where $G_{p\psi}^K(\omega)$ is the Keldysh Green's function [18] between the tip electron and $\psi_{0\alpha}$. Expanding the current to leading order in the tunneling matrix elements, we obtain [18]: $G_{p\psi}^K = G_p^R G_\psi^K + G_p^K G_\psi^A$, where R, A, K denote the retarded, the advanced, and the Keldysh Green's functions of the tip and the Kondo lattice. Since the tip and the lead are in thermal equilibrium, their Keldysh Green's functions can be rewritten in terms of retarded and advanced Green's functions, using the fluctuation dissipation relations [18] $G_p^K(\omega) = -2i\pi\rho_p(\omega + eV)h(\omega + eV)$ and $G_\psi^K(\omega) = -2i\pi\rho_\psi(\omega)h(\omega)$. Here $h(\omega) = 1 - 2f(\omega)$, where $f(\omega)$ is the Fermi distribution function, while $\rho_{\text{tip}}(\omega)$ is the local density of states of the tip; $\rho_\psi(\omega)$ is the "cotunneling" density of states of the sample given by $\rho_\psi(\omega) \equiv \frac{1}{\pi}\,\text{Im}G_\psi(\omega - i\delta)$, and $G_\psi(\omega)$ is the retarded Green's function of the ψ field, usually obtained through analytic continuation of the Matsubara imaginary time propagator $G_\psi = -\langle T\psi_{0\alpha}(\tau)\psi_{0\alpha}^\dagger(0)\rangle$.

Using these relations, the current (6) can be rewritten as

$$I(eV) = \frac{2\pi e}{\hbar}\int d\omega\,\rho_{\text{tip}}(\omega - eV)\rho_\psi(\omega)[f(\omega - eV) - f(\omega)]. \tag{7}$$

In this way, the tunneling current into a Kondo lattice probes the spectral function of the composite operator.

To illustrate the tunneling into the Kondo lattice, we now solve for the tunneling behavior in the large-N limit [19–23] of the Kondo lattice, where $N = 2j + 1$ is the spin degeneracy of the localized f state. In this approach, the spin operator is represented as a bilinear of pseudofermions [24]: $\vec{S}_f(j) = f_{j\alpha}^\dagger \vec{S}_{\alpha\beta} f_{j\beta}$, where $\vec{S}_{\alpha\beta}$ are the generators of the $SU(N)$ symmetry group. The mean field theory provides a representation of the composite fermion $[\vec{\sigma}_{\alpha\beta} \cdot \vec{S}_f(j)]c_{j\beta}$ in (3) as a single fermionic operator

$$\sum_\beta[\vec{\sigma}_{\alpha\beta} \cdot \vec{S}_f(j)]c_{j\beta} \to \frac{\mathcal{V}}{J}f_{j\alpha}, \tag{8}$$

where the amplitude $\frac{\mathcal{V}}{J} = -\langle f_{j\beta}^\dagger c_{j\beta}\rangle$. In this way, the large-N mean field theory captures the formation of a composite f electron, an essential element of the Kondo effect. In terms of pseudofermions, we can rewrite single particle operator in (3) as

$$\psi_{j\alpha} = t_c c_{j\alpha} + \tilde{t}_f f_{j\alpha}, \tag{9}$$

where the complex amplitude for tunneling into the composite fermion state is $\tilde{t}_f = \frac{\mathcal{V}}{J}t_f$.

The requirement that the number of pseudofermions at any given site should be equal to $N/2$ introduces a constraint λ, to be determined self-consistently together with the hybridization amplitude $\mathcal{V}$ (see, e.g., [21,25]). The resulting mean field Hamiltonian can then be diagonalized by means of the Bogoliubov transformation $c_{\mathbf{k}\sigma} = v_{\mathbf{k}} a_{\mathbf{k}\sigma} + u_{\mathbf{k}} b_{\mathbf{k}\sigma}$, and $f_{\mathbf{k}\sigma} = u_{\mathbf{k}} a_{\mathbf{k}\sigma} - v_{\mathbf{k}} b_{\mathbf{k}\sigma}$, where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the Kondo lattice coherence factors given by $u_{\mathbf{k}}^2 = [R_{\mathbf{k}} + (\varepsilon_{\mathbf{k}} - \lambda)]/2R_{\mathbf{k}}$, $v_{\mathbf{k}}^2 = 1 - u_{\mathbf{k}}^2$ with $R_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} - \lambda)^2 + 4\mathcal{V}^2}$. The Hamiltonian (1) in the mean field approximation then becomes $H_{\mathrm{KL}}^{(\mathrm{mf})} = \sum_{\mathbf{k}\alpha}(\omega_{\mathbf{k}}^- a_{\mathbf{k}\alpha}^\dagger a_{\mathbf{k}\alpha} + \omega_{\mathbf{k}}^+ b_{\mathbf{k}\alpha}^\dagger b_{\mathbf{k}\alpha})$, where $\omega_{\mathbf{k}}^\pm = (\varepsilon_{\mathbf{k}} + \lambda \pm R_{\mathbf{k}})/2$ is the quasiparticle dispersion in the newly developed heavy Fermi liquid. The mean field tunneling Hamiltonian then becomes

$$\hat{H}_T^{(\mathrm{mf})} = \sum_{j\alpha} p_{j\alpha}^\dagger [t_c c_{j\alpha} + \tilde{t}_f f_{j\alpha}] + \mathrm{H.c.} \tag{10}$$

Although our mean field Hamiltonian has the form of the Anderson lattice model with $U = 0$, the states on which it operates have an underlying composite structure, formed when local spins hybridize with conduction electrons. Thus, the Hamiltonian (11) provides a mean field description of the tunneling into the conduction band together with the cotunneling processes involving local moments.

It is instructive to contrast the tunneling conductance expected in a Kondo lattice with that of a single Kondo impurity. Using the tunneling Hamiltonian (11), we compute $G_\psi(\omega)$. In the case of a single Kondo impurity, we obtain

$$G_\psi^{\mathrm{imp}}(\omega) = \frac{(t_c i\pi\rho\mathcal{V} + \tilde{t}_f)^2}{\omega - \lambda - i\Delta} + t_c^2 i\pi\rho, \tag{11}$$

where ρ is the density of states of the conduction electrons, $\Delta = \pi\rho\mathcal{V}^2 \simeq T_K$ is the width of the Kondo resonance. The differential conductance $\frac{dI}{dV} \equiv g(eV)$ is

$$g_{\mathrm{imp}}(eV) = N\frac{2\pi e^2}{\hbar} t_c^2 \rho_{\mathrm{tip}}\rho \frac{|q + \epsilon'|^2}{1 + \epsilon'^2}\Big|_{\epsilon' = (eV-\lambda)/\Delta}, \tag{12}$$

where N is the spin degeneracy and $q = A(eV)/B(eV)$ is the ratio of two complex tunneling amplitudes, where $A(eV) = \tilde{t}_f + t_c\mathcal{V}P(\frac{1}{eV - \epsilon_{\mathbf{k}}})$ describes the cotunneling into the atomic orbital and $B(eV) = t_c\mathcal{V}\pi\delta(eV - \epsilon_{\mathbf{k}})$ describes direct tunneling into the metal [26]. Here $\epsilon' = (eV - \lambda)/\Delta$, ρ_{tip} is the density of states at the Fermi level of electrons in the tip. For a broad flat band, $A = \tilde{t}_f$, $B = t_c\mathcal{V}\pi\rho$, and $q = \tilde{t}_f/(t_c\mathcal{V}\pi\rho)$.

Now we turn to the case of the Kondo lattice. Within the large-N mean field theory, we obtain

$$G_\psi^{\mathrm{KL}}(\omega) = N\sum_{\mathbf{k}} \frac{(t_c + \tilde{t}_f \frac{\mathcal{V}}{\omega - \lambda})^2}{\omega - \epsilon_{\mathbf{k}} - \frac{\mathcal{V}^2}{\omega - \lambda}}, \tag{13}$$

where $\epsilon_{\mathbf{k}}$ is the dispersion of the conduction band. We obtain the following expression for the differential tunneling conductance,

$$g(eV) = N\frac{2\pi e^2}{\hbar} t_c^2 \rho_{\mathrm{tip}} \sum_{s=\pm,\mathbf{k}} \frac{|q + E_{s\mathbf{k}}|^2}{1 + E_{s\mathbf{k}}^2}\delta(eV - \omega_{s\mathbf{k}}), \tag{14}$$

where $E_{s\mathbf{k}} = (\omega_{s\mathbf{k}} - \lambda)/\Delta$. The prefactor of the delta function has a characteristic Fano functional form [27,28]. This form introduces an asymmetry in the resulting voltage dependence of the tunneling conductance $g(eV)$. The momentum summation in $G_\psi^{\mathrm{KL}}(\omega)$ (13) and $g(eV)$ (14) can be carried out analytically assuming a constant conduction electron density of states ρ to give

$$g(eV) = N\left(\frac{2\pi e^2}{\hbar}\right) t_c^2 \rho_{\mathrm{tip}}\rho \frac{1}{\pi}\,\mathrm{Im}\tilde{G}_\psi^{\mathrm{KL}}(eV - i\delta), \tag{15}$$

where

$$\tilde{G}_\psi^{\mathrm{KL}}(\omega) = \left(1 + \frac{q\Delta}{\omega - \lambda}\right)^2 \ln\left[\frac{\omega + D_1 - \frac{\mathcal{V}^2}{\omega - \lambda}}{\omega - D_2 - \frac{\mathcal{V}^2}{\omega - \lambda}}\right] + \frac{2D/t_c^2}{\omega - \lambda}. \tag{16}$$

Here $-D_1$ and D_2 are the lower and the upper conduction band edges, respectively, and $2D = D_1 + D_2$ is the bandwidth. The differential tunneling conductance predicted by this formula has two well-pronounced peaks at $eV \sim \lambda$ separated by a narrow hybridization gap $\Delta_g \sim 2\mathcal{V}^2/D$ in the single particle spectrum, as shown in Fig. 2.

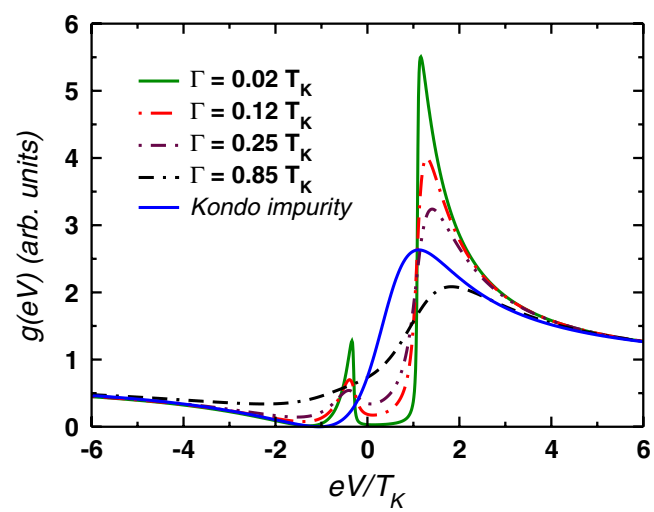

FIG. 2 (color online). Differential tunneling conductance $g(V)$ for a single Kondo impurity case given by (12), a Kondo lattice given by (15). A typical Fano shape in the single Kondo impurity case gets replaced with a double-peaked resonance line in the Kondo lattice case. The dashed lines illustrate the effect of disorder, which destroys the coherence, closing the gap in the density of states curve. Here $\tilde{t}_f/t_c = 0.2$, $q = 4.9$, $\lambda/T_K = 0.3$, while $D = 100T_K$.

In practice, experimental tunneling results will be modified by the effects of disorder [20]. A phenomenological quasiparticle elastic relaxation rate Γ may be introduced into the theory by replacing $\omega \to \omega - i\Gamma$ in (13). The results of this procedure are shown in Fig. 2. As we see, disorder removes the sharp peak structure in the tunneling conductance $g(eV)$ (15). The resulting line shape of the tunneling conductance $dI/dV(eV)$ is an asymmetric smooth curve.

The current work can be extended in a number of interesting directions. One important aspect is to examine the effects of cotunneling on the fluctuations in the density of states probed in Fourier transform STM experiments. In one-band systems, the Fourier transform of these fluctuations is phase sensitive to quasiparticle scattering [4,29], and is expected to be an important probe of both the quasiparticle dispersion and the phase of the cotunneling matrix elements.

A particularly fascinating aspect of cotunneling is its likely interplay with various forms of heavy-fermion order, such as heavy-fermion superconductivity. Unlike in conventional tunneling, the quasiparticle matrix elements of the composite operators associated with cotunneling are expected to be *sensitive* to the nature of the heavy-electron ground state. For example, recent work has proposed that heavy-electron superconductivity may involve composite pairing between local moments and electron pairs [25]. A key feature of composite pairing is the presence of two conduction screening channels Γ_1 and Γ_2, so that now the tunneling will be described by the ψ field (3) of the form

$$\psi_{0\alpha} = t_c c_{0\alpha} + \overbrace{\sum_{i=1}^{2}\{t_{f\Gamma_i}[\vec{\sigma}_{\alpha\beta}\cdot\vec{S}_f(0)]c_{\Gamma_i\beta}\}}^{uf_\alpha + v\,\mathrm{sgn}(\alpha) f^\dagger_{-\alpha}}, \tag{17}$$

where v describes hybridization in the particle-particle channel. In this way, we see that the cotunneling term in ψ may develop both particle and hole components, resulting in Andreev reflection even in the limit of weak tunneling.

In conclusion, we have studied electron tunneling into a Kondo lattice of localized moments, bringing out the importance of cotunneling as a primary mechanism of tunneling into the heavy-electron fluid. We have expressed the conductance in terms of a spectral function of a cotunneling composite operator, illustrating the result by a calculation carried out in the large-N limit. Our results predict that in a clean system the differential tunneling conductance will display two peaks separated by the hybridization gap. Addition of disorder leads to the smearing of the gap and produces a Fano-like smooth asymmetric line shape.

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