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Hybridization Induced Competitive Scanning Tunneling Interference Process into a Heavy Fermion System *

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We theoretically present the results for a scanning interference tunneling process between a metallic tip and a heavy fermion system. The density of states (DOS) and the differential conductance at zero temperature under different c–f band hybridizations, as well as the interference Fano ratio strength in the heavy fermion system, are calculated. It is found that the hybridization strength gives rise to the splitting effect in the DOS around the Fermi energy. Also the interference Fano ratio strength makes the differential conductance characteristics strongly asymmetric.

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The recent scanning tunneling microscopy (STM) research in heavy-fermion materials which include delocalized conduction electrons and strongly localized f electrons[1–3] provides an important experimental basis for studying the abundant principles of strongly correlated systems.[4–7] The interplay between the conduction electrons and f electrons gives rise to a wide range of behaviors in heavy fermion systems. Experimentally, recent study on the differential conductance (DC) has allowed one to measure the many-body quantum properties generated by the hybridization between the two types of electrons. For example, unconventional super-conductivity,[8] hidden order transition,[9,10] quantum criticality,[11] and correlated topological insulator[12,13] have made a breakthrough from the study of Fano DC in $CeCoIn_5$,[14,15] URu_2Si_2,[16,17] and SmB_6.[18,19] These works affirm the microscopic properties of the heavy-fermion as the composition of conduction electrons and f electrons.[20] However, detailed theoretical STM results in the heavy fermion materials being scarce because of the lack of a thorough microscopic realization of the internal coupling effect. In URu_2Si_2, it is uncertain whether the observation of the hybridization gap is necessarily associated with the hidden order.[21] In $CeCoIn_5$, can the superconducting gap be used to explain the kink at energies inside the superconducting gap?[22] In addition, the well-known STM DC process requires a proper treatment of electron correlation effects in the interference process.

In this Letter, we address the competitive effects of c–f hybridization strength and the Fano ratio strength on the STM transport in a heavy fermion system. We compute the density of states (DOS) for the c (f) electrons and the DC under different Fano ratio strengths, which can control the width of the dip and the asymmetry of the DC. We find that the DOS splits into double peaks with increasing the hybridization strength. The Fano ratio gives rise to asymmetric coherent peaks separated by the hybridization gap, which depends on the energy location of the bound state. In particular, it reduces the capability of the f-electron spectral weight near the edges of the hybridization gap. We employ the periodical Anderson-lattice model to describe the heavy fermion system, whose characteristics can be described by its DOS and interference effect through an STM process. The DOS and DC can be derived by the non-equilibrium Green function method. The corresponding STM Hamiltonian reads

$$H = H_{\rm tip} + H_{\rm tunnel} + H_{\rm fm}, \tag{1}$$

where $H_{\rm tip} = \sum_{\sigma} \varepsilon_\sigma d_\sigma^+ d_\sigma$ is the tip Hamiltonian, and $H_{\rm fm}$ is the heavy fermion system, which can be described by the periodical Anderson-lattice Hamiltonian as follows:

$$H_{\rm fm} = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum_{l,\sigma} \varepsilon_{\rm f} f_{l\sigma}^+ f_{l\sigma} + U \sum_{l} n_{l\uparrow}^{\rm f} n_{l\downarrow}^{\rm f} + \frac{V}{\sqrt{N}} \sum_{k,l,\sigma} c_{k\sigma}^+ f_{l\sigma} e^{-i\boldsymbol{k}\cdot\boldsymbol{l}} + {\rm H.c.} \tag{2}$$

Here we consider a two-dimensional square lattice, and the first term is the Hamiltonian of the conduction band with the energy dispersion relation $\varepsilon_k = -2t[\cos(k_x) + \cos(k_y)] - \mu$, μ and t are the chemical potential and hopping amplitude, respectively, and $\varepsilon_{\rm f}$ is the f-orbital local energy. The c–f hybridization is represented by the last two terms. Since the on-site Coulomb repulsion U in the Hamiltonian is very large for f electrons, the creation and annihilation operators for f electrons need to be applied with special projection operators.[23] Here we adopt the slave boson approach developed in the mid 1980s.[24] We replace the f-electron operator with two auxiliary operators $\tilde{f}_{i\sigma} b^+$ (b^+ is a boson operator). To proceed, we make a static approximation by replacing the boson operator with their expectation values $b_{\rm m}^+(b_{\rm m}) \to \langle b_{\rm m}^+ \rangle = b$, then the Hamiltonian can be rewritten in the momen-

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tum space as

$$H_{\rm fm} = \sum_{k,\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + E_{\rm f} \tilde{f}^+_{k\sigma} \tilde{f}_{k\sigma} + Vb(c^+_{k\sigma} \tilde{f}_{k\sigma} + {\rm H.c.}) + \lambda N(b^2 - 1), \quad (3)$$

where $E_{\rm f} = -2\chi[\cos(k_x) + \cos(k_y)] + \varepsilon_{\rm f} + \lambda - \mu$ is the f electrons dispersion with the spin liquid parameter χ. Moreover, for the purposes of the present discussion, we assume that the uniform spin liquid ($\chi_{ij} = \chi$) is a good reference state for the formation of the Kondo Fermi liquid, Vb is the renormalized hybridization-term in the c–f electron band. The Lagrange multiplier λ is the constraint imposed on the slave particles $\sum_\sigma \tilde{f}^+_{i\sigma} \tilde{f}_{i\sigma} + b^2 = 1$, which can be derived by the set of self-consistent equations in the momentum space as follows:

$$\lambda b + \frac{V}{N} \sum_{k,\sigma} \langle \tilde{f}^+_{k\sigma} c_{k\sigma} \rangle = 0,$$
$$b^2 + \frac{1}{N} \sum_{k,\sigma} \langle \tilde{f}^+_{k\sigma} \tilde{f}_{k\sigma} \rangle = 1. \quad (4)$$

Also the constraint function $n_t = \frac{1}{N} \sum_{k,\sigma} \langle c^+_{k\sigma} c_{k\sigma} \rangle + \frac{1}{N} \sum_{k,\sigma} \langle \tilde{f}^+_{k\sigma} \tilde{f}_{k\sigma} \rangle$ is introduced to express that the chemical potential must be determined by the total particle number. To obtain the single electron Green function in Eq. (4), we diagonalize the heavy fermion Hamiltonian by $G = (E - H + i\eta)^{-1}$ as follows:

$$G = \begin{bmatrix} G_{\rm c} & G_{\rm fc} \\ G_{\rm cf} & G_{\rm f} \end{bmatrix} = \begin{bmatrix} \omega - \varepsilon_k & -\tilde{V} \\ -\tilde{V} & \omega - E_{\rm f} \end{bmatrix}^{-1}. \quad (5)$$

In our scanning interference tunneling process, we adopt the coupling Hamiltonian between the metallic tip electron and the heavy fermion system as

$$H_{\rm tunnel} = \sum_{k\sigma} t_{\rm c} c^+_{k\sigma} d_\sigma + t_{\rm f} \tilde{f}^+_{k\sigma} d_\sigma + {\rm H.c.} \quad (6)$$

The amplitudes of tunneling into c (f) electrons are denoted as $t_{\rm c}$ and t_f, respectively. Then the tunneling current can be derived by the change in particle number of the tip,[25]

$$I = -e\langle \dot{N}_{\rm tip} \rangle = -\frac{ie}{\hbar} \langle [H, N_{\rm tip}] \rangle = \frac{2e}{\hbar} \sum_{k\sigma} \int \frac{d\omega}{2\pi} {\rm Re}[t_{\rm c} G^<_{\rm tc}(k,\sigma,\omega) + t_{\rm f} G^<_{\rm tf}(k,\sigma,\omega)], \quad (7)$$

where all Green's functions are written in a matrix form. By the Dyson equation, we can obtain less Green functions and give the resolved DC in the weak-tunneling limit at zero temperature[26]

$$\frac{dI}{dV} = \frac{2\pi e^2}{\hbar} D_{\rm tt}(\omega) t_{\rm c}^2 [D_{\rm cc}(\omega) + 2(t_{\rm f}/t_{\rm c}) D_{\rm cf}(\omega) + (t_{\rm f}/t_{\rm c})^2 D_{\rm ff}(\omega)], \quad (8)$$

where $D_{\rm cc}(\omega)$, $D_{\rm ff}(\omega)$ and $D_{\rm tt}(\omega)$ are the DOSs corresponding to c electrons, f electrons, and the tip. We treat the tip DOS as a constant to reflect the broadening of the tip state by contacting with the remainder of the tip electrode, then the low-temperature DC can be derived in Eq. (8). A similar choice can be found in Ref. [27]. Here $D_{\rm cf}(\omega)$ is a quantity similar to a DOS by the c–f Green function ($G_{\rm fc}$) between the two bands. It represents the interference effect in the tunneling process, which produces a very significant appearance of the DC. Equation (8) 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.[28] The Fano ratio $t_f/t_{\rm c}$ controls the relative tunneling strength into the bands of c electrons and f electrons, whose value determines the exact location of the conductance minimum.

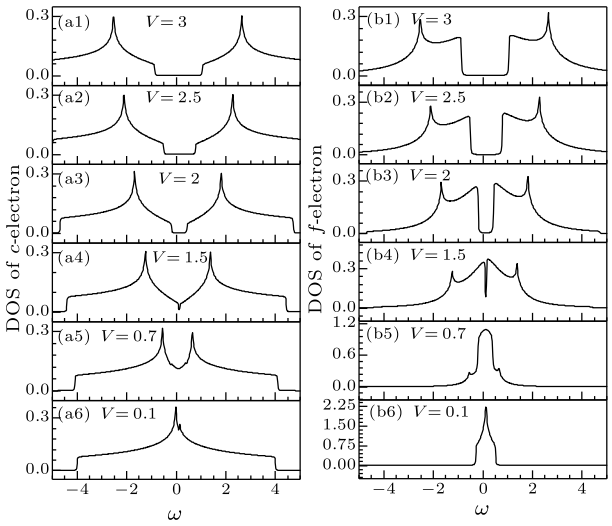

Fig. 1. DOSs of the conduction electrons (a1)–(a6) and f electrons (b1)–(b6) for different c–f hybridization strengths of the heavy fermion system.

In our numerical calculations, we take the following values of parameters for the system: the energy scale is defined by the conduction hopping amplitude by setting $t = 1$, the local f level is taken to be $\varepsilon_{\rm f} = 0$, the spin liquid parameter $\chi = 0.1$, and the chemical potential $\mu = 0$. The calculations reproduce similar results when we choose other values of the parameters. We first show the DOS ($D(\omega) = -\frac{1}{\pi} {\rm Im}[\sum_k G(\omega)]$) for the states of c electrons and f electrons in the weak-to-strong hybridization case shown in Fig. 1, which are symmetric with respect to the zero energy ($\omega = 0$). In the weak coupling strength ($V = 0.1$), the c electron DOS and the f electron DOS exhibit obvious resonance states around the zero energy. The DOS intensity is peaked at the coherent gap edge and is finite at the zero energy, indicating that the electron DOSs are in the heavy Fermi liquid regime. The dominant contribution to the DOS comes from strongly

anisotropic hybridization between conduction electron and f-electron states. Here it is important to note that the dispersion of the heavy energy band is rather flat over a wide range of the Brillouin zone. As a result, we find a very sharp van-Hove type feature in the DOS displayed. When we increase the hybridization strength, the DOS resonance state splits into two peaks, which is related to the energy dispersion $E_k^{\pm} = [(\varepsilon_k + \chi_k) \pm \sqrt{(\varepsilon_k - \chi_k)^2 + 4b^2V^2}]/2$ and the increasing energy splitting $\Delta E(= E_k^+ - E_k^- = \sqrt{(\varepsilon_k - \chi_k)^2 + 4b^2V^2})$. Furthermore, there has been a significant increasing platform structure in the DOS as well as increasing width with increasing the hybridization. The reasons can be attributed as follows: when V is weak, the band energy dispersion between the c-electron channel and f-electron channel separates into decoupled energy bands, and the energy splitting does not clearly occur. However, when we increase the hybridization strength, an attractive potential hybridization strength will turn the bound state away from the zero-energy center. As a consequence, the gap leads to a quantum phase transition, which will induce the flat-band structure of the DOS. Such fingerprints can also be found in the suppression of the DOS when the energy is very low or high, which is related to the energy gap induced by increasing the hybridization.

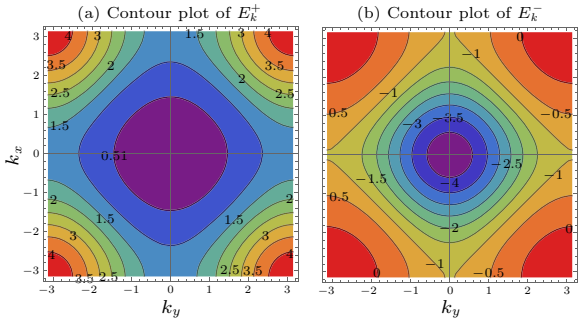

Fig. 2. (Color online) Contour plot of the band structure: (a) contour plot of E_k^+ and (b) contour plot of E_k^-. The parameters are $t = 1$, $\varepsilon_{\rm f} = 0$, $\chi = 0.1$, $V = 2.5$, and $\mu = 0$.

To show how the hybridization affects the system, we give a contour plot of the energy band dispersion acquired by $E_k^{\pm}$ in Fig. 2. The contrast in color reflects the changes in magnitude of the band energy, which has been manifested that in the DOS, the two peaks appear with the increasing hybridization shown in Fig. 1. For the two-dimensional conduction electrons, we have the van Hove singularity at $k = (0, \pm\pi)$ and $(\pm\pi, 0)$ in the energy band, which leads to divergence in the DOS of the hybridization band, respectively. Hybridization between conduction electrons and the f electrons in the system may result in new states of matter, which is decided by the exact location of the concomitant hybridization gap with respect to the Fermi energy, a heavy fermion or an insulating ground state ensues. The hybridization gap and the van Hove singularity, determine the primary shape of the DC spectrum in Fig. 3. For the fixed parameters, we can obtain a maximum or minimum centered around the van Hove singularity. Specifically, E_k^- displays a concave dense distribution with increasing the bump height, while E_k^+ shows a convex distribution with continuously reducing height. We have encountered such similar results reported previously in the DOS with the corresponding platform under strong hybridization strength. The recent study[17] has shown that the hybridization gap of localized states with conduction bands induces the resultant gap between the renormalized bands,[29] not proving but leaving open the possibility of the existence of a topologically protected hybridized gap.

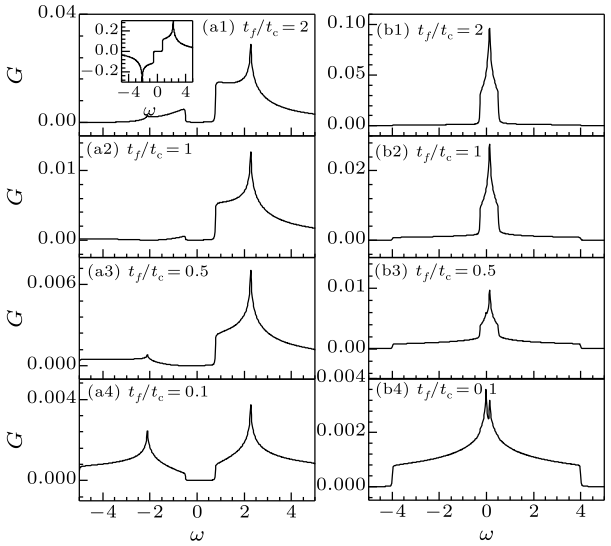

Fig. 3. Differential conductance of the system for different Fano ration parameters, (a1)–(a4) are for the hybridization strength $V = 2.0$, and (b1)–(b4) are for the hybridization strength $V = 0.7$. The inset of (a1) stands for the c–f DOS ($D_{\rm cf}(\omega)$) when $V = 2.0$.

To show the presence of hybridization strength in the system, we also show the Fano ratio $(t_f/t_{\rm c})$ effect on the transport DC under weak and strong coupling strengths in Fig. 3. The line shape of DC is determined not only by the hybridization symmetry of the c–f band but also by the relative strength of the tunneling amplitude. On the one hand, we find that the DC resonance peak still exists in the case of strong coupling, as well as a platform structure under small Fano ratio, which indicates that the system's top insulator gate state is not affected by the Fano ratio, whereas the right edge is always enhanced and becomes sharper with increasing the Fano ratio due to the increasing probability of tunneling into the f electrons channel, and the left edge of the hybridization gap is suppressed with the increase of the Fano ratio $(t_f/t_{\rm c} = 0.5)$. To further increase the Fano ratio, the resonance peak at negative energy is completely suppressed $(t_f/t_{\rm c} = 1$ and 2). Such characteristics are related to the variation of the hybridization gap and the suppression of the van Hove peaks around the Fermion energy. Moreover, the DC spectra are

dominated by a gap-like feature around zero-bias resulting from the hybridization of conduction and f electrons. It is also necessary to note that the hybrid c–f DOS exhibits a negative-sign peak for the intra-gap state (inset of Fig. 3(a)), which induces the shift of the Fano destructive and instructive interference processes. An attractive potential scattering on the conduction channel will further tune the bound state peak away from the gap center. The Fano ratio makes the DC characteristics strongly asymmetric, with the continuum part of DC intensity at negative energies much smaller than that at positive energies. The Fano ratio also leads to different DC intensity maps at the energy.

On the other hand, for the weak coupling case, the situation changes under large Fano ratio strength. The conductance shows a more pronounced resonance structure near the Fermi energy, which is related to the enhanced DOS of the f electrons. The passage of an electron from the tip is accompanied by a simultaneous interference cotunneling mechanism, which is equivalent to an effective tunneling channel renormalized by a local boson parameter. Obviously, the transport process only occurs in the conduction band so that the spectrum follows exactly the DOS of the conduction electrons for the small Fano ratio. Larger hybridization strength between the c–f electrons induces a larger energy shift in the f-level band structure. When the hybridization strength is weak, the f-band does not show any energy dispersion in the band structures. The hybridization is further confirmed by the formation of the hybridization gap revealed in the DOS of weak hybridization strength. Especially, the DOS resonance emerges at the locations where the conduction bands approach or cross the Fermi level, while the f band does not show observable energy dispersions in Figs. 1(a6) and 1(b6). Moreover, it is found that the conduction band is negatively charged while the f band is positively charged in the interference process, by which the conduction DOS on the system may be prohibited by the enhanced Fano ratio, which has also been discussed in the STM transport of an electronic bound state at thorium atoms substituted by U atoms in URu_2Si_2.[30]

In summary, we have demonstrated the qualitative c–f competitive hybridization and the different Fano ratio interference processes in the heavy fermion system. The DOS splits into double peaks with increasing the hybridization strength, and also a coherent platform induced by the large hybridization strength in the system. The continuum part of DC intensity at negative energies is much smaller than that at positive energies, which shows a prohibited effect under large Fano ratio strength. All reflect the unconventional top transport properties in the heavy fermion system. Such general behavior of the competitive hybridization and interference effect is of some interesting models we have considered. Also, our work opens some new prospects for the physical properties on the heavy-fermion transport.

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