Tunneling into clean Heavy Fermion Compounds: Origin of the Fano Lineshape

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Recently observed tunneling spectra on clean heavy fermion compounds show a lattice periodic Fano lineshape similar to what is observed in the case of tunneling to a Kondo ion adsorbed at the surface. We show that the translation symmetry of a clean surface in the case of weakly correlated metals leads to a tunneling spectrum given by the superposition of the local weighted density of states of all energy bands involved, which does not have a Fano lineshape. In particular the spectrum will show any hybridization gap present in the band structure. By contrast, in a strongly correlated heavy fermion metal the heavy quasiparticle states will be broadened by interaction effects. The broadening grows as one moves away from the Fermi surface, up to a value of the order of $T_K$, the Kondo scale. We show that the hybridization gap is completely filled in this way, and an ideal Fano lineshape of width $T_K$ results, similar to the impurity case. We also discuss the possible influence of the tunneling tip on the surface, in (i) leading to additional broadening of the Fano line, and (ii) enhancing the hybridization locally, hence adding to the impurity type behavior. The latter effects depend on the tip-surface distance.

Introduction. — Recent progress in scanning tunneling spectroscopy (STS) techniques has made it possible for the first time to measure the differential conductance, $dI/dV$, in heavy-fermion compounds [1, 2]. These materials are governed by the strong Coulomb interaction on the f-electron orbitals, hybridizing with a conduction band. Provided the f-energy is sufficiently below the Fermi energy and the hybridization strength is weak enough, magnetic moments will appear at the f-sites. The Kondo effect will screen the local moments at a temperature below the Kondo temperature $T_K$ [3, 4]. The ensuing Fermi liquid state is characterized by large effective masse ratios $m^*/m$. Out of this heavy Fermi liquid a variety of interesting phenomena may emerge, such as magnetic order, quantum phase transitions and the associated non-Fermi liquid behavior, as well as unconventional superconductivity [5]. Their microscopic origin likely lies in the competition between the exchange interaction of the magnetic moments and their screening by conduction electrons [6], though no theoretical consensus has emerged as yet [7]. STS experiments by providing insight into the local electronic structure [1, 2] of heavy-fermion materials, might hold the key to understanding their complex properties, by providing complementary information. The theoretical challenge in the interpretation of the differential conductance in Kondo lattice systems [8, 9] lies in the proper treatment of the strong correlation effects governing these systems. Whereas tunneling into single Kondo impurities [10, 11] is relatively well understood, there is a serious problem of interpretation of tunneling into states on a clean crystal surface, which has the lattice periodicity. In the single impurity case the quantum interference between electrons tunneling from the STS tip into the conduction band and into the magnetic f-electron states is essential. As a consequence, the lineshape of the $dI/dV$ spectrum shows an asymmetric form, as first discussed by Fano [18]. It is rather surprising that a similar spectrum is found, periodically continued along the surface, in the clean case. Within the framework of electron band theory one would rather expect the spectrum to show the superposition of local density of states contributions from the different electronic bands involved. Recent attempts to calculate the tunneling spectrum by treating the problem of strong correlations within pseudoparticle mean field theory bear out this expectation [8, 9]. The resulting spectra are characterized by two peaks belonging to the two heavy bands, separated by a hybridization gap. As we will show below, a mapping of the problem onto a non-interacting system, as done in 1/N theories is not sufficient to capture the dominant many-body effects at energy scales of the order of $T_K$.

In this paper, we address this issue within Fermi liquid theory extended to somewhat higher energy scales. It is convenient to start with the lattice Anderson model in the low energy domain where heavy quasiparticles (QP) are well defined. Our main point is that the QP width $Gamma$ at energy $E$, which varies as $Gamma propto E^2/T_K$ in the Fermi liquid regime (we use units with $h = k_B = 1$), will grow up to $Gamma propto T_K$ at the scale $E = T_K$, which is larger than the hybridization gap, given by $Delta propto (V/e_F^0 T_K <<< T_K$, where $V$ is the hybridization amplitude and $e_F^0$ is the bare Fermi energy of the unhybridized conduction band. Consequently, the local f-electron density of states (DOS) takes the form of a Lorentzian of width $T_K$, just like in the impurity case, and the Fano lineshape arises as usual. We will first consider the case of a weakly correlated metal, to make our point that in this case no Fano lineshape is expected.

While the translation invariance is preserved in an
ideal noninvasive tunneling experiment, in reality the translation invariance may be broken by the local influence the tip may exert on the surface. Such an effect has been recently invoked to explain the somewhat distorted energy spectrum observed in tunneling spectra of a topological insulator [19]. We discuss two ways by which the presence of the tip may change the tunneling spectra. Both effects will depend on the tip-surface distance.

**Tunneling into weakly correlated metals.** – We consider tunneling into a metal characterized by two hybridized bands, as described by the Hamiltonian

\[
H = H_0 + H_{hyb} + H_t
\]

\[
H_0 = \sum_{k,\sigma} \epsilon_{k\sigma} c_{k\sigma}^{+} c_{k\sigma} + \epsilon_{f\sigma} \sum_{i,\sigma} n_{f\sigma}
\]

\[
H_{hyb} = V \sum_{i,k,\sigma} (e^{i\mathbf{k} \cdot \mathbf{R}_i} f_{i\sigma}^{+} c_{k\sigma} + h.c.)
\]

\[
H_t = t_s \sum_{k,\sigma} (p_{\sigma}^{+} c_{k\sigma} + h.c.) + t_f \sum_{\sigma} (p_{\sigma}^{+} f_{0\sigma} + h.c.)
\]

(1)

where \(c_{k\sigma}^{+}, f_{i\sigma}^{+}, p_{\sigma}^{+}\) create an electron of spin \(\sigma\) in a Bloch state of momentum \(\mathbf{k}\), a localized f-orbital at site \(i\) or the level at the tip of the tunneling electrode, respectively. The operator \(n_{f\sigma} = f_{i\sigma}^{+} f_{i\sigma}\) counts the number of electrons with spin \(\sigma\) on the local f-level, and \(\epsilon_f\) is the energy of the f-level (which is position and momentum independent). In Eq. (1) we only take into account tunneling into the orbitals directly under the tip at \(\mathbf{R}_0 = 0\), which is the only source for breaking of the translational invariance, otherwise preserved in the Hybridized system. Assuming the tunneling electrode and the metal to be in thermal equilibrium (in the limit of vanishing tunneling current), their chemical potentials differing by \(\Delta\), we can neglect their effect.

\[
I(V) = \frac{2e}{h} \int d\omega N_{\omega}(\omega - eV) \left[ f(\omega - eV) - f(\omega) \right] \times \Im \left\{ \left[ t_s^2 G_{cc}(\omega) + t_s^{\prime 2} G_{ff}(\omega) + 2t_s t_f G_{cf}(\omega) \right] \right\}
\]

(2)

where \(G_{ab}(\omega)\) are the advanced local single particle Green's functions of \(H_{ac} = H_0 + H_{hyb}\) and \(N_{\omega}(\omega)\) is the STM tip DOS. The Hamiltonian \(H_{ac}\) may easily be diagonalized to yield two hybridized bands with Bloch energies

\[
\epsilon_{k}^{+,-} = \frac{1}{2} \left( \epsilon_{f} + \epsilon_{k} \pm \sqrt{(\epsilon_{f} - \epsilon_{k})^2 + 4V^2} \right)
\]

(3)

and density of states

\[
N_{+,-}(\omega) = \int d^3k \delta(\omega - \epsilon_{k}^{+,-})
\]

(4)

The density of states exhibits a hybridization gap at \(\omega = \epsilon_f\) of width \(\Delta = 2V\). The Green’s functions are found as

\[
G_{ab}(\omega) = \sum_{\nu = +,-} \frac{a_{ab,\nu \omega}}{\omega - \nu \epsilon_{k}^\nu}, \quad a_{ab,\nu \omega} = \frac{\nu \epsilon_{k}^\nu - \epsilon_{k}}{2\Delta \epsilon_{k}^\nu}
\]

(5)

where \(\Delta \epsilon_{k}^\nu = \epsilon_{k}^{+} - \epsilon_{k}^-\). While the coherence factors \(a_{ab,\nu \omega}\) shift the weight in the partial spectral functions \(\Im \{G_{ab}(\omega)\}\) somewhat, compared to the band density of states \(N_{\nu,\omega}\), the hybridization gap will remain. In Fig. 1 we show the differential conductance \(dI/dV\) calculated for a three-dimensional parabolic band of bandwidth 2eV (crossing the Fermi energy at \(|t| = 0.866\pi/a_0\)). Hybridization strength \(V = 0.1eV\), the tunneling amplitude ratio \(t_f/t_e = 0.15\) and f-level energy \(\epsilon_f = -10eV\) without any finite level width (dashed line). The shape of the curve is similar to what has been found in Refs. [20, 21] within pseudoparticle mean field theory of the Kondo lattice model. These results are nowhere near what is observed in experiments on strongly correlated heavy fermion compounds. We stress again the main conclusion from this section: in the absence of finite f-level lifetime and breaking of translation invariance, the DOS cannot exhibit a Fano lineshape. Therefore, understanding the origin of either finite QP lifetime or a breaking of translational invariance of the system by the influence of the tip on the surface is crucial to understanding the Fano lineshapes observed in recent experiments.

**Tunneling into heavy fermion compounds.** – A microscopic Hamiltonian believed to capture the physics of...
heavy fermion compounds is the lattice Anderson model

\[ H_{AL} = H_{wc} + U \sum_i n_{fi}^\dagger n_{fi} , \]

where \( U \) is the Coulomb interaction matrix element, assumed to be much larger than the conduction band width.

As above the single particle Green’s functions as well as the self-energy form 2 × 2 matrices in the conduction electron (c), f-electron (f) space. It is worth noting that the only self energy element is \( \Sigma_{ff}(\omega) \). Expanding \( \Sigma_{ff}(\omega) \) about the Fermi energy \( \omega = 0 \) (neglecting its weak momentum dependence), we end up with a QP description in terms of the QP weight factor \( z \), the shifted position of the f-level \( \tilde{\epsilon}_f \) and the QP line width (the inverse of the QP life time) \( \gamma \), which are defined in terms of \( \Sigma_{ff}(\omega) \) by

\[ z^{-1} = 1 - \frac{\partial}{\partial \omega} \Re \Sigma_{ff}(\omega)|_{\omega=0}, \]

\[ \tilde{\epsilon}_f = z[\epsilon_f + \Re \Sigma_{ff}(0)] \]

\[ \gamma(E_k) = z \Im \Sigma_{ff}(E_k). \]

The complex-valued QP energies of the two hybridized bands are defined by

\[ \epsilon_k^{+, -} = \frac{1}{2}(\tilde{\epsilon}_f + \epsilon_k - i\gamma \pm \sqrt{(\tilde{\epsilon}_f - \epsilon_k - i\gamma)^2 + 4zV^2} \right) = E_k - i\Gamma_k \]

The hybridization gap follows (neglecting the QP width) as \( \Delta = zV^2(\frac{1}{m_{k,c}} + \frac{1}{m_{k,f}}) \), where \( G \) is a vector at the edge of the Brillouin zone. In the heavy fermion regime, assuming that the Fermi energy \( (E_{k_F} = 0) \) intersects the lower band and observing \( z^{-1} \gg 1 \), and \( \epsilon_{k_F} \gg |\tilde{\epsilon}_f|, \sqrt{2}\Gamma_k \) one may expand \( E_k \) about the Fermi momentum \( K_F \) to get

\[ E_k = (k - k_F)v_F \sqrt{m_{k,c}/m_{k,f}}, \]

where we defined the effective mass ratio \( \frac{m_{k,c}}{m_{k,f}} = z(\frac{\epsilon_{k_F}}{|\epsilon_{k_F}|})^2 \). Here \( \epsilon_{k_F} \) is the value of the bare conduction band energy at the Fermi surface, which is assumed to be close to the upper band edge, so that \( \epsilon_{k_F} \approx W/2 \), where \( W \) is the conduction band width. Approaching the heavy fermion regime from high temperatures the renormalization is observed to occur below a scale \( T_K \), usually called the lattice Kondo temperature. We assume \( T_K \) to be approximately equal to the Kondo temperature of a single Kondo ion.

It follows from the Pauli principle that the QP width tends to zero in the limit temperature \( T \) and excitation energy \( E_k \to 0 \), as given by

\[ \Gamma(E_k) = A[E_k^2 + (\pi T)^2] << E_k \]

As long as this condition is satisfied, one may employ the formalism of Fermi liquid theory. There are indications from both theory and experiment (for a recent
determination of \( \Gamma \) from ESR data see [21]) that the prefactor scales with the inverse Kondo temperature as \( A \approx 1/T_K \). At the energy scale \( T_K \) we therefore have

\[ \Gamma(T_K) \approx T_K. \]

Beyond that scale the lattice coherence is suppressed by inelastic processes and the metal behaves like a crystal of independent Kondo ions. The coherence scale of the single Kondo ion is set by the local spin relaxation time, which is known to be \( T_s \approx T_K \) at energy/temperature less or equal to \( T_K \). At higher energy the relaxation rate is given by \( \Gamma_s(E) \approx g^2(E)|E| \), where \( g(E) \approx 1/\ln(|E|/|T_K|) \), \( E > 2T_K \). At temperatures \( T << T_K \) one may therefore approximate the QP width by

\[ \Gamma(E_k) \approx E_k^2/T_K , \quad E_k < T_K \]

\[ \Gamma(E_k) = |E_k|/[1 + \ln(|E|/|T_K|)^2 , \quad E_k > T_K . \]

The solid points in Fig. 1 denote the DOS calculated in the presence of the finite QP width of Eq. 12, taking \( T_K = 130K \). The solid black line is a fit to the Fano lineshape, given by \( f(E) \propto (q^2+q^2)^2 \) where \( q = \frac{\epsilon - \epsilon_0}{T} \). The fit yields \( q = 1.25 \) and \( \Gamma = 29.7 \) meV, in good agreement with the values obtained in experiment [1]. For a qualitative comparison, in the inset we plot the experimental Fano lineshape of Ref. [1]. From calculations of the DOS and fitting to a Fano lineshape with various parameters, we find the relation \( \Gamma \sim 2T_K \) to hold for a wide range of parameter values.

In the experiment [1] the Fano width \( \Gamma \) also varies with the STM tip position, although the modulation is smaller than that of the Fano asymmetry parameter \( q \). While for the latter the origin of the modulation is clear (since the tunneling amplitudes \( t_c \) and \( t_f \) depend on the tip position), a modulation of \( \Gamma \) is somewhat surprising. A possible interpretation is provided in the following.

**Tip-induced effects.** We point out two ways in which the tunneling tip may influence the properties of the surface and consequently the tunneling lineshape. First, the f-electron self-energy acquires a contribution originating from tunneling into the tip, \( \Im \Sigma_{ff-tip}(\omega) \propto |t_f|^2 N_f(\omega) \), resulting in a modulation of the QP width with tip position. The fact that this is only a part of the self-energy accounts for the relatively weak modulation in \( \Gamma \).

A second and potentially more important effect is related to the local potential generated by the tip at the surface underneath [19]. This potential acts like an additional local hybridization between f- and c-states, and will give rise to Kondo impurity type behavior. More specifically, in addition to the interaction-induced broadening, there will be a tip-induced local scattering term added to the Hamiltonian of Eq. 4 of the form

\[ H_{tip} = V_{tip} \delta_{f=0} + h.c. \]

\[ = V_{tip} \sum_{k,k'} c_{k}^\dagger f_{k'} + h.c. \].
induced quasi-particle line broadening as the origin of the Fano lineshape observed in tunneling experiments on strongly correlated metals. We model the quasi-particle energy width phenomenologically by using Fermi liquid theory and Kondo physics. In fact the broadening is related to the Kondo temperature via Eq.\,\,[12] and yields a Fano linewidth $\Gamma \sim 2T_K$, in agreement with recent experiments.

In addition, we address the modulation in the Fano width $\Gamma$ observed experimentally. While the lattice periodic modulation of the Fano asymmetry parameter $q$ is immediately understood as a consequence of the modulation of the tunneling amplitudes between tip and f- or c-orbitals, the modulation of the width $\Gamma$ requires a different interpretation, possibly related to the influence of the tip on the properties of the metal beneath it. Specifically, we show that a tip-induced local hybridization may generate such a modulation. A direct consequence would be that the Fano parameters $q$ and $\Gamma$ would depend on STM tip parameters (height, voltage etc.). A dependence of $q$ on tip parameters is rather expected, since it depends on the tunneling amplitudes $t_c$ and $t_f$, which are unlikely to change in the same way with changing tip parameters, hence $t_f/t_c$ should depend on the tip parameters. However, a dependence of $\Gamma$ on tip parameters would be surprising if $\Gamma$ is a purely intrinsic quantity, and would indicate that indeed the STM tip effect is non negligible. These predictions can be directly tested within current experimental setups.

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