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Signature of Kondo breakdown quantum criticality in optical conductivity

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We show that the behavior of the finite-frequency interband transition peak in the optical conductivity of the heavy fermions can provide definitive experimental proof of the Kondo breakdown phenomenon in which the lattice Kondo temperature vanishes at a quantum critical point. Approaching such a phase transition from the heavy Fermi-liquid side, we find a new crossover regime where the peak position is related to, but is not directly proportional to the lattice Kondo scale. The peak position moves to lower energies but remains finite, while the peak value changes nonmonotonically and it eventually disappears at the quantum critical point. These are unique signatures which distinguish a Kondo breakdown transition from a spin-density wave driven transition.

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I. INTRODUCTION

Developments in material synthesis have led to the discovery of numerous rare-earth compounds, the heavy fermions (HFs), which can be tuned to a quantum critical point (QCP), separating a magnetic ground state from a paramagnetic one,[1] by varying an external parameter such as pressure or chemical doping. In the quantum critical regime the metallic properties are significantly different from what one expects from a standard Landau Fermi liquid (LFL), and therefore these systems are prototypes to study how strong correlation effects give rise to deviations from LFL.

The early theoretical attempts to describe the QCP are based on the possibility that the instability of the paramagnetic phase is due to spin-density wave (SDW) formation,[2] and the critical fluctuations are the paramagnons. However, in three dimensions these theories fail to explain simultaneously the linear temperature (T) dependence of the resistivity and the log T dependence of the specific heat coefficient observed in experiments.[3] This has stimulated theorists to construct alternative descriptions of the quantum criticality,[4] among which the scenario of Kondo breakdown (KB) has proven to be promising.[5,6] In the KB scenario the non-LFL behavior is due to the presence of a *second* QCP, in close proximity to the magnetic one, where the effective Kondo temperature of the lattice (T_K) goes to zero. In this picture the critical fluctuations, nonmagnetic in origin, are associated with the hybridization fluctuation between a broad conduction band and a narrow f-electron band.

In view of the current interest in KB,[5–8] it is apt to pose the question if a *direct* experimental signature of the KB could distinguish it from other possible routes to quantum criticality. The issue is nontrivial partly due to the absence of low-T angle-resolved photoemission data of the HFs and partly because standard quantities such as resistivity and specific heat do not measure T_K directly. For example, the violation of the Wiedemann-Franz (WF) law and the divergence of the Grüneisen ratio (GR) at the QCP have been identified as experimental consequences of KB.[8] However, a true violation of the WF law signifies the absence of electron quasiparticles which need not necessarily be due to $T_K \to 0$ physics. An apparent violation of the WF law near a SDW transition[9] can also take place because of inelastic scattering. Similarly, the divergence of the GR is expected for all kinds of QCPs.[10] Consequently, while KB phenomenon implies the violation of the WF law and the divergence of the GR, the converse does not hold. The main purpose of this work is to point out that finite-frequency features in the optical conductivity of the HFs, the so-called midinfrared peak which arise due to interband optical transitions, can provide a direct and unique experimental signature of the KB phenomenon.

The midinfrared peak in the optical conductivity of the HFs has been well-studied experimentally[11] and theoretically[12] in the case where the system is far from any phase instability. The physical origin of the peak is readily understood within a two-band picture of the Kondo effect in a lattice, which describes the formation of the heavy LFL as the hybridization between a conduction c band and a narrow f band. The interband transition takes place between one band with more f character and another with more c character, and therefore it involves an energy scale *at least* of the order of the binding energy T_K of the composite heavy electrons. Thus the peak position is related to T_K, even though the two quantities may not always be proportional, as we show below.

A crucial aspect of the SDW approach is that the paramagnetic energy scale T_K remains finite at the QCP. Therefore, for such a transition one does not expect the midinfrared peak position and the peak height to change significantly while the system is tuned to the QCP by varying the external parameter. In contrast, the KB phenomenon is based on the possibility of a QCP where $T_K \to 0$. Consequently, a hallmark of KB is a significant shift of the interband peak position to lower energies, as the system is tuned to the QCP. Furthermore, since at the KB-QCP the f band effectively decouples from the c band, one expects the interband feature to gradually disappear. These qualitative differences can be useful to distinguish experimentally a KB transition from a SDW instability. This motivates us to study how the midinfrared peak for a heavy LFL varies as the system approaches a KB-QCP.

From the perspective of the charge dynamics of the f electrons, the KB-QCP has been identified as an orbital-selective Mott transition, where the f electrons localize and decouple from the metallic environment.[13,14] Orbital selective localization is a relevant phenomenon in materials with both weakly and strongly correlated bands, including classical Mott insulators [such as VO_2 (Ref. 15) and V_2O_3 (Ref. 16)], ruthenates $Ca_{2-x}Sr_xRuO_4$,[17] cobaltates, fullerenes, and layered organic superconductors (for a complete list see, e.g., Ref. 18). KB is likely only one of the several possible microscopic mechanisms that leads to orbital selective Mott transition. However it is interesting to conjecture that, besides the HFs, there are other cases where the localization can be described in terms of a vanishing "effective Kondo temperature." We expect that in such systems the study of the optical conductivity will be equally germane.

II. MODEL

The system we study is described by the Anderson-Heisenberg model which is given by

$$\mathcal{H} = -\sum_{\langle ij\rangle,\sigma} (t_c c^\dagger_{i\sigma} c_{j\sigma} + t_f f^\dagger_{i\sigma} f_{j\sigma}) - E_0 \sum_{i,\sigma} n^f_{i\sigma} + V_0 \sum_{i,\sigma} (c^\dagger_{i\sigma} f_{i\sigma} + \text{H.c.}) + U \sum_i n^f_{i\uparrow} n^f_{i\downarrow} + J_H \sum_{\langle ij\rangle} \vec{S}^f_i \cdot \vec{S}^f_j. \quad (1)$$

Here t_c and t_f ($t_c \gg t_f$) denote hopping of c and f electrons, respectively, (i,j) are lattice sites (which are, say, nearest and next-nearest neighbors), E_0 is the local energy level of the f band, and σ is the spin index. V_0 is the hybridization between the bands, U is the on-site Coulomb repulsion in the f band ($U \gg t_f$), and $J_H \sim (t_f)^2/U$ is a superexchange spin-spin interaction in the f band. We study the above model in the Kondo limit where the f electrons form local moments.

The mean-field theory is generated by replacing $f_{i\sigma} \to b^\dagger_i F_{i\sigma}$, where $(b^\dagger_i, b_i)$ describe charged holons and $(F^\dagger_{i\sigma}, F_{i\sigma})$ describe spin-1/2 spinons. The large Coulomb repulsion is taken into account by projecting out the double-occupied f-electron states via the constraint $\Sigma_\sigma F^\dagger_{i\sigma} F_{i\sigma} + b^\dagger_i b_i = 1$ (the associated Lagrange multiplier renormalizes E_0). At the mean-field level this model shows a KB quantum phase transition at a critical value x_c of the parameter $x \equiv V_0/J_H$.[13] For $x > x_c$ one obtains a heavy LFL phase where $\langle b_i \rangle \neq 0$ and the f electrons participate in band formation, and for $x < x_c$ one obtains a phase with $\langle b_i \rangle = 0$ where the f electrons localize and form a nonmagnetic uniform spin-liquid phase (with $\langle F^\dagger_{i\sigma} F_{j\sigma} \rangle \neq 0$). As the QCP is approached from the LFL side, the lattice Kondo temperature $T_K \approx \pi \langle b \rangle^2 V_0^2 \nu_0 \to 0$, where ν_0 is the bare density of states of the c band. We write the spinon bandwidth as $\alpha t_c \sim (\langle b \rangle^2 t_f + J_H)$ and consider $\alpha \ll 1$ as a small parameter of the theory.

We use linear-response theory to study the $T=0$ optical conductivity of the system as it approaches the QCP from the LFL side. We ignore the f band contribution to the current operator and write it as $\hat{J}_\mu \approx \Sigma_{\mathbf{k}\sigma} (\nabla_{\mathbf{k}} \epsilon_{\mathbf{k}})_\mu c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$, where $\epsilon_{\mathbf{k}}$ is the bare dispersion of the c band and μ denotes spatial direction. This does not change our results at a qualitative level and can be formally justified as an expansion in t_c/t_f. Furthermore, we write $|\nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}| \approx v_F$, the Fermi velocity of the c band, and we ignore the vertex corrections to the current-current correlator. The optical conductivity $\sigma_1(\Omega)$ is the real part of the frequency-dependent conductivity tensor, which can be written as (for $\Omega \geq 0$, and setting $\hbar = 1$)

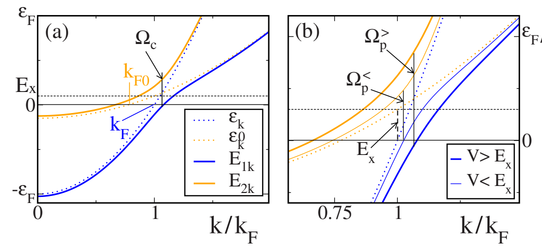

FIG. 1. (Color online) (a) $\epsilon_{\mathbf{k}}$ and $\epsilon^0_{\mathbf{k}}$ are the bare conduction and spinon bands (with respective Fermi vectors k_F and k_{F0}). $E_x = \epsilon^0_{k_F}$ is a microscopic energy scale. $E_{1,2\mathbf{k}}$ are the hybridized bands, V is the effective hybridization, and $\Omega_c = 2V$ is the minimal interband transition energy (corresponds to momenta for which $\epsilon_{\mathbf{k}} = \epsilon^0_{\mathbf{k}}$). (b) For $V > E_x$, the optical conductivity peak is at $\Omega^>_p = \Omega_c$. For $V < E_x$ the Ω_c transition is forbidden at $T=0$ (since $E_{1\mathbf{k}} > 0$ is above the chemical potential). The peak is at $\Omega^<_p = V^2/E_x + E_x$.

$$\sigma_1(\Omega) \approx \frac{2e^2 v_F^2}{\pi \Omega d} \int_{-\Omega}^{0} d\omega \sum_{\mathbf{k}} \text{Im } G^R_c(\omega, \mathbf{k}) \text{Im } G^R_c(\omega + \Omega, \mathbf{k}), \quad (2)$$

where R denotes the retarded function. Within the mean-field theory the Green's function for the c electrons is $G^R_c(\omega,\mathbf{k})^{-1} = \omega - \epsilon_{\mathbf{k}} + i/(2\tau_c) - \Sigma^R_c(\omega,\mathbf{k})$, $\Sigma^R_c(\omega,\mathbf{k}) = V^2/[\omega - \epsilon^0_{\mathbf{k}} + i/(2\tau_F)]$. $V = \langle b \rangle V_0$ is the effective hybridization between the c band and the F band of the spinons, $\epsilon^0_{\mathbf{k}}$ is the dispersion of the spinons whose bandwidth is αt_c, and τ_c and τ_F mimic the elastic scattering due to the presence of impurities. In principle, αt_c is V dependent, but, for simplicity, we treat it as a constant.

We adopt few simplifications in order to perform the calculations analytically: (i) the c-band dispersion is linearized $\epsilon_{\mathbf{k}} = v_F(k - k_F)$, where k_F is the Fermi wave vector of the c band; (ii) the mildly dispersive F band is replaced by a flat level $\epsilon^0_{\mathbf{k}} \approx \epsilon^0_{k_F} \equiv E_x$ [Fig. 1(a)]. Here $E_x \approx \alpha v_F (k_F - k_{F0})$, where k_{F0} is the Fermi wave vector of the F band, and $k_{F0} < k_F$. The latter approximation is equivalent to ignoring all nonsingular α dependence in Eq. (2). The microscopic nonuniversal parameter E_x, which is the energy necessary for a momentum-conserving interband transition from the Fermi surface of the c band to the F band, becomes an important energy scale in the limit where the effective hybridization V is small (see below). We do not expect our results to depend on the details of the band dispersions. To demonstrate this explicitly, we also evaluate numerically $\sigma_1(\Omega)$ in Eq. (2) by taking the continuum limit of the model. We use parabolic dispersions $\epsilon_{\mathbf{k}} = (k^2 - k_F^2)/(2m)$ and $\epsilon^0_{\mathbf{k}} = (k^2 - k_{F0}^2)/(2m_0)$, set the energy scale by $\epsilon_F \equiv k_F^2/(2m) = 1$, and we choose $E_x = \epsilon_F/100$, $m/m_0 \equiv \alpha = 0.25$. We show that at a qualitative level the numerical and approximate analytical results match well [Figs. 2 and 3], and this validates our physical conclusions.

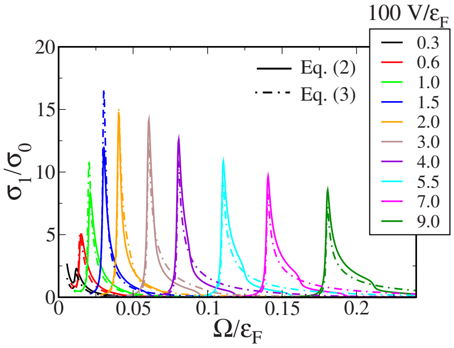

FIG. 2. (Color online) Evolution of the optical conductivity $\sigma_1(\Omega)$ with effective hybridization V ranging from $0.3\times10^{-2}\varepsilon_F$ (left) to $9\times10^{-2}\varepsilon_F$ (right). $\sigma_1(\Omega)$ is expressed in unit of $\sigma_0=e^2/(m\epsilon_F)$. The solid lines [Eq. (2)] are obtained using parabolic bands ($\alpha=0.25$ and $1/\tau_{c[F]}=10^{-3}\epsilon_F$). The dotted-dashed lines [Eq. (3)] are obtained using a linearized c band and a nondispersive F band. In both cases, as V is reduced, the peak heights first increase for $V\gg E_x=\epsilon_F/100$ and then diminish for $V\lesssim E_x$. For clarity the plots are truncated to exclude the Drude feature.

III. RESULTS

Let us for the moment ignore the finite lifetimes of the fermions and write

$$\mathrm{Im}\, G_c^R(\omega,\mathbf{k}) = -\pi[u_{\mathbf{k}}^2\delta(\omega-E_{1\mathbf{k}})+v_{\mathbf{k}}^2\delta(\omega-E_{2\mathbf{k}})],$$

where $u_{\mathbf{k}}^2=[1+(E_x-\epsilon_{\mathbf{k}})/D]/2$, $D=[(\epsilon_{\mathbf{k}}-E_x)^2+4V^2]^{1/2}$, $v_{\mathbf{k}}^2=1-u_{\mathbf{k}}^2$, and $E_{1,2k}=[\epsilon_{\mathbf{k}}+E_x\mp D]/2$ are the two hybridized bands. From Eq. (2) we get (for $\Omega>0$),

$$\sigma_1(\Omega)\propto\frac{1}{\Omega}\int_{-\Omega}^{0}d\omega\sum_{\mathbf{k}}u_{\mathbf{k}}^2v_{\mathbf{k}}^2\delta(\omega-E_{1\mathbf{k}})\delta(\omega+\Omega-E_{2\mathbf{k}}),$$

which is finite provided (a) $-\Omega\le E_{1\mathbf{k}}\le0$ and (b) $\Omega=E_{2\mathbf{k}}-E_{1\mathbf{k}}$. Thus, any finite-frequency feature in the optical conductivity is due to momentum-conserving interband transitions. We note that, for a given effective hybridization V, there is a cut-off frequency $\Omega_c\equiv[E_{2k}-E_{1k}]_{\min}=2V$ below which interband transitions are not possible. This corresponds to momenta where the bare bands $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}}^0$ cross [Fig. 1(a)]. For this process $u_{\mathbf{k}}^2v_{\mathbf{k}}^2\approx1/4$ is maximal and it reduces for interband transitions with frequencies larger than Ω_c.

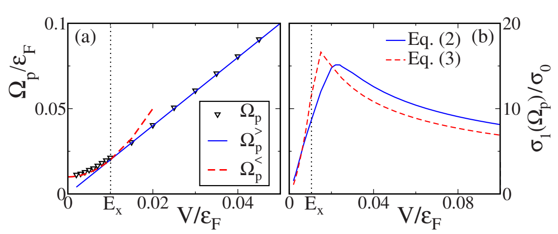

FIG. 3. (Color online) (a) The position Ω_p of the interband peak in $\sigma_1(\Omega)$ and (b) the peak height $\sigma_1(\Omega_p)$ as a function of the effective hybridization V. The triangles in (a) and the solid line in (b) are obtained using parabolic bands [Eq. (2) with $\alpha=0.25$ and $1/\tau_{c[F]}=10^{-3}\epsilon_F$]. The peak position matches the analytical result $\Omega_p=\Omega_p^>$ ($\Omega_p^<$) for $V>E_x(V<E_x)$. In (b) the dashed line is obtained using a linearized c band and nondispersive F band [Eq. (3)].

In order to include effects of finite lifetime of the c electrons (we find that finite τ_F is of secondary importance, and we ignore it in the analytic evaluation), it is more convenient to replace the momentum sum in Eq. (2) by an energy integral, which can be performed by the method of contours for the simplified case of a linearized c band and a nondispersive F band. This gives

$$\sigma_1(\Omega)\approx-\frac{\Omega_0^2}{\Omega}\mathrm{Im}\int_{-\Omega}^{0}\frac{d\omega}{\Omega+i/\tau_c+\Sigma_c^A(\omega)-\Sigma_c^R(\omega+\Omega)},\tag{3}$$

where $\Omega_0^2=ne^2/m$, n being the c-electron density. As V is reduced we find two different regimes (Figs. 2 and 3).

(i) $V>E_x$. In this regime $\Omega=\Omega_c$ corresponds to $E_{1\mathbf{k}}=E_x-V<0$, which implies that the threshold frequency for an interband transition is Ω_c [Fig. 1(a)]. Close to the threshold we get (dotted-dashed line in Fig. 2)

$$\sigma_1(\Omega\gtrsim\Omega_c)\approx\frac{\Omega_0^2\Omega^2}{4\Omega_c^2}\mathrm{Im}\left[\frac{1}{2Z}\left\{\ln\left(1-\frac{\Omega}{\Omega/2-E_x+Z}\right)-\ln\left(1-\frac{\Omega}{\Omega/2-E_x-Z}\right)\right\}\right],$$

where $Z=(\Omega_+^2+i/\tau_1^2)^{1/2}$, $\Omega_+=\Omega(\Omega^2-\Omega_c^2)^{1/2}/(2\Omega_c)$, and $1/\tau_1^2=\Omega^3/(4\tau_c\Omega_c^2)$. The difference in the position of the peak Ω_p in $\sigma_1(\Omega)$ and the threshold Ω_c is $\mathcal{O}[1/(\Omega_c\tau_c)]$, and assuming well-defined quasiparticles with $\Omega_c\tau_c\gg1$ we get [Figs. 1(b) and 3(a)]

$$\Omega_p\approx\Omega_p^>\equiv2V.\tag{4}$$

Thus, in this regime, which has been discussed in the literature,[11,12] $\Omega_p\propto\sqrt{T_K}$ and the peak position is a direct measure of the lattice Kondo temperature. For $V\gg E_x$, $\sigma_1(\Omega_p)\propto\Omega_0^2[\tau_c/V]^{1/2}$, which implies that the peak value *increases* as V is reduced [Figs. 2 and 3(b)]. This behavior continues until $(\tau_c/V)^{1/2}(V-E_x)\sim1$, after which the peak value *decreases* with decreasing V. We note that, the divergence of $\sigma_1(\Omega_p)$ for infinitely long-lived c electrons is an artifact of a theory where the effective hybridization is momentum independent. For the case where the momentum dependence of the hybridization is important, we expect $\sigma_1(\Omega_p)\propto1/V$.

(ii) $V<E_x$. This new regime, which has not been studied earlier, is relevant when the system is close to the KB-QCP. We find that $\Omega=\Omega_c$ corresponds to $E_{1\mathbf{k}}=E_x-V>0$, which implies that an interband transition at this frequency is not possible at $T=0$. The threshold frequency is $\Omega_p^<\equiv V^2/E_x+E_x>\Omega_c$, and this corresponds to an interband transition from the Fermi surface of the lower hybridized band [Fig. 1(b)]. In the vicinity of the threshold we get

$$\sigma_1(\Omega\gtrsim V^2/E_x+E_x)\approx\frac{\pi\Omega_c^2}{4\Omega^2\sqrt{\Omega^2-\Omega_c^2}}.$$

As before, neglecting the finite lifetime, the peak position is at the threshold frequency, and we get [Fig. 3(a)]

$$\Omega_p \approx \Omega_p^< = V^2/E_x + E_x. \quad (5)$$

Thus, Ω_p is no longer a direct measure of T_K, and, in particular, it stays finite ($\Omega_p \to E_x$ as $T_K \to 0$) at the QCP. Also, in this regime Ω_p varies little with V, which may not be discernible whenever Ω_p cannot be very well resolved. Since $\Omega_p \neq \Omega_c$, the corresponding matrix element $u_{\mathbf{k}}^2 v_{\mathbf{k}}^2$ decreases from the maximal value 1/4 as V is reduced. As a result the peak value $\sigma_1(\Omega_p)$ decreases rapidly [Figs. 2 and 3(b)], and the peak vanishes at the QCP indicating the gradual decoupling of the f band from the c band. Note that if $1/\tau_c \gg E_x$, the interband feature is eventually masked by the Drude peak.

Next we discuss the limitations of our results. These are based on model calculations and mean-field considerations giving more prominent interband feature than those observed experimentally. Furthermore, the fluctuations are non-negligible near the QCP, and the crucial question is whether this only smears the feature further or washes it out entirely. The issue requires further investigation that is beyond the scope of the current paper. However, even if the feature is washed out very near the QCP, any observation of significant shift of the peak position toward lower energy will have demonstrated that the physics of these systems is richer than what can be captured by SDW theory.

IV. CONCLUSION

We studied the finite-frequency interband transition peak in the optical conductivity of a heavy-fermion system near a Kondo breakdown type of quantum critical point, where the lattice Kondo temperature vanishes. As the system approaches the QCP from the heavy Fermi-liquid side, we find a new crossover regime where the peak position is related to, but is no longer a direct measure of the lattice Kondo scale. In particular, the peak position moves to lower energies, but remains finite at the QCP. On the other hand, the peak value changes nonmonotonically as $T_K \to 0$, and eventually the peak disappears at the QCP indicating the decoupling of the f electrons from the conduction band. These features are fingerprints of a Kondo breakdown type of QCP, and therefore can be used to distinguish it experimentally from a spin-density wave type of QCP.

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