Kondo-lattice screening in a *d*-wave superconductor

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We show that local-moment screening in a Kondo lattice with *d*-wave superconducting conduction electrons is qualitatively different from the corresponding single Kondo impurity case. Despite the conduction-electron pseudogap, Kondo-lattice screening is stable if the gap amplitude obeys $\Delta < \sqrt{T_K D}$, in contrast to the single-impurity condition $\Delta < T_K$ (where T_K is the Kondo temperature for $\Delta = 0$ and D is the bandwidth). Our theory explains the heavy electron behavior in the *d*-wave superconductor $Nd_{2-x}Ce_xCuO_4$.

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I. INTRODUCTION

The physical properties of heavy-fermion metals are commonly attributed to the Kondo effect, which causes the hybridization of local $4f$ and $5f$ electrons with itinerant conduction electrons. The Kondo effect for a single magnetic ion in a metallic host is well understood.[1] In contrast, the physics of the Kondo lattice, with one magnetic ion per crystallographic unit cell, is among the most challenging problems in correlated electron systems. At the heart of this problem is the need for a deeper understanding of the stability of collective Kondo screening. Examples are the stability with respect to competing ordered states (relevant in the context of quantum criticality[2]) or low conduction electron concentration (as discussed in the so-called exhaustion problem[3]). In these cases, Kondo screening of the lattice is believed to be more fragile in comparison to the single-impurity case. In this paper, we analyze the Kondo lattice in a host with a *d*-wave conduction electron pseudogap.[4] We demonstrate that Kondo-lattice screening is then significantly more robust than single-impurity screening. The unexpected stabilization of the state with screened moments is a consequence of the coherency of the hybridized heavy Fermi liquid, i.e., it is a unique lattice effect. We believe that our results are relevant for the observed large low-temperature heat capacity and susceptibility of $Nd_{2-x}Ce_xCuO_4$, an electron-doped cuprate superconductor.[5]

The stability of single-impurity Kondo screening has been investigated by modifying the properties of the conduction electrons. Most notably, beginning with the work of Withoff and Fradkin,[6] the suppression of the single-impurity Kondo effect by the presence of *d*-wave superconducting order has been studied. A variety of analytic and numeric tools have been used to investigate the single-impurity Kondo screening in a system with conduction-electron density of states (DOS) $\rho(\omega) \propto |\omega|^r$, with variable exponent r (see Refs. 6–12). Here, $r=1$ corresponds to the case of a *d*-wave superconductor, i.e., is the impurity version of the problem discussed in this paper. For $r \ll 1$, the perturbative renormalization group of the ordinary[13] Kondo problem ($r=0$) can be generalized.[6] While the Kondo coupling J is marginal, a fixed point value $J_* = r/\rho_0$ emerges for finite but small r. Here, ρ_0 is the DOS for $\omega = D$ with bandwidth D. Kondo screening only occurs for $J > J_*$, and the transition from the unscreened doublet state to a screened singlet ground state is characterized by critical fluctuations in time.

Numerical renormalization group (NRG) calculations demonstrated the existence of such an impurity quantum critical point even if r is not small, but also revealed that the perturbative renormalization group breaks down, failing to correctly describe this critical point.[9] For $r=1$, Vojta and Fritz demonstrated that the universal properties of the critical point can be understood using an infinite-U Anderson model, where the level crossing of the doublet and singlet ground states is modified by a marginally irrelevant hybridization between those states.[10,11] NRG calculations further demonstrate that the nonuniversal value for the Kondo coupling at the critical point is still given by $J_* \simeq r/\rho_0$, even if r is not small.[8] This result applies to the case of broken particle-hole symmetry, relevant for our comparison with the Kondo lattice. In the case of perfect particle-hole symmetry, it holds that[8] $J_* \to \infty$ for $r \geq 1/2$.

The result $J_* \simeq r/\rho_0$ may also be obtained from a large N mean-field theory,[6] which, otherwise, fails to properly describe the critical behavior of the transition, in particular, if r is not small. The result for J_* as the transition between the screened and unscreened states relies on the assumption that the DOS behaves as $\rho(\omega) \propto |\omega|^r$ all the way to the bandwidth. However, in a superconductor with nodes, we expect that $\rho(\omega) \simeq \rho_0$ is essentially constant for $|\omega| > \Delta$, with gap amplitude Δ altering the predicted location of the transition between the screened and unscreened states. To see this, we note that, for energies above Δ, the approximately constant DOS implies the renormalization group flow will be governed by the standard metallic Kondo result[1,13] with $r=0$, renormalizing the Kondo coupling to $\tilde{J} = J/(1 - J\rho_0 \ln D/\Delta)$ with the effective bandwidth Δ (see Ref. 9). Then, we can use the above result in the renormalized system, obtaining that Kondo screening occurs for $\tilde{J}\rho_0 \gtrsim r$, which is easily shown to be equivalent to the condition $\Delta \lesssim \Delta_*$ with

$$\Delta_* = e^{1/r} T_K, \tag{1}$$

where

$$T_K = D \exp\left(-\frac{1}{J\rho_0}\right) \tag{2}$$

is the Kondo temperature of the system in the absence of a pseudogap (which we are using here to clarify the typical

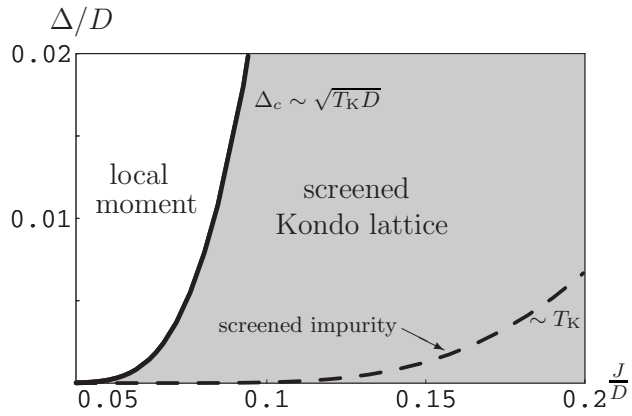

FIG. 1. The solid line is the critical pairing strength Δ_c for $T \to 0$ [Eq. (32)] separating the Kondo-screened (shaded) and local-moment regimes in the Kondo-lattice model Eq. (4). Following well-known results (Refs. 6 and 7; see also the Appendix), the *single-impurity* Kondo effect is only stable for $\Delta \lesssim D \exp(-2D/J) \sim T_K$ (dashed line).

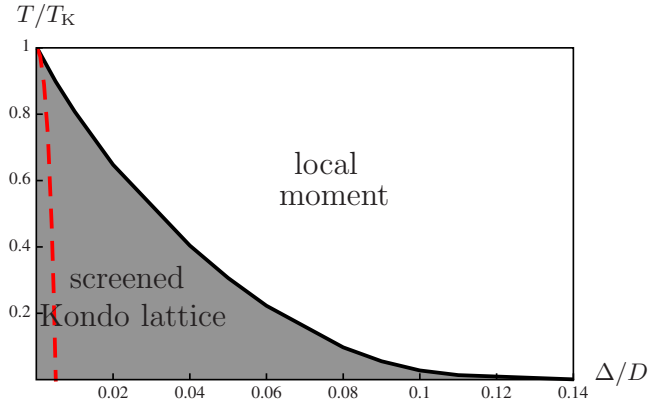

FIG. 2. (Color online) The solid line is a plot of the Kondo temperature $T_K(\Delta)$, above which $V=0$ (and Kondo screening is destroyed), normalized to its value at $\Delta=0$ [Eq. (14a)], as a function of the d-wave pairing amplitude Δ, for the case of $J=0.3D$ and $\mu=-0.1D$. With these parameters, $T_K(0)=0.0014D$, and Δ_c, the point where $T_K(\Delta)$ reaches zero, is $0.14D$ [given by Eq. (32)]. The dashed line indicates a spinodal, along which the term proportional to V^2 in the free energy vanishes. At very small $\Delta < 2.7 \times 10^{-4} D$, where the transition is continuous, the dashed line coincides with the solid line.

energy scale for Δ_*). Setting $r=1$ to establish the implication of Eq. (1) for a d-wave superconductor, we see that, due to the d-wave pseudogap in the density of states, the conduction electrons can only screen the impurity moment if their gap amplitude is smaller than a critical value of the order of the corresponding Kondo temperature T_K for constant density of states. In particular, for Δ large compared to the (often rather small) energy scale T_K, the local moment is unscreened, demonstrating the sensitivity of the single-impurity Kondo effect with respect to the low energy behavior of the host.

Given the complexity of the behavior for a single impurity in a conduction electron host with a pseudogap, it seems hopeless to study the Kondo lattice. We will show below that this must not be the case and that, moreover, Kondo screening is stable far beyond the single-impurity result Eq. (1), as illustrated in Fig. 1 [the dashed line in this plot is Eq. (1) with $\rho_0 = 1/2D$]. To do this, we utilize the large-N mean-field theory of the Kondo lattice to demonstrate that the transition between the screened and unscreened case is discontinuous. Thus, at least within this approach, no critical fluctuations occur (in contrast to the single-impurity case discussed above). More importantly, our large-N analysis also finds that the stability regime of the Kondo-screened lattice is much larger than that of the single impurity. Thus, the screened heavy-electron state is *more* robust and the local-moment phase only emerges if the conduction-electron d-wave gap amplitude obeys

$$\Delta > \Delta_c \simeq \sqrt{T_K D} \gg T_K, \tag{3}$$

with D the conduction-electron bandwidth. Below, we shall derive a more detailed expression for Δ_c; in Eq. (3) we are simply emphasizing that Δ_c is large compared to T_K [and, hence, Eq. (1)].

In addition, we find that for $\Delta < \Delta_c$, the renormalized mass only weakly depends on Δ, except for the region close to Δ_c. We give a detailed explanation for this enhanced stability of Kondo-lattice screening, demonstrating that it is a direct result of the opening of a hybridization gap in the heavy Fermi liquid state. Since the result was obtained using a large-N mean-field theory, we stress that such an approach is not expected to properly describe the detailed nature close to the transition. It should, however, give a correct order of magnitude result for the location of the transition.

To understand the resilience of Kondo-lattice screening, recall that, in the absence of d-wave pairing, it is well known that the lattice Kondo effect (and concomitant heavy-fermion behavior) is due to a hybridization of the conduction band with an f-fermion band that represents excitations of the lattice of spins. A hybridized Fermi liquid emerges from this interaction (see Fig. 4 below). We shall see that, due to the coherency of the Fermi liquid state, the resulting hybridized heavy fermions are only *marginally* affected by the onset of conduction-electron pairing. This weak proximity effect, with a small d-wave gap amplitude $\Delta_f \simeq \Delta T_K/D$ for the heavy fermions, allows the Kondo effect in a lattice system to proceed via f-electron-dominated heavy-fermion states that screen the local moments, with such screening persisting up to much larger values of the d-wave pairing amplitude than implied by the single-impurity result,[6,7] as depicted in Fig. 1 (which applies at low T). A typical finite-T phase diagram is shown in Fig. 2.

Our theory directly applies to the electron-doped cuprate $Nd_{2-x}Ce_xCuO_4$, possessing both d-wave superconductivity[14,15] with $T_c \simeq 20$ K and heavy-fermion behavior below[5] $T_K \sim 2-3$ K. The latter is exhibited in a large linear heat capacity coefficient $\gamma \simeq 4$ J/(mol K^2) together with a large low-frequency susceptibility χ with Wilson ratio $R \simeq 1.6$. The lowest crystal field state of Nd^{3+} is a Kramers doublet, well separated from higher crystal field levels,[16] supporting Kondo-lattice behavior of the Nd spins. The superconducting Cu-O states play the role of the conduction electrons. Previous theoretical work on $Nd_{2-x}Ce_xCuO_4$ discussed the role

of conduction-electron correlations.[17] Careful investigations show that the single ion Kondo temperature slightly increases in systems with electronic correlations,[18,19] an effect essentially caused by the increase in the electronic density of states of the conduction electrons. However, the fact that these conduction electrons are gapped has not been considered, even though the Kondo temperature is significantly smaller than the *d*-wave gap amplitude $\Delta \simeq 3.7$ meV (see Ref. 20). We argue that Kondo screening in $Nd_{2-x}Ce_xCuO_4$ with $T_K \ll \Delta$ can only be understood in terms of the mechanism discussed here.

We add, for completeness, that an alternative scenario for the large low-temperature heat capacity of $Nd_{2-x}Ce_xCuO_4$ is based on very low lying spin wave excitations.[21] While such a scenario cannot account for a finite value of $C(T)/T$ as $T \to 0$, it is consistent with the shift in the overall position of the Nd-crystal field states upon doping. However, an analysis of the spin wave contribution of the Nd spins shows that for realistic parameters, $C(T)/T$ vanishes rapidly below the Schottky anomaly,[22] in contrast to experiments. Thus, we believe that the large heat capacity and susceptibility of $Nd_{2-x}Ce_xCuO_4$ at low temperatures originate from Kondo screening of the Nd spins.

Despite its relevance for the *d*-wave superconductor $Nd_{2-x}Ce_xCuO_4$, we stress that our theory does not apply to heavy-electron *d*-wave superconductors, such as $CeCoIn_5$ (see Ref. 23), in which the *d*-wave gap is not a property of the conduction electron host, but a more subtle aspect of the heavy-electron state itself. The latter gives rise to a heat capacity jump at the superconducting transition $\Delta C(T_c)$ that is comparable to γT_c, while in our theory, $\Delta C(T_c) \ll \gamma T_c$ holds.

II. MODEL

The principal aim of this paper is to study the screening of local moments in a *d*-wave superconductor. Thus, we consider the Kondo-lattice Hamiltonian, possessing local spins ($\mathbf{S}_i$) coupled to conduction electrons ($c_{\mathbf{k}\alpha}$) that are subject to a pairing interaction:

$$\mathcal{H} = \sum_{\mathbf{k},\alpha} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + \frac{J}{2} \sum_{i,\alpha,\beta} \mathbf{S}_i \cdot c^\dagger_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta} + U_{\text{pair}}. \tag{4}$$

Here, J is the exchange interaction between conduction electrons and local spins, and $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$ with $\epsilon_{\mathbf{k}}$ the conduction-electron energy and μ the chemical potential. The pairing term

$$U_{\text{pair}} = -\sum_{\mathbf{k},\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} \tag{5}$$

is characterized by the attractive interaction between conduction electrons $U_{\mathbf{k}\mathbf{k}'}$. We shall assume that the latter stabilizes *d*-wave pairing with a gap $\Delta_{\mathbf{k}} = \Delta \cos 2\theta$, with θ the angle around the conduction-electron Fermi surface.

We are particularly interested in the low-temperature strong-coupling phase of this model, which can be studied by extending the conduction-electron and local-moment spin symmetry to $SU(N)$ and focusing on the large-N limit.[24] In the case of the single Kondo impurity, the large-N approach is not able to reproduce the critical behavior at the transition from a screened to an unscreened state. However, it does correctly determine the location of the transition, i.e., the nonuniversal value for the strength of the Kondo coupling where the transition from screened to unscreened impurity takes place.[8] Since the location of the transition and not the detailed nature of the transition is the primary focus of this paper, a mean-field theory is still expected to be useful.

Although the physical case corresponds to $N=2$, the large-N limit yields a valid description of the heavy Fermi liquid Kondo-screened phase.[25] We, thus, write the spins in terms of auxiliary f fermions as $\mathbf{S}_i \cdot \sigma_{\alpha\beta} \to f^\dagger_{i\alpha} f_{i\beta} - \delta_{\alpha\beta}/2$, subject to the constraint

$$\sum_\alpha f^\dagger_{i\alpha} f_{i\alpha} = N/2. \tag{6}$$

To implement the large-N limit, we rescale the exchange coupling via $J/2 \to J/N$ and the conduction-electron interaction as $U_{\mathbf{k},\mathbf{k}'} \to s^{-1} U_{\mathbf{k},\mathbf{k}'}$ [where $N \equiv (2s+1)$]. The utility of the large-N limit is that the (mean-field) stationary-phase approximation to $\mathcal{H}$ is believed to be exact at large N. Performing this mean-field decoupling of $\mathcal{H}$ yields

$$\mathcal{H} = \sum_{\mathbf{k},m=-s}^{s} [\xi_{\mathbf{k}} c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + V(f^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + \text{H.c.}) + \lambda f^\dagger_{\mathbf{k}m} f_{\mathbf{k}m}] - \sum_{\mathbf{k},m=1/2}^{s} (\Delta^\dagger_{\mathbf{k}} c_{-\mathbf{k}-m} c_{\mathbf{k}m} + \text{H.c.}) + E_0, \tag{7}$$

with E_0 a constant in the energy that is defined below. The pairing gap, $\Delta_{\mathbf{k}}$, and the hybridization between conduction and f electrons, V, result from the mean-field decoupling of the pairing and Kondo interactions, respectively. The hybridization V (that we took to be real) measures the degree of Kondo screening (and can be directly measured experimentally[26]) and λ is the Lagrange multiplier that implements the above constraint, playing the role of the f-electron level. The free energy F of this single-particle problem can now be calculated, and has the form

$$F(V,\lambda,\Delta_{\mathbf{k}}) = \frac{NV^2}{J} - \frac{N\lambda}{2} + s\sum_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{k}} \Delta_{\mathbf{k}'} U^{-1}_{\mathbf{k}\mathbf{k}'} + N \sum_{\mathbf{k},\alpha=\pm} \left(\frac{1}{4}(\xi_k + \lambda) - \frac{1}{2} E_{\mathbf{k}\alpha} - T \ln(1 + e^{-\beta E_{\mathbf{k}\alpha}}) \right), \tag{8}$$

where $T = \beta^{-1}$ is the temperature. The first three terms are the explicit expressions for E_0 in Eq. (7), and $E_{\mathbf{k}\pm}$ is

$$E_{\mathbf{k}\pm} = \frac{1}{\sqrt{2}} \sqrt{\Delta^2_{\mathbf{k}} + \lambda^2 + 2V^2 + \xi^2_{\mathbf{k}} \pm \sqrt{S_{\mathbf{k}}}},$$

$$S_{\mathbf{k}} = (\Delta^2_{\mathbf{k}} + \xi^2_{\mathbf{k}} - \lambda^2)^2 + 4V^2[(\xi_{\mathbf{k}} + \lambda)^2 + \Delta^2_{\mathbf{k}}], \tag{9}$$

describing the bands of our *d*-wave paired heavy-fermion system.

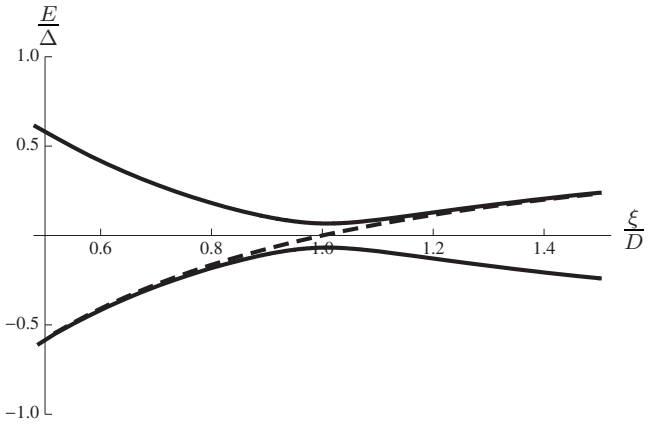

FIG. 3. The dashed line is the lower heavy-fermion band (crossing zero at the heavy-fermion Fermi surface) for the unpaired ($\Delta=0$) case, and the solid lines are $\pm E_{\mathbf{k}-}$ for $\Delta_{\mathbf{k}}=0.1D$, showing a small f-electron gap $\Delta_{f\mathbf{k}}\simeq 0.014D$.

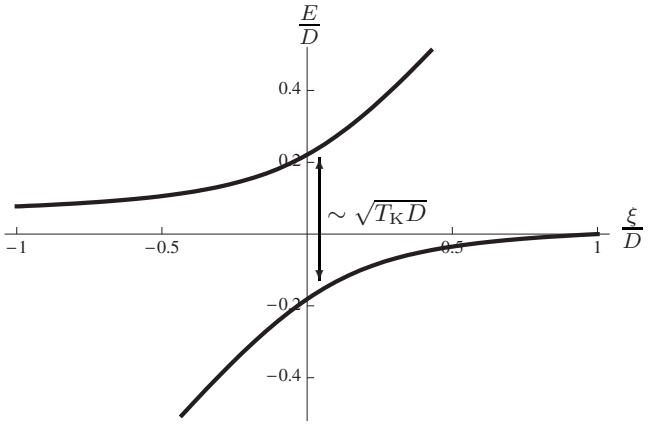

FIG. 4. Plot of the energy bands $E_+(\xi)$ (top curve) and $E_-(\xi)$ (bottom curve), defined in Eq. (13), in the heavy Fermi liquid state (for $\Delta=0$), for the case $V=0.2D$ and $\lambda=0.04D$, that has a heavy-fermion Fermi surface near $\xi=D$ and an experimentally measurable hybridization gap (Ref. 26) (the minimum value of E_+-E_-, i.e., the direct gap) equal to $2V\sim\sqrt{T_K D}$. Note, however, the indirect gap is $\lambda\sim T_K$.

The phase behavior of this Kondo-lattice system for given values of T, J, and μ is determined by finding points at which F is stationary with respect to the variational parameters V, λ, and $\Delta_{\mathbf{k}}$. For simplicity, henceforth we take $\Delta_{\mathbf{k}}$ as given (and having d-wave symmetry as noted above), with the goal of studying the effect of nonzero pairing on the formation of the heavy-fermion metal characterized by V and λ that satisfy the stationarity conditions

$$\frac{\partial F}{\partial V}=0, \tag{10a}$$

$$\frac{\partial F}{\partial \lambda}=0, \tag{10b}$$

with the second equation enforcing the constraint [Eq. (6)]. We shall, furthermore, restrict attention to $\mu<0$ (i.e., a less than half-filled conduction band).

Before we proceed, we point out that the magnitude of the pairing gap near the unpaired heavy-fermion Fermi surface (located at $\xi=V^2/\lambda$) is remarkably small. Taylor expanding $E_{\mathbf{k}-}$ near this point, we find

$$E_{\mathbf{k}-}\simeq\frac{\lambda^2}{V^2}\left[\left(\xi-\frac{V^2}{\lambda}-\frac{\lambda\Delta_{\mathbf{k}}^2}{V^2}\right)^2+\Delta_{\mathbf{k}}^2\right]^{1/2}, \tag{11}$$

giving a heavy-fermion gap $\Delta_{f\mathbf{k}}=(\lambda/V)^2\Delta_{\mathbf{k}}$ [with amplitude $\Delta_f=\Delta(\lambda/V)^2$]. We show below that $(\lambda/V)^2\ll 1$ such that $\Delta_{f\mathbf{k}}\ll\Delta_{\mathbf{k}}$. In Fig. 3, we plot the lower heavy-fermion band for the unpaired case $\Delta_{\mathbf{k}}=0$ (dashed line) along with $\pm E_{\mathbf{k}-}$ for the case of finite $\Delta_{\mathbf{k}}$ (solid lines) in the vicinity of the unpaired heavy-fermion Fermi surface, showing the small heavy-fermion gap $\Delta_{f\mathbf{k}}$. Thus, we find a weak proximity effect in which the heavy-fermion quasiparticles, which are predominantly of f character, are only weakly affected by the presence of d-wave pairing in the conduction-electron band.

III. KONDO-LATTICE SCREENING

A. Normal conduction electrons

A useful starting point for our analysis is to recall the well-known[27] unpaired ($\Delta=0$) limit of our model. By minimizing the corresponding free energy [simply the $\Delta=0$ limit of Eq. (8)], one obtains, at low temperatures, that the Kondo screening of the local moments is represented by the nontrivial stationary point of F at $V=V_0$ and $\lambda=\lambda_0=V_0^2/D$, with

$$V_0\simeq\sqrt{\frac{D+\mu}{2\rho_0}}\exp\left(-\frac{1}{2J\rho_0}\right). \tag{12}$$

Here, we have taken the conduction-electron density of states to be a constant, $\rho_0=(2D)^{-1}$, with $2D$ the bandwidth. The resulting phase is a metal accommodating both the conduction and f electrons with a large density of states $\propto\lambda_0^{-1}$ near the Fermi surface at $\epsilon_{\mathbf{k}}\simeq\mu+V_0^2/\lambda_0$, revealing its heavy-fermion character. In Fig. 4, we plot the energy bands

$$E_\pm(\xi_{\mathbf{k}})=\frac{1}{2}(\xi_{\mathbf{k}}+\lambda\pm\sqrt{(\xi_{\mathbf{k}}-\lambda)^2+4V^2}) \tag{13}$$

of this heavy Fermi liquid in the low-T limit.

With increasing T, the stationary V and λ decrease monotonically, vanishing at the Kondo temperature

$$T_K=\frac{2e^\gamma}{\pi}\sqrt{D^2-\mu^2}\exp\left[-\frac{1}{\rho_0 J}\right] \tag{14a}$$

$$=\frac{2e^\gamma}{\pi}\sqrt{\frac{D-\mu}{D+\mu}}\lambda_0. \tag{14b}$$

Here, the second line is meant to emphasize that T_K is of the same order as the $T=0$ value of the f-fermion chemical potential λ_0, and therefore, $T_K\ll V_0$, i.e., T_K is small compared to the zero-temperature hybridization energy V_0.

It is well established that the phase-transition-like behavior of V at T_K is, in fact, a crossover once N is finite.[1,24] Nevertheless, the large-N approach yields the correct order of magnitude estimate for T_K and provides a very useful description of the strong-coupling heavy Fermi liquid regime, including the emergence of a hybridization gap in the energy spectrum.

B. *d*-wave paired conduction electrons

Next, we analyze the theory in the presence of d-wave pairing with gap amplitude Δ. Thus, we imagine continuously turning on the d-wave pairing amplitude Δ, and study the stability of the Kondo-screened heavy Fermi liquid state characterized by the low-T hybridization V_0 [Eq. (12)]. As we discussed in Sec. I, in the case of a *single* Kondo impurity, it is well known that Kondo screening is qualitatively different in the case of d-wave pairing, and the single impurity is only screened by the conduction electrons if the Kondo coupling exceeds a critical value

$$J_* \simeq \frac{1}{\rho_0}\frac{1}{1+\ln D/\Delta}. \tag{15}$$

For $J<J_*$, the impurity is unscreened. This result for J_* can equivalently be expressed in terms of a critical pairing strength Δ_*, beyond which Kondo screening is destroyed for a given J:

$$\Delta_* = D\exp\left[1-\frac{1}{\rho_0 J}\right] \tag{16}$$

[equivalent to Eq. (1) for $r=1$], which is proportional to the Kondo temperature T_K. This result, implying that a d-wave superconductor can only screen a local spin if the pairing strength is much smaller than T_K, can also be derived within the mean-field approach to the Kondo problem, as shown in the Appendix (see also Ref. 7). Within this approach, a continuous transition to the unscreened phase (where $V^2\to 0$ continuously) takes place at $\Delta\simeq\Delta_*$.

Thus, calculations for the single-impurity case indicate that Kondo screening is rather sensitive to a d-wave pairing gap. The question we wish to address is, how does d-wave pairing affect Kondo screening in the lattice case? In fact, we will see that the results are quite different in the Kondo lattice case, such that Kondo screening persists beyond the point Δ_*. To show this, we have numerically studied the Δ dependence of the saddle point of the free energy Eq. (8), showing that, at low temperatures, V only vanishes, in a discontinuous manner, at much larger values of Δ, as shown in Fig. 5 (solid dots) for the case of $J=0.30D$, $\mu=-0.1D$, and $T=10^{-4}D$ (i.e., $T/T_K\simeq 0.069$). In Fig. 2, we plot the phase diagram as a function of T and Δ, for the same values of J and μ, with the solid line denoting the line of discontinuous transitions.

The dashed line in Fig. 2 denotes the spinodal T_s of the free energy F at which the quadratic coefficient of Eq. (8) crosses zero. The significance of T_s is that, if the Kondo-to-local-moment transition were continuous (as it is for $\Delta=0$), this would denote phase boundary; the $T\to 0$ limit of this quantity coincides with the single-impurity critical pairing Eq. (16). An explicit formula for T_s can be easily obtained by finding the quadratic coefficient of Eq. (8):

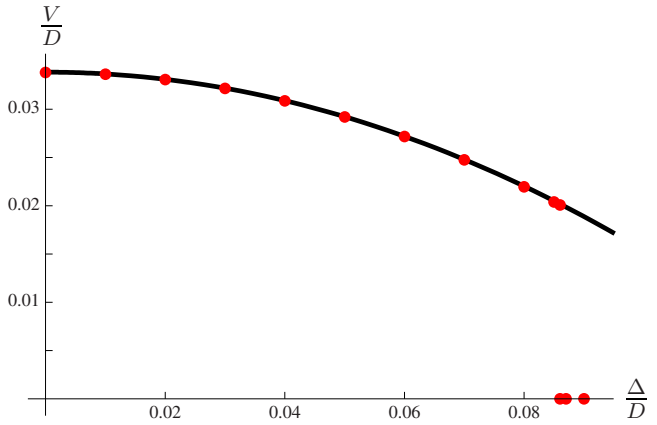

FIG. 5. (Color online) Mean-field Kondo parameter V as a function of the d-wave pairing amplitude Δ, for exchange coupling $J=0.30D$ and chemical potential $\mu=-0.1D$, according to the approximate formula Eq. (30) (solid line) and via a direct minimization of Eq. (8) at $T=10^{-4}D$ (points), the latter exhibiting a first-order transition near $\Delta=0.086D$.

$$\frac{1}{J} = \sum_{\mathbf{k}} \frac{\tanh E_{\mathbf{k}}/2T_s(\Delta)}{2E_{\mathbf{k}}}, \tag{17}$$

with $E_{\mathbf{k}}\equiv\sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$ and where we set $\lambda=0$ [which must occur at a continuous transition where $V\to 0$, as can be seen by analyzing Eq. (10b)]. As seen in Fig. 2, the spinodal temperature is generally much smaller than the true transition temperature; however, for very small $\Delta\to 0$, $T_s(\Delta)$ coincides with the actual transition (which becomes continuous), as noted in the figure caption.

Our next task is to understand these results within an approximate analytic analysis of Eq. (8); before doing so, we stress again that the discontinuous transition from a screened to an unscreened state as a function of T becomes a rapid crossover for finite N. The large-N theory is, however, expected to correctly determine where this crossover takes place.

1. Low-T limit

According to the numerical data (points) plotted in Fig. 5, the hybridization V is smoothly suppressed with increasing pairing strength Δ before undergoing a discontinuous jump to $V=0$. To understand, analytically, the Δ dependence of V at low T, we shall analyze the $T=0$ limit of F, i.e., the ground-state energy E. The essential question concerns the stability of the Kondo-screened state with respect to a d-wave pairing gap, characterized by the following Δ-dependent hybridization

$$V(\Delta) = V_0\left(1-\frac{\Delta^2}{\Delta_{\text{typ}}^2}\right), \tag{18}$$

with Δ_{typ} an energy scale, to be derived, that gives the typical value of Δ for which the heavy-fermion state is affected by d-wave pairing.

To show that Eq. (18) correctly describes the smooth suppression of the hybridization with increasing Δ, and to obtain the scale Δ_{typ}, we now consider the dimensionless quantity

$$\chi_\Delta \equiv -\frac{1}{2\rho_0}\frac{\partial^2 E}{\partial \Delta^2} \tag{19}$$

that characterizes the change of the ground-state energy with respect to the pairing gap. Separating the amplitude of the gap from its momentum dependence, i.e., writing $\Delta_{\mathbf{k}}=\Delta\phi_{\mathbf{k}}$, we obtain from the Hellmann-Feynman theorem that

$$\chi_\Delta = -\frac{1}{2\rho_0\Delta}\left\langle\frac{\partial \mathcal{H}}{\partial \Delta}\right\rangle = -\frac{N}{2\rho_0\Delta}\sum_{\mathbf{k}}\phi_{\mathbf{k}}\langle c^\dagger_{\mathbf{k}m}c^\dagger_{-\mathbf{k}-m}\rangle. \tag{20}$$

For $\Delta\to 0$, this yields

$$\chi_\Delta = \frac{N}{2\rho_0}\int\frac{d\omega}{2\pi}\sum_{\mathbf{k}}\phi^2_{\mathbf{k}}G_{cc}(\mathbf{k},i\omega)G_{cc}(-\mathbf{k},-i\omega). \tag{21}$$

Here, $G_{cc}(\mathbf{k},i\omega)$ is the conduction-electron propagator. As expected, χ_Δ is the particle-particle correlator of the conduction electrons. Thus, for $T=0$, the particle-particle response will be singular. This is the well-known Cooper instability. For $V=0$, we obtain, for example,

$$\chi_\Delta(V=0) = \frac{N}{8}\log\frac{D^2-\mu^2}{\Delta^2}, \tag{22}$$

where we used Δ as a lower cutoff to control the Cooper logarithm. Below we will see that, except for extremely small values of Δ, the corresponding Cooper logarithm is overshadowed by another logarithmic term that does not have its origin in states close to the Fermi surface, but rather results from states with typical energy $V\simeq\sqrt{T_K D}$.

In order to evaluate χ_Δ in the heavy Fermi liquid state, we start from

$$G_{cc}(\mathbf{k},\omega) = \frac{v^2_{\mathbf{k}}}{\omega-E_+(\xi_{\mathbf{k}})}+\frac{u^2_{\mathbf{k}}}{\omega-E_-(\xi_{\mathbf{k}})}, \tag{23}$$

where $E_\pm$ is given in Eq. (13) and the coherence factors of the hybridized Fermi liquid are

$$u^2_{\mathbf{k}} = \frac{1}{2}\left(1-\frac{\xi_{\mathbf{k}}-\lambda}{\sqrt{(\xi_{\mathbf{k}}-\lambda)^2+4V^2}}\right),$$

$$v^2_{\mathbf{k}} = \frac{1}{2}\left(1+\frac{\xi_{\mathbf{k}}-\lambda}{\sqrt{(\xi_{\mathbf{k}}-\lambda)^2+4V^2}}\right). \tag{24}$$

Inserting $G_{cc}(\mathbf{k},\omega)$ into the above expression for χ_Δ yields

$$\chi_\Delta = \frac{N}{8}\int_{-D-\mu}^{D-\mu}d\xi\left(\frac{v^4}{E_+}+\frac{u^4}{|E_-|}+\frac{4v^2u^2\theta(E_-)}{E_++E_-}\right). \tag{25}$$

We used that $E_+>0$ is always fulfilled, as we consider a less than half-filled conduction band.

Considering first the limit $\lambda=0$, it holds $E_-(\xi)<0$ and the last term in the above integral disappears. The remaining terms simplify to

$$\chi_\Delta(\lambda=0) = \frac{N}{8}\int_{-D-\mu}^{D-\mu}d\xi\frac{1}{\sqrt{\xi^2+4V^2}} = \frac{N}{8}\log\frac{D^2-\mu^2}{4V^2}. \tag{26}$$

Even for λ nonzero, this is the dominant contribution to χ_Δ in the relevant limit $\lambda\ll V\ll D$. To demonstrate this, we analyze Eq. (25) for nonzero λ, but assuming $\lambda\ll V$ as is, indeed, the case for small Δ. The calculation is lengthy but straightforward. It follows

$$\chi_\Delta = \frac{N}{8}\left(1+\frac{\lambda}{D}\right)\log\frac{D^2-\mu^2}{4V^2}+\frac{N}{8}\frac{\lambda}{D}\log\frac{D|\mu|}{\Delta^2}. \tag{27}$$

The last term is the Cooper logarithm, but now in the heavy-fermion state. The prefactor $\lambda/D\simeq T_K/D$ is a result of the small weight of the conduction electrons on the Fermi surface (i.e., where $\xi\simeq V^2/\lambda$) as well as the reduced velocity close to the heavy electron Fermi surface. Specifically, it holds $u^2(\xi\simeq V^2/\lambda)\simeq\lambda^2/V^2$ as well as $E_-(\xi\simeq V^2/\lambda)\simeq\lambda^2/V^2(\xi-V^2/\lambda)$.

Thus, except for extremely small gap values where $\Delta^2<D^2(\frac{D}{4T_K})^{-D/T_K}$, χ_Δ is dominated by the $\lambda=0$ result [Eq. (26)] and the Cooper logarithm plays no role in our analysis. The logarithm in Eq. (26) is not originating from the heavy-electron Fermi surface (i.e., it is not from $\xi\simeq\frac{V^2}{\lambda}$). Instead, it has its origin in the integration over states where $E_-<0$. The important term $\frac{v^4}{2E_+}-\frac{u^4}{2E_-}$ in Eq. (25) is peaked for $\xi\simeq 0$, i.e., where $E_\pm(\xi\simeq 0)=\pm V$ and is large as long as $|\xi|\lesssim V$. For $\xi\simeq 0$ holds $\frac{v^4}{2E_+}\simeq-\frac{u^4}{2E_-}\simeq\frac{1}{32V}$. This peak at $\xi\simeq 0$ has its origin in the competition between two effects. Usually, u or v are large when $E_\pm\simeq\xi$. The only regime where u or v are still sizable while $E_\pm$ remain small is close to the bare conduction-electron Fermi surface at $|\xi|\simeq V$ (the position of the level repulsion between the two hybridizing bands, see Fig. 4). Thus, the logarithm is caused by states that are close to the *bare* conduction-electron Fermi surface. Although these states have the strongest response to a pairing gap, they do not have much to do with the heavy-fermion character of the system. It is interesting that this heavy-fermion pairing response is the same even in the case of a Kondo insulator where $\lambda=0$ and the Fermi level is in the middle of the hybridization gap.

The purpose of the preceding analysis was to derive an accurate expression for the ground-state energy E at small Δ. Using Eq. (19) gives

$$E = E(\Delta=0)-\chi_\Delta\rho_0\Delta^2, \tag{28}$$

which, using Eq. (26) and considering the leading order in $\lambda\ll V$ and $\Delta\ll V$, safely neglecting the last term of Eq. (27) according to the argument of the previous paragraph, and dropping overall constants, yields

$$\frac{E}{N}\simeq\frac{V^2}{J}-\frac{\lambda}{2}+V^2\rho_0\ln\frac{\lambda}{D+\mu}-\frac{\rho_0\Delta^2}{8}\ln\frac{D^2-\mu^2}{V^2}. \tag{29}$$

Using Eq. (10), the stationary value of the hybridization (to leading order in Δ^2) is then obtained via minimization with respect to V and λ. This yields

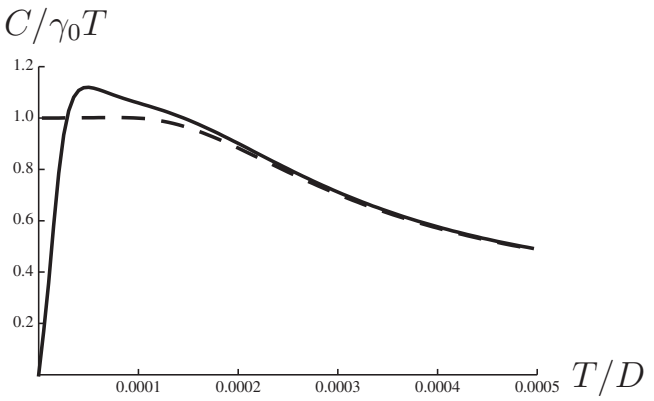

FIG. 6. Plot of the low-temperature specific heat coefficient $\frac{C}{T}=-\frac{\partial^2 F}{\partial T^2}$, for the case of $\lambda=10^{-2}D$, $V=10^{-1}D$, and $\mu=-0.1D$, for the metallic case ($\Delta=0$, dashed line), and for the case of nonzero *d*-wave pairing ($\Delta=0.1D$, solid line). This shows that, even with nonzero Δ, the specific heat coefficient will appear to saturate at a large value at low T (thus, exhibiting signatures of a heavy-fermion metal) before vanishing at asymptotically low $T \ll \Delta_f$ [$=\Delta(\lambda/V)^2 = 10^{-4}D$]. Each curve is normalized to the $T=0$ value for the metallic case, $\gamma_0 \simeq \frac{2}{3}\pi^2\rho_0 V^2/\lambda^2$.

$$V(\Delta) \simeq V_0 - \frac{\Delta^2}{16V_0}, \tag{30}$$

with the stationary value of $\lambda=2\rho_0 V^2$, which establishes Eq. (18). A smooth suppression of the Kondo hybridization from the $\Delta=0$ value V_0 [Eq. (12)] occurs with increasing *d*-wave pairing amplitude Δ at low T. This result, thus, implies that the conduction-electron gap only causes a significant reduction of V and λ for $\Delta \simeq \Delta_{\rm typ} \propto \sqrt{T_K D}$.

In Fig. 5, we compare $V(\Delta)$ of Eq. (30) (solid line) with the numerical result (solid dots). As long as V stays finite, the simple relation Eq. (30) gives an excellent description of the heavy-electron state. Above the small *f*-electron gap Δ_f, these values of V and λ yield a large heat capacity coefficient (taking $N=2$) $\gamma \simeq \frac{2}{3}\pi^2\rho_0 V^2/\lambda^2$ and susceptibility $\chi \simeq 2\rho_0 V^2/\lambda^2$, reflecting the heavy-fermion character of this Kondo-lattice system even in the presence of a *d*-wave pairing gap. According to our theory, this standard heavy-fermion behavior (as observed experimentally[5] in $Nd_{2-x}Ce_xCuO_4$) will be observed for temperatures that are large compared to the *f*-electron gap Δ_f. However, for very small $T \ll \Delta_f$, the temperature dependence of the heat capacity changes (due to the *d*-wave character of the *f*-fermion gap), behaving as $C=AT^2/\Delta$ with a large prefactor $A \simeq (D/T_K)^2$. This leads to a sudden drop in the heat capacity coefficient at low T, as depicted in Fig. 6.

The surprising robustness of the Kondo screening with respect to *d*-wave pairing is rooted in the weak proximity effect of the *f* levels and the coherency as caused by the formation of the hybridization gap. Generally, a pairing gap affects states with energy $\Delta_{\mathbf{k}}$ from the Fermi energy. However, low energy states that are within T_K of the Fermi energy are predominantly of *f*-electron character (a fact that follows from our large-N theory, but also from the much more general Fermi liquid description of the Kondo lattice[28]) and are protected by the weak proximity. These states only sense a gap $\Delta_{f\mathbf{k}} \ll \Delta_{\mathbf{k}}$ and can readily participate in local-moment screening.

Furthermore, the opening of the hybridization gap coherently pushes conduction electrons to energies $\simeq V$ from the Fermi energy. Only for $\Delta \simeq V \simeq \sqrt{T_K D}$ will the conduction electrons' ability to screen the local moments be affected by *d*-wave pairing. This situation is very different from the single-impurity Kondo problem, where conduction-electron states come arbitrarily close to the Fermi energy.

2. First-order transition

The result Eq. (30) of the preceding section strictly applies for $\Delta \to 0$, although as seen in Fig. 5, in practice it agrees quite well with the numerical minimization of the free energy until the first-order transition. To understand the way in which V is destroyed with increasing Δ, we must consider the $V \to 0$ limit of the free energy.

We start with the ground-state energy. Expanding E [the $T \to 0$ limit of Eq. (8)] to leading order in V and zeroth order in λ (valid for $V \to 0$), we find (dropping overall constants)

$$\frac{E}{N} \simeq -4\rho_0 V^2 \ln\frac{\Delta_c}{\Delta} + \frac{16}{3}\frac{\rho_0}{\Delta}V^3, \tag{31}$$

where we defined the quantity Δ_c

$$\Delta_c = 4\sqrt{D^2-\mu^2}\exp\left(-\frac{1}{2\rho_0 J}\right), \tag{32}$$

at which the minimum value of V in Eq. (31) vanishes continuously, with the formula for $V(\Delta)$ given by

$$V(\Delta) \simeq \frac{1}{2}\Delta \ln\frac{\Delta_c}{\Delta} \tag{33}$$

near the transition. According to Eq. (32), the equilibrium hybridization V vanishes (along with the destruction of Kondo screening) for pairing amplitude $\Delta_c \sim \sqrt{T_K D}$, of the same order of magnitude as the $T=0$ hybridization V_0, as expected [and advertised above in Eq. (3)].

Equation (32) strictly applies only at $T=0$, apparently yielding a continuous transition at which $V \to 0$ for $\Delta \to \Delta_c$. What about for $T \neq 0$? We find that, for small but nonzero T, Eq. (32) approximately yields the correct location of the transition, but that the nature of the transition changes from continuous to first order. Thus, for Δ near Δ_c, there is a discontinuous jump to the local-moment phase that is best obtained numerically, as shown above in Figs. 5 and 2. However, we can get an approximate analytic understanding of this first-order transition by examining the low-T limit. Since excitations are gapped, at low T the free energy F_K of the Kondo-screened ($V \neq 0$) phase is well approximated by inserting the stationary solution Eq. (33) into Eq. (31):

$$\frac{F_K}{N} \simeq -\frac{1}{6}\rho_0\Delta^2 \ln^3\frac{\Delta_c}{\Delta}, \tag{34}$$

for F_K at $\Delta \to \Delta_c$. The discontinuous Kondo-to-local-moment transition occurs when the Kondo free energy Eq. (34) is

equal to the local-moment free energy. For the latter, we set $V=\lambda=0$ in Eq. (8), obtaining (recall $E_{\mathbf{k}}=\sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}$)

$$\frac{F_{\mathrm{LM}}}{N} \simeq -\frac{1}{2}\rho_0(D+\mu)^2 - \frac{1}{4}\rho_0\Delta^2 \ln\frac{4\sqrt{D^2-\mu^2}}{\Delta} - T\ln 2 - T\sum_{\mathbf{k}} \ln[1+e^{-\beta E_{\mathbf{k}}}], \tag{35}$$

where we dropped an overall constant depending on the conduction-band interaction.

The term proportional to T in Eq. (35) comes from the fact that $E_{\mathbf{k}-}=0$ for $V=\lambda=0$, and corresponds to the entropy of the local moments. At low T, the gapped nature of the d-wave quasiparticles implies that the last term in Eq. (35) can be neglected (although the nodal quasiparticles give a subdominant power-law contribution). In deriving the Kondo free energy F_K [Eq. (34)], we dropped overall constant terms; reestablishing these to allow a comparison to F_{LM}, and setting $F_{\mathrm{LM}}=F_K$, we find

$$\frac{1}{6}\rho_0\Delta^2 \ln^3\frac{\Delta_c}{\Delta} = T\ln 2 \tag{36}$$

that can be solved for temperature to find the transition temperature T_K for the first-order Kondo-screened-to-local-moment phase transition:

$$T_K(\Delta) = \frac{\rho_0\Delta^2}{6\ln 2}\ln^3\frac{\Delta_c}{\Delta} \tag{37}$$

that is valid for $\Delta \to \Delta_c$, providing an accurate approximation to the numerically determined T_K curve in Fig. 2 (solid line) in the low-temperature regime (i.e., near $\Delta_c=0.14D$ in Fig. 2).

Equation (37) yields the temperature at which, within mean-field theory, the screened Kondo lattice is destroyed by the presence of nonzero d-wave pairing; thus, as long as $\Delta < T_K(\Delta)$, heavy-fermion behavior is compatible with d-wave pairing in our model. The essential feature of this result is that $T_K(\Delta)$ is only marginally reduced from the $\Delta=0$ Kondo temperature Eq. (2), establishing the stability of this state. In comparison, according to expectations based on a single-impurity analysis, one would expect the Kondo temperature to follow the dashed line in Fig. 2.

Away from this approximate result valid at large N, the Ruderman-Kittel-Kasuya-Yosida interaction between moments is expected to lower the local-moment free energy, altering the predicted location of the phase boundary. Then, even for $T=0$, a level crossing between the screened and unscreened ground states occurs for a finite V. Still, as long as the $\Delta=0$ heavy-fermion state is robust, it will remain stable at low T for Δ small compared to Δ_c, as summarized in Figs. 1 and 2.

IV. CONCLUSIONS

We have shown that a lattice of Kondo spins coupled to an itinerant conduction band experiences robust Kondo screening even in the presence of d-wave pairing among the conduction electrons. The heavy-electron state is protected by the large hybridization energy $V \gg T_K$. The d-wave gap in the conduction band induces a relatively weak gap at the heavy-fermion Fermi surface, allowing Kondo screening and heavy-fermion behavior to persist. Our results demonstrate the importance of Kondo-lattice coherency, manifested by the hybridization gap, which is absent in the case of dilute Kondo impurities. As pointed out in detail, the origin for the unexpected robustness of the screened heavy-electron state is the coherency of the Fermi liquid state. With the opening of a hybridization gap, conduction-electron states are pushed to energies of order $\sqrt{T_K D}$ away from the Fermi energy. Whether or not these conduction electrons open up a d-wave gap is, therefore, of minor importance for the stability of the heavy-electron state.

Our conclusions are based on a large-N mean-field theory. In case of a single impurity, numerical renormalization group calculations demonstrated that such a mean-field approach fails to reproduce the correct critical behavior where the transition between screened and unscreened impurity takes place. However, the mean-field theory yields the correct value for the strength of the Kondo coupling at the transition. In our paper, we are not concerned with the detailed nature in the near vicinity of the transition. Our focus is solely the location of the boundary between the heavy Fermi liquid and unscreened local-moment phase, and we do expect that a mean-field theory gives the correct result. One possibility to test the results of this paper is a combination of dynamical mean-field theory and numerical renormalization group for the pseudogap Kondo-lattice problem.

In case where Kondo screening is inefficient and $\Delta > \sqrt{T_K D}$, i.e., the "local moment" phase of Figs. 1 and 2, the ground state of the moments will likely be magnetically ordered. This can have interesting implications for the superconducting state. Examples are reentrance into a normal phase (similar to $ErRh_4B_4$, see Ref. 29) or a modified vortex lattice in the low-temperature magnetic phase. In our theory, we ignored these effects. This is no problem as long as the superconducting gap amplitude Δ is small compared to $\sqrt{T_K D}$ and the Kondo lattice is well screened. Thus, the region of stability of the Kondo-screened state will not be significantly affected by including the magnetic coupling between the f electrons. Only the nature of the transition and, of course, the physics of the unscreened state will depend on it. Finally, our theory offers an explanation for the heavy-fermion state in $Nd_{2-x}Ce_xCuO_4$, where $\Delta \gg T_K$.

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APPENDIX: SINGLE IMPURITY CASE

For a single Kondo impurity, a critical value J_* for the coupling between conduction electron and impurity spin

emerges, separating Kondo-screened from local-moment behavior for a single spin impurity in a *d*-wave superconductor, see Eq. (15). As discussed in the main text, this is equivalent to a critical pairing Eq. (16), above which Kondo screening does not occur. The result was obtained in careful numerical renormalization group calculations.[8,9] In the present section, we demonstrate that the same result also follows from a simple large-N mean-field approach. It is important to stress that this approach fails to describe the detailed critical behavior. However, here we are only concerned with the approximate value of the nonuniversal quantity J_*. Indeed, mean-field theory is expected to give a reasonable value for the location of the transition.

Our starting point is the model Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}m} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}m} c_{\mathbf{k}m} + + \frac{J}{N} \sum_{m,m',\mathbf{k},\mathbf{k}'} f^\dagger_m f_m c^\dagger_{\mathbf{k}m} c_{\mathbf{k}'m'} - \sum_{\mathbf{k}\mathbf{k}'} U_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}, \tag{A1}$$

with the corresponding mean-field action $S=S_f+S_b+S_{\rm int}$ with (introducing the Lagrange multiplier λ and hybridization V as usual, and making the BCS mean-field approximation for the conduction fermions):

$$S_f = \int d\tau \sum_m \left[\sum_{\mathbf{k}} c^\dagger_{\mathbf{k}m} (\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}m} + f^\dagger_m (\partial_\tau + \lambda) f_m \right],$$

$$S_b = \int d\tau \left(\frac{N}{J} V^\dagger V - \lambda N q_0 \right), \tag{A2}$$

$$S_{\rm int} = \int d\tau \sum_{m\mathbf{k}} (f^\dagger_m c_{\mathbf{k}m} V + V^\dagger c_{\mathbf{k}m} f_m) + \sum_{\mathbf{k}\mathbf{k}'} \Delta_{\mathbf{k}} \Delta'_{\mathbf{k}} U^{-1}_{\mathbf{k}\mathbf{k}'} - \sum_{m=1/2}^{J} (\Delta^\dagger_{\mathbf{k}} c_{-\mathbf{k}-m} c_{\mathbf{k}m} + c^\dagger_{\mathbf{k}m} c^\dagger_{-\mathbf{k}-m} \Delta_{\mathbf{k}}), \tag{A3}$$

where the λ integral implements the constraint $Nq_0 = \Sigma_m f^\dagger_m f_m$, with $q_0=1/2$. Here, we have taken the large-N limit, with $N=2J+1$.

The mean-field approximation having been made, it is now straightforward to trace over the fermionic degrees of freedom to yield

$$F = \frac{N|V|^2}{J} - \lambda N q_0 - \frac{N}{2} T \sum_\omega \ln\{[i\omega - \lambda - \Gamma_1(i\omega)] \times [i\omega + \lambda + \Gamma_1(-i\omega)] - \Gamma_2(i\omega)\bar{\Gamma}_2(i\omega)\}, \tag{A4}$$

for the free energy contribution due to a single impurity in a *d*-wave superconductor. Here, we dropped an overall constant due to the conduction fermions only, as well as the quadratic term in $\Delta_{\mathbf{k}}$ (which, of course, determines the equilibrium value of $\Delta_{\mathbf{k}}$; here, as in the main text, we are interested in the impact of a given $\Delta_{\mathbf{k}}$ on the degree of Kondo screening), and defined the functions

$$\Gamma_1(i\omega) = |V|^2 \sum_{\mathbf{k}} \frac{i\omega + \epsilon_{\mathbf{k}}}{(i\omega)^2 - E^2_{\mathbf{k}}}, \tag{A5}$$

$$\Gamma_2(i\omega) = V^2 \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{(i\omega)^2 - E^2_{\mathbf{k}}}, \tag{A6}$$

$$\bar{\Gamma}_2(i\omega) = (V^\dagger)^2 \sum_{\mathbf{k}} \frac{\Delta_{\mathbf{k}}}{(i\omega)^2 - E^2_{\mathbf{k}}}. \tag{A7}$$

At this point, we note that, for a *d*-wave superconductor, $\Gamma_2=\bar{\Gamma}_2=0$ due to the sign change of the *d*-wave order parameter. The self-energy $\Gamma_1(i\omega)$ is nonzero and essentially measures the DOS $\rho_d(\omega)$ of the *d*-wave superconductor. In fact, one can show that the corresponding retarded function $\Gamma_{1R}(\omega)$ satisfies

$$\Gamma_{1R}(\omega) = |V|^2 \int_{-\infty}^{\infty} dz \frac{\rho_d(z)}{\omega + i\delta - z}, \tag{A8}$$

with $\delta=0^+$, so that the imaginary part $\Gamma''_{1R}(\omega)=-\pi|V|^2\rho_d(\omega)$ measures the DOS. Writing $\Gamma_{1R}(\omega) \equiv |V|^2 G(\omega)$, we have for the free energy

$$F = \frac{N|V|^2}{J} - \lambda N q_0 + N \int_{-\infty}^{\infty} \frac{dz}{\pi} n_F(z) \tan^{-1}\left(\frac{-|V|^2 G''(z)}{z - \lambda - |V|^2 G'(z)} \right), \tag{A9}$$

and for the stationarity conditions [Eq. (10)],

$$\frac{1}{J} = \int_{-\infty}^{\infty} \frac{dz}{\pi} \frac{n_F(z) G''(z)(z-\lambda)}{[z - \lambda - |V|^2 G'(z)]^2 + |V|^4 [G''(z)]^2}, \tag{A10}$$

$$q_0 = -\int_{-\infty}^{\infty} \frac{dz}{\pi} \frac{n_F(z) |V|^2 G''(z)}{[z - \lambda - |V|^2 G'(z)]^2 + |V|^4 [G''(z)]^2}, \tag{A11}$$

which can be evaluated numerically to determine V and λ as a function of T and Δ.

The Kondo temperature T_K is defined by the temperature at which $V^2 \to 0$ continuously; at such a point, the constraint Eq. (A11) requires $\lambda \to 0$. Here, we are interested in finding the pairing Δ at which $T_K \to 0$; thus, this is obtained by setting $T=V=\lambda=0$ in Eq. (A10):

$$\frac{1}{J} = \int_{-D-\mu}^{0} \frac{dz}{\pi} \frac{-\pi\rho_d(z)}{z} \tag{A12a}$$

$$= -\rho_0 \log \frac{\Delta}{D+\mu} + \rho_0, \tag{A12b}$$

where, for simplicity, in the final line we approximated $\rho_d(z)$ to be given by

$$\rho_d(\omega) \simeq \begin{cases} \rho_0 |\omega|/\Delta & \text{for } |\omega| < \Delta \\ \rho_0 & \text{for } |\omega| > \Delta \end{cases} \tag{A13}$$

that captures the essential features (except for the narrow peak near $\omega=\Delta$) of the true DOS of a d-wave superconductor, with ρ_0 the (assumed constant) DOS of the underlying conduction band.

The solution to Eq. (A12) is

$$\Delta_* = (D+\mu)\exp\left[1-\frac{1}{\rho_0 J}\right], \tag{A14}$$

showing a destruction of the Kondo effect for $\Delta \to \Delta_*$, as $V \to 0$ continuously, thus separating the Kondo-screened (for $\Delta < \Delta_*$) from the local-moment (for $\Delta > \Delta_*$) phases.

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