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Kondo effect in gapless superconductors

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We present a self-consistent theory of Kondo impurities in gapless unconventional superconductors valid in the Fermi-liquid regime $T \lesssim T_K$. The impurity degrees of freedom are treated using the large-N slave-boson technique, leading to tractable equations describing the interplay between the Kondo effect and superconductivity. We show that for a single impurity in a superconductor with density of states $N(\omega) \sim |\omega|^r$, there exists a critical coupling J_c below which the Kondo effect does not occur. However, for $r \leq 1$ or $N=2$ any finite concentration of impurities drives $J_c \to 0$. The theory provides microscopic support for phenomenological models of resonant impurity scattering in heavy-fermion systems.

The problem of a magnetic impurity in a superconductor has a long history, beginning with the work of Anderson[1] and Abrikosov and Gor'kov,[2] who pointed out that the time-reversal breaking nature of the perturbation would lead to pair breaking and T_c suppression. It is well known that if the exchange interaction between impurity spin and conduction electrons is sufficiently strong, the Kondo effect will both modify the effective interaction in the Cooper channel and shield the impurity local moment. Theories describing the effect of Kondo impurities on superconductivity[3,4] have been attempted by many authors, generally utilizing methods specialized to the "high temperature," $T_K \ll T_{c0}$ or "Fermi liquid," $T_K \gg T_{c0}$, regimes, where T_{c0} is the superconducting transition temperature in the absence of impurities and T_K is the Kondo temperature. In general, these theories neglect the self-consistent effect of superconductivity on impurity electron properties (see, however, Ref. 5). The lack of a complete theory describing the crossover reflects the absence of a theory correctly describing the dynamics of a Kondo impurity in a normal metal at all temperatures. Jarrell has circumvented this difficulty by using Monte Carlo methods to treat the impurity degrees of freedom in a calculation of T_c suppression,[6] but this method does not appear well suited to calculate properties below the transition temperature.

The Kondo effect is accompanied by the formation of a narrow many-body resonance of width T_K near the Fermi level in the impurity spectral density $A_f(\omega)$. It is reasonable to expect that the opening of a gap Δ in the conduction-electron density of states leads through hybridization processes to a similar gap in $A_f(\omega)$, which destroys the Kondo effect if sufficiently large. Recently, Withoff and Fradkin[7] (WF) pointed out that the two problems of impurity spins coupled to baths of conduction electrons with (a) constant density of states and (b) with a fully developed gap represent two extreme members of a family of problems given by specifying a generalized conduction-electron density of states $N(\omega)=C|\omega|^r$, $|\omega|<D$, and $0 \leq r < \infty$. Making use of renormalization-group arguments as well as explicit calculations for the large-degeneracy SU(N) Kondo (Coqblin-Schrieffer) model, they showed, for $r>0$, the existence of a critical coupling J_c below which impurities are decoupled from the conduction band and no Kondo effect occurs. As potential physical examples of this phenomenon they suggested unconventional superconducting states with line and point zeroes in the momentum-dependent gap function, corresponding to densities of states $N(\omega)$ varying as ω and ω^2, respectively. Such states are possibly realized in the heavy-fermion superconductors UPt_3, UBe_{13}, URu_2Si_2, and $CeCu_2Si_2$.[8]

In the context of heavy-fermion superconductivity, theories of impurity scattering in such states have been given by Ueda and Rice[9] for the case of weak potential scattering, and by Hirschfeld, Vollhardt, and Wölfle,[10] and Schmitt-Rink, Miyake, and Varma[11] for strong scattering. Moment formation was not considered in these theories, but pair breaking still occurs because of the vanishing of the anomalous one-electron impurity-averaged self-energy. The strength of the scattering was crudely parametrized in the latter works by a phase shift δ_0 for s-wave potential scattering of electrons at the Fermi surface. One of the principal results of these treatments was that in the resonant scattering limit, $\delta_0 \to \pi/2$, corresponding to the single-impurity spin-$\frac{1}{2}$ Kondo effect,[12] a "bound-state" resonance was found to form in the superconducting density of states, $N(\omega)$, leading to gapless effects in thermodynamic properties. These are the analogs of the bound states found in discussions of Kondo effects in s-wave superconductors.[13,14]

There are several questions left open in the work of WF (Ref. 7) and in Refs. 9–11 that we hope to address here. First, what signatures of the transitions from the Kondo ($J>J_c$) to "local moment" ($J<J_c$) regime are to be expected in superconducting properties? To what extent do physical aspects of real superconductors modify the WF predictions; in particular, what are the effects of finite spin degeneracy N and a density of states varying on a scale $\Delta \ll D$? And finally, to what extent can the phenomenological theories of Refs. 9–11 be justified by microscopic analysis?

To analyze the problem we start from the SU(N) Coqblin-Schrieffer Hamiltonian,[15]

$$H=\sum_{k,m}\epsilon_k c^\dagger_{km}c_{km}+\frac{J}{N}\sum_{k,k'}\sum_{m,m'}c^\dagger_{km}f^\dagger_{m'}f_m c_{k'm'} + \sum_{k,m}[\Delta(k)c^\dagger_{km}c^\dagger_{-k-m}+\text{H.c.}] , \qquad (1)$$

with $m=1,\ldots,N$. The conduction- and impurity-electron operators are denoted by c and f, respectively. We have added the last term, a simple BCS-like pairing of electrons on opposite sides of the Fermi sphere. The f-site occupancy constraint $n_f=\sum_m f^\dagger_m f_m=1$ enforces the correct commutation relations for the impurity spin operators. We now generalize the procedure of Read and Newns[15] to include superconducting correlations in the functional integral representation of (1). The saddle-point approximation to this theory is equivalent in the $N\to\infty$ limit to a mean-field theory of (1) with mean-field amplitude $\sigma=(J/N)\sum_{km}\langle c_m f^\dagger_m\rangle$ and Lagrange multiplier ϵ_f implementing the average constraint. It leads to the two equations

$$\frac{1}{N}=-\text{Im}\int_{-\infty}^{\infty}d\omega\, f(\omega)\tfrac{1}{2}\text{Tr}\{(\tau_0+\tau_3)\underline{G}_f(\omega+i0^+)\} , \qquad (2)$$

and

$$\frac{1}{J}=\text{Im}\int_{-\infty}^{\infty}d\omega\, f(\omega)\tfrac{1}{2}\text{Tr}\{(\tau_0+\tau_3)\underline{G}^0(k,\omega+i0^+)\times\underline{G}_f(\omega+i0^+)\} , \qquad (3)$$

where G^0 denotes the conduction electron Green's function in the pure superconductor and G_f is the full impurity Green's function, given by

$$\underline{G}_f^{-1}(\omega)=\omega\tau_0-\epsilon_f\tau_3-\underline{\Sigma}_f(\omega) .$$

Both are matrices in particle-hole space spanned by the Pauli matrices τ_i, and $\underline{\Sigma}_f(\omega)=\sigma^2\sum_k\underline{G}(k,\omega)$ is the impurity self-energy. In the normal state $\Delta\to 0$ Eqs. (2) and (3) were solved by Read and Newns,[15] leading to a Lorentzian impurity spectral density centered at ϵ_f, of width $\Gamma=\pi N_0\sigma^2$. This solution assumed a constant conduction-electron density of states $N(\omega)=N_0=1/2D$, $|\omega|<D$, giving rise to a characteristic energy scale

$$T_K=\sqrt{\Gamma^2+\epsilon_f^2}=D\exp(-1/N_0J) .$$

In the superconducting state, we must solve the full saddle-point equations (2) and (3) together with Dyson's equations for $\underline{G}_f$ and $\underline{G}$ as well as the gap equation

$$\Delta(k)=\int_{-\infty}^{\infty}d\omega\, f(\omega)\sum_{k'}V_{kk'}\text{Tr}\tfrac{1}{2}\{(\tau_1-i\tau_2)\underline{G}(k',\omega)\} . \qquad (4)$$

We focus first on the case of a single impurity, analogous to the case discussed by WF, except that the gap maximum in momentum space Δ_0 and the conduction-electron bandwidth D are here treated more generally as independent energy scales. We also consider the case of small N, despite the fact that Eqs. (2) and (3) are strictly valid only in the large-N limit. Here we adopt the point of view that, since the saddle point for $N=2$ is known to reproduce the correct analytic low-temperature normal-state behavior[12] of the f resonance, including its position at $\epsilon_f=0$, the $N=2$ theory will provide a good starting point for a description of the $T_K\gg T$ regime. For the superconducting order parameter we take for simplicity model p-wave states with lines ["polar", $\Delta(k)=\Delta_0\hat{k}_z$] and points of nodes ["axial", $\Delta(k)=\Delta_0(\hat{k}_x+i\hat{k}_y)$] on the Fermi surface, with densities of states varying at low energies $\omega\ll\Delta_0$ as ω and ω^2, respectively. The critical coupling J_c in this case[7] is now defined to be that J for which $\sigma=\epsilon_f=0$ is the only solution of Eqs. (2) and (3), with $G(k,\omega)$ replaced by $G^0(k,\omega)$. We note that to show that σ and ϵ_f always scale to zero together at the transition for $N<\infty$ requires a careful analysis of impurity bound states in $A_f(\omega)$, which occur in the gap and outside the band edges. It follows from this analysis and from Eq. (3) that J_c is independent of N. For the (unphysical) case $\Delta_0=D$ we recover the WF $r=1$ result, $J_c/D=1$, for the polar state, while for the axial state we find $J_c/D=1.44$. This differs slightly from the WF $r=2$ result $J_c/D=1.33$, as the axial density of states deviates from pure ω^2 behavior at larger energies. In the physical limit $\Delta_0\ll D$, we obtain $J_c\simeq 2D/\ln(2D/\Delta_0)$ for axial, polar, and isotropic s-wave states. In Fig. 1 we plot J_c vs Δ_0/D for all three states. It is worth noting that for typical narrow bandwidths in strongly correlated metals and superconducting transition temperatures of a few degrees, J_c is of the order of magnitude of experimentally deduced exchange constants in rare-earth–actinide systems. This leads to the possibility that the transition might be observed in heavy-fermion superconductors. Since for $T_K>T_{c0}$, $\Delta_0\to 0$ the system is always in the Kondo regime, decreasing temperature may drive the system through the transition.

We have also investigated the existence of bound states in the gap analogous to those discussed in an earlier work[14] on s-wave superconductors in the low-temperature regime. The T matrix for conduction-electron scattering is simply $\underline{T}(\omega)=\sigma^2\underline{G}_f(\omega)$; thus the position ω_B of the bound states in the p-wave case is found by solving

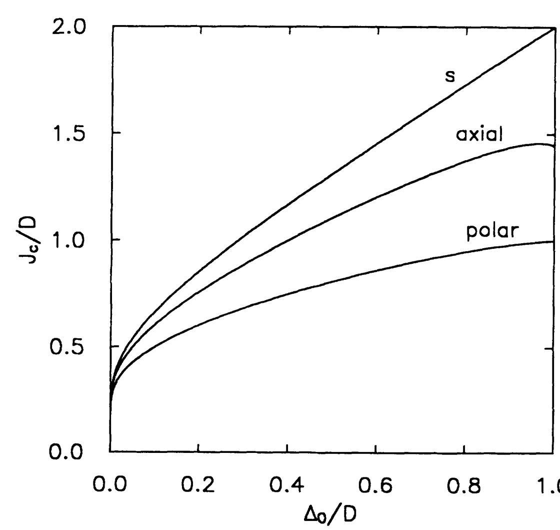

FIG. 1. Critical coupling J_c/D for one impurity vs the amplitude of the scaled order parameter Δ_0/D.

$$\omega+\Gamma\,\mathrm{Re}\left\langle\frac{\omega}{\sqrt{\Delta^2(k)-\omega^2}}\right\rangle_{\hat{k}}=\pm\epsilon_f\ . \tag{5}$$

For $T_K \gg \Delta_0$, $|\omega_B|\to\Delta_0$ and the bound states disappear into the gap edge, except for the case $N=2$, where $\epsilon_f=0$ and the bound state always sits at the center of the gap. In the opposite limit, $T_K \ll \Delta_0$, all bound states approach the center of the gap. In the s-wave case, the results for all N are qualitatively similar to the $N>2$ p-wave case, in agreement with the result of Ref. 14 for $T_{c0}\lesssim T_K$. For $T_{c0}/T_K\to\infty$ the high-temperature theory[13] predicts that the bound states approach the gap edge. It is interesting to note that the fixed position of the $N=2$, p-wave bound state at the center of the gap agrees with the results of phenomenological approach,[10,11] and will obtain more generally whenever the off-diagonal part of the impurity self-energy $\underline{\Sigma}_f$ vanishes for symmetry reasons (as in odd-parity states).

To study the case of finite impurity concentrations, we calculate self-consistent Green's functions averaged over impurity positions in the usual way, leading to $\underline{G}_f^{-1}(\omega)=\bar{\omega}\tau_0-\epsilon_f\tau_3$ and $\underline{G}^{-1}(\omega)=\tilde{\omega}\tau_0-\epsilon_k\tau_3-\Delta(k)\tau_1$, where

$$\tilde{\omega}=\omega+\Gamma\langle\tilde{\omega}/[\Delta^2(k)-\tilde{\omega}^2]^{1/2}\rangle_{\hat{k}}$$

and

$$\bar{\omega}=\omega+a\Gamma\bar{\omega}/(-\bar{\omega}^2+\epsilon_f^2)\ .$$

Here $a=\bar{n}T_{c0}N/2\pi$, and $\bar{n}=n/T_{c0}N_0$ is the scaled impurity concentration. In general, G_f^{-1} and G^{-1} will also contain additional off-diagonal renormalizations, which vanish in the p-wave case considered here. We have obtained self-consistent numerical solutions to the coupled system of Eqs. (2)–(4) together with Dyson's equations for the averaged propagators, which we now use to calculate the critical exchange coupling, as well as various thermodynamic properties of the superconducting state.

For $\bar{n}>0$, the bound states in the gap discussed above acquire a finite width and should be observable as resonances in the conduction-electron density of states close to the bound-state positions ω_B determined by Eq. (5). In Fig. 2 we show the $N=2$ density of states for axial and polar states. The sharpness of the bound states is seen to increase with T_{c0}/T_K. We note that although the scattering phase shift in the present theory, $\delta(\omega)=-\arg(\underline{G}_f^{-1})^{11}(\omega+i0^+)$, is strongly energy dependent, in the limit $T_{c0}\lesssim T_K$ the resulting density of states is quite similar to the phenomenological theories of Refs. 10 and 11, assuming $\delta(0)\simeq\pi/2$. In the insets of Figs. 2 we have plotted for comparison the f spectral densities in both cases; we see that removing conduction-electron states from the vicinity of the Fermi level has the effect of narrowing $A_f(\omega)$, or effectively decreasing the Kondo temperature.

An interesting consequence of the self-consistent treatment of impurity scattering is that the conclusions of WF regarding the existence of a critical exchange coupling J_c based on a single-impurity analysis are modified. It is clear from physical considerations or from Eqs. (2) and (3) that the Kondo effect occurs for all $J>0$ whenever the density of states at the Fermi level $N(0)$ is finite. Since in the polar state any finite impurity concentration $\bar{n}$ may be shown to lead self-consistently to $N(0)>0$, as also found in Refs. 9–11, the transition discussed by WF does not take place. This may easily be seen by solving the equations for $\tilde{\omega}$ and $\bar{\omega}$ at $\omega=0$, with $\mathrm{Im}\tilde{\omega}(0)>0$. A closer analysis shows that $J_c=0$ for all superconducting states with density of states $N(\omega)\sim|\omega|^r$ for $\omega\ll\Delta_0$, $r\le 1$. In the axial state ($r=2$), and indeed for any state with $1<r<\infty$, the cases $N=2$ and $N>2$ are qualitatively different. If $N>2$, a critical concentration is required to create a gapless state $N(0)>0$, and thus drive $J_c\to 0$. However, when the bound state is located exactly at the Fermi surface ($N=2,\epsilon_f=0$), we find again a finite density of states $N(0)$ for any finite concentration. These results are also in accord with earlier studies,[10,11] where the phenomenological phase shift δ_0 is crudely given here by $\cot^{-1}\epsilon_f/\Gamma$.

Finally, we discuss the suppression of the critical temperature T_c with impurity concentration $\bar{n}$. This is calculated in the usual way by solving the gap equation (4) at T_c together with Eqs. (2) and (3) for the normal state. The results are presented in Fig. 3 for both p-wave states considered. For $T_K\lesssim T_{c0}$, we obtain reentrant behavior in $T_c(\bar{n})$ similar to that found by earlier theories of s-wave superconductors.[3] However, we note that the large-N mean-field-theory approach applied here cannot be expected to describe the temperature-dependent polar-

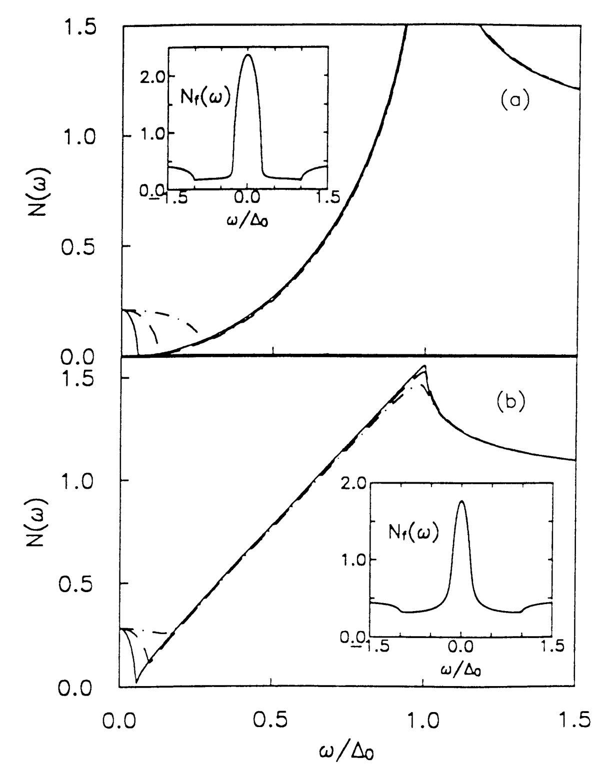

FIG. 2. Density of states for conduction electrons, (a) axial, (b) polar state for $N=2$ and $T_K/T_{c0}=0.3$ (solid line), 1 (dashed line), and 20 (dash-dotted line). The inset shows the impurity spectrum for $T_K/T_{c0}=20$ in both (a) and (b). The scaled impurity concentration was chosen to be $\bar{n}=0.2$.

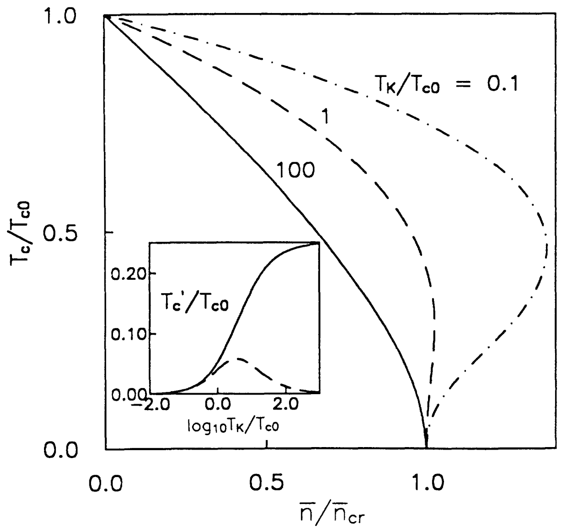

FIG. 3. Suppression of the critical temperature as a function of impurity concentration for different values of T_K/T_{c0} and $N=2$. The lines represent $T_K/T_{c0}=0.1$ (dash-dotted line), 1 (dashed line), and 100 (full line). Concentration is scaled to the critical concentration at $T=0$. The inset presents the slope of T_c suppression at T_{c0}, for $N=2$, for both the p-wave (full line) and the s-wave (broken line) states.

ization of the Kondo singlet and the crossover to local moment behavior. We therefore do not obtain the Abrikosov-Gor'kov result for $T_K \ll T_{c0}$, and the $T_K/T_{c0}=0.1$ curve shown in Fig. 3 may be taken seriously only for $T_c/T_{c0}<0.1$. In the opposite limit $T_K \gg T_{c0}$ the form of the T_c suppression is identical to that found by Abrikosov and Gor'kov[2] with renormalized energy-independent pair-breaking parameter $\bar{n}N\Gamma^2/(2\pi T_K)^2$; this result must obtain simply because the theory in this limit describes pair-breaking by resonant potential scatterers in the p-wave superconducting state, as discussed in Refs. 10 and 11. In the inset of Fig. 3, we show the normalized slope $T_c'(\bar{n}=0)/T_{c0}$ for both s- and p-wave cases. We note that the much larger T_c depression in the Fermi-liquid regime for the p-wave states is again due to an absence of an "Anderson theorem"[1] for p-wave superconductors.

Our results suggest that the transition discussed by WF might be observable in ordinary superconductors doped with Kondo impurities with spin degeneracy $N>2$, e.g., Ce. For $N=2$ we have shown that effective Kondo temperature in the superconducting state is reduced but never vanishes. Nevertheless, in relatively clean systems deviations in thermodynamic properties per impurity from those of the pure superconductor may be qualitatively similar to what one might expect from a WF-type analysis if the effective T_K is driven to zero. The theory presented here provides an easily tractable framework to calculate such properties, as well as transport coefficients, in the superconducting state. Furthermore, it improves upon phenomenological theories[10,11] by including a Kondo impurity description of the energy dependence of scattering phase shifts. We will present the results of a detailed numerical evaluation of thermodynamic properties of doped s- and p-wave superconducting states in a later work.

Heavy-fermion superconductors, which are thought to have unconventional order parameters,[8] are dense lattices of Kondo ions rather than weakly interacting superconductors with dilute magnetic impurities as discussed here. It has been nevertheless suggested[16] that nonmagnetic impurities may be treated as scattering centers with the phase shift close to the unitarity limit relative to the host lattice. Our results may therefore be relevant to these systems. On the other hand, it is clear that normal-state coherence effects require a more sophisticated treatment of the problem of a defect in a Kondo lattice. A final justification of the applicability of the theory presented here to dense heavy-fermion systems requires microscopic studies of the lattice problem.

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