Phase Transitions in Gapless Fermi Systems with Magnetic Impurities

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We consider a model of a Kondo-like impurity interacting with a band of fermions for which the density of states is zero or small near the Fermi energy. Renormalization-group arguments and a large-degeneracy technique are used to demonstrate that this model has a nontrivial zero-temperature phase transition at a finite coupling constant, in contrast to the zero-coupling-constant transition of the ordinary Kondo model. Possible experimental realizations of this model include anisotropic superconductors, narrow-gap semiconductors, and systems with flux phases.

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It is well known that the dramatic low-temperature properties (Kondo effect) associated with interaction between band electrons and magnetic impurities appear only when the density of states is nonzero (metallic) at the Fermi energy. In insulators and semiconductors the density of states vanishes in a finite energy gap containing the Fermi energy, and the full Kondo effect is not seen since electronic excitations are frozen out at low temperatures. Between these extremes, however, is an interesting marginal or "gapless" case for which the density of states vanishes at a point (infinitely narrow gap) near the Fermi energy. In this paper we study a simple model of a Kondo impurity interacting with a *gapless* band of electrons. We show that the model has a nontrivial zero-temperature critical point at a finite value J_c of the coupling constant, and that a Kondo effect occurs only for $J > J_c$, in contrast to the usual Kondo model for which $J_c = 0$. Near the critical point we study the properties of the model as a function of magnetic field and chemical potential and predict a difference between the crossover behavior of this model and that of the usual Kondo model.

A variety of materials are thought to have a gapless excitation spectrum. In bulk semiconductors this situation can occur when the valence and conduction bands touch at symmetry points of the Brillouin zone, such as the L points of fcc lattices. For example, α-Sn is gapless under appropriate conditions,[1] and certain tertiary semiconductors such as $Pb_{1-x}Sn_xTe$ can be gapless at a critical composition.[2] If the bands cross, the gap is almost linear and the electrons behave as if they were relativistic massless particles moving at the Fermi velocity. This situation arises in the latter example as well as in domain walls of PbTe,[3] in PbTe-SnTe heterojunctions,[4] and in graphite. The density of states then behaves like $|\epsilon|^{d-1}$.

The single-particle excitations in anisotropic superconductors are also gapless, and it has been argued that heavy-fermion materials may be physical realizations of such a system.[5] Coupling between magnetic impurities and these excitations could provide an interesting direct probe of the nature of the gap. Magnetic impurities are also known to interfere with superconductivity,[6] but the description suggested here should apply if the superconducting condensate is rigid enough to persist at least partially at the impurity site. In these systems, the gap vanishes at points or lines in the Brillouin zone, and the density of states behaves like $|\epsilon|^{d-1}$ near the gap[7] (axial) and like $|\epsilon|^{d-2}$ (polar).[8] Other possible candidate systems are the conjectured "flux phases" of models of strongly correlated systems.[9]

In all of these cases the density of states is proportional to $|\epsilon|^r$ with $r = 0$, $\frac{1}{2}$, 1, or 2 for physical dimensionalities. As a simple model the density of states $\rho(\epsilon)$ will here be taken to be

$$\rho(\epsilon) = C|\epsilon|^r, \text{ if } |\epsilon| < D, \tag{1}$$

where D is a large band cutoff. Although this approximation ignores the asymmetry across the gap which exists, for example, in most semiconductors,[2] the qualitative results are nevertheless expected to be reliable. Also, in realistic situations the parameter r need not equal any of the values listed above,[10] but the listed values certainly suggest the correct range.

Scaling.—A primary motivation for studying the Kondo model with a gapless density of states is that the scaling properties of such a model are significantly different from those of the model with a constant density of states. The difference can be demonstrated using a simple generalization of the "poor-man's-scaling" method introduced by Anderson.[11] Consider the spin-$\frac{1}{2}$ Kondo model for gapless band electrons

$$H = \sum_k \epsilon_k (c_{k\uparrow}^\dagger c_{k\uparrow} + c_{k\downarrow}^\dagger c_{k\downarrow}) + \tfrac{1}{2} J \sum_{kk'} (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}) S_z + \tfrac{1}{2} J \sum_{kk'} (c_{k\uparrow}^\dagger c_{k'\downarrow} S^- + c_{k\downarrow}^\dagger c_{k'\uparrow} S^+) \tag{2}$$

with a density of states $\rho(\epsilon)$ given by Eq. (1). The influence of band electrons having energies within δE of the cutoffs can be accounted for approximately using a generalization of the Rayleigh-Schrödinger perturbation theory to obtain an effective Hamiltonian for the remaining degrees of freedom. The effective Hamiltonian is characterized by a cutoff $D' = D - \delta E$ and an effective

coupling constant J_{eff} given by

$$J'=J+\rho(-D)J^2\delta E/D+\cdots . \tag{3}$$

Rescaling to restore the cutoff and the density of states can be accomplished by first noting that the density of states is proportional to volume and the coupling constant is inversely proportional to volume. When the density of states is given by Eq. (1), the number of band electron states is $2CD^{r+1}/(r+1)$. The original number of states can be restored if the unit of length scaled by a factor of $(D/D')^{r+1}$. With this rescaling the coupling constant changes by the inverse of the same factor. The cutoff can be restored if physical quantities with units of energy, including the coupling constant, are increased by a factor of D/D'. The renormalized coupling constant J_R is then

$$J_R=(D'/D)^r J'\approx J+J(JCD^r-r)\delta E/D . \tag{4}$$

The most significant difference between this expression and the standard result[11] is that, in addition to the fixed points at $J=0$ and ∞, there is a new infrared unstable fixed point at $J_c=r/CD^r$, neglecting terms beyond J^2. For $J>J_c$ the effective coupling flows towards the strong-coupling fixed point and we find a standard Kondo effect, but for $0<J<J_c$, low-temperature behavior of the model is controlled by the $J=0$ fixed point and no Kondo effect is seen.

Large-N limit.—The results of the previous section can be confirmed and extended by considering the large-degeneracy [SU(N)] version of the same model, which we write here as

$$H=\sum_{km}\epsilon_{km}c^\dagger_{km}c_{km}+\frac{J}{N}\sum_{kk'}\sum_{mm'}c^\dagger_{km}f^\dagger_{m'}f_m c_{k'm'} , \tag{5}$$

where $m=1,\ldots,N$. The impurity spin operators have been represented here by the pseudofermion operators $f^\dagger_{m'}$ and f_m together with the constraint of single occupancy

$$n_f\equiv\sum_m f^\dagger_m f_m=1 , \tag{6}$$

where n_f is the occupancy of the impurity site. Several years ago, Read and Newns[12] introduced a path-integral method for obtaining a $1/N$ expansion for this model. In this method, a Stratonovich-Hubbard transformation is used to eliminate the four-fermion term in favor of a path integral over an auxiliary Bose field σ. An integral over a variable λ is used to enforce the constraint. The fermionic fields then occur only in a quadratic exponent and can be integrated out in closed form leaving a path integral over σ and an integral over λ to be evaluated. A $1/N$ expansion can then be obtained from a saddle-point expansion for these integrals. Here we will consider only the $N\rightarrow\infty$ limit and will therefore only be studying the extrema of the integrand.

The maximum of the integrand as a function of σ turns out to occur for a constant value σ_0 of the function σ, and the $N\rightarrow\infty$ partition function can be written in the form $Z=\exp(-\beta V)$, where

$$V=\frac{N}{J}\sigma_0^2-\epsilon_F-N\int\frac{d\epsilon}{1+e^{\beta\epsilon}}\frac{1}{\pi}\cot^{-1}\left(\frac{-\epsilon+\epsilon_F-P\int C|\epsilon'|^r d\epsilon'/(\epsilon'-\epsilon)}{\pi C|\epsilon|^r\sigma_0^2}\right) \tag{7}$$

and ϵ_F parametrizes the position of the saddle point of the λ (constraint) integral. Physically, ϵ_F corresponds to the position of the Kondo resonance relative to the Fermi energy, and $\pi\rho(\epsilon_F)\sigma_0^2$ characterizes the width of the resonance. Values for σ_0 and ϵ_F can then be obtained by solving the simultaneous equations

$$\partial V/\partial\epsilon_F=0 \tag{8}$$

and

$$\partial V/\partial\sigma_0=0 . \tag{9}$$

At zero temperature these equations become

$$0=\frac{\partial V}{\partial\epsilon_F}=-N\left(\frac{1}{N}-\int_{-D}^{0}\frac{C|\epsilon|^r\sigma_0^2 d\epsilon}{(\pi C|\epsilon|^r\sigma_0^2)^2+[-\epsilon+\epsilon_F-\sigma_0^2P\int C|\epsilon'|^r d\epsilon'/(\epsilon'-\epsilon)]^2}\right) \tag{10}$$

and

$$0=\frac{\partial V}{\partial\sigma_0}=N\sigma_0\left(\frac{1}{J}-\int_{-D}^{0}\frac{C|\epsilon|^r(-\epsilon+\epsilon_F)d\epsilon}{(\pi C|\epsilon|^r\sigma_0^2)^2+[-\epsilon+\epsilon_F-\sigma_0^2P\int C|\epsilon'|^r d\epsilon'/(\epsilon'-\epsilon)]^2}\right) . \tag{11}$$

One immediate solution to the second equation is $\sigma_0=0$. Since all interactions are mediated by the field σ, stability of this solution would imply that the impurity is decoupled from the band electrons within mean-field theory, and corresponds to the perturbative regime of the model. The phase transition to an interacting state is signaled by the appearance of an additional solution at a nonzero value of σ_0.

Near the phase transition a solution to the saddle-point equations is expected at a small but nonzero value of σ_0. In this region Eq. (11) has a solution only if ϵ_F is also small, and at the transition σ_0 and ϵ_F must go to zero together in such a way that Eq. (10) remains satisfied. The critical value of the coupling constant can be determined by substitut-

ing $\sigma_0=\epsilon_F=0$ into Eq. (11) to obtain $1/J_c=CD^r/r+O(1/N)$ to within corrections which vanish when D is large. This result has more general validity than the prediction of poor man's scaling since it is nonperturbative and therefore not restricted to the limit of small J.

Let us now consider the scaling properties of the system in the large-N limit. It will suffice to consider the saddle-point equations. The divergences which arise in the $D\rightarrow\infty$ limit turn out to depend crucially on the value of r. For $0<r<1$ the principal-value integral in Eqs. (10) and (11) is

$$P\int\frac{C|\epsilon'|^r d\epsilon'}{\epsilon'-\epsilon}=\pi C|\epsilon|^r\tan\left(\frac{\pi r}{2}\right)\mathrm{sgn}(\epsilon) \tag{12}$$

up to corrections which vanish in the $D\rightarrow\infty$ limit. If the density of states is constant then $r=0$ and this term can be dropped. Equation (10) is convergent for $r<1$, and Eq. (11) contains a divergence of order D^r which will be absorbed into a definition of the crossover temperature. For $r\geq 1$ both the principal-value integral and Eq. (10) contain a divergence of order D^{r-1} which is discussed below.

The leading divergence in Eq. (11) can be canceled by subtracting the same equation at the critical point

$$\int_{-D}^{0}d\epsilon\left[C\epsilon^{r-1}-\frac{C|\epsilon|^r(-\epsilon+\epsilon_F)}{(\pi C|\epsilon|^r\sigma_0^2)^2+[-\epsilon+\epsilon_F+\pi C|\epsilon|^r\sigma_0^2\tan(\pi r/2)]^2}\right]=\frac{1}{J_c}-\frac{1}{J}\equiv\frac{CT_0^r}{r}, \tag{13}$$

where T_0 sets the energy scale of the problem and in fact reduces to the usual Kondo result $T_K=D\exp(-1/\rho JN)$ at $r=0$. The integral is then convergent for $D\rightarrow\infty$, provided $r<\frac{1}{2}$. For $r\geq\frac{1}{2}$ the integral in Eq. (13) contains an uncanceled divergence which diverges like $\ln D$ for $r=\frac{1}{2}$ and like D^{2r-1} for $r\geq\frac{1}{2}$. This divergence can be absorbed into a renormalized value of σ_0^2, and ϵ_F must then also be renormalized in such a way as to satisfy Eq. (10). A similar renormalization applies to the divergences mentioned above which appear for $r\geq 1$.

Return for simplicity to the case $r\leq\frac{1}{2}$, and consider the limit of small n_F/N. In this region Eq. (10) can be approximated by

$$\frac{n_F}{N}\approx\frac{\pi r}{\sin(\pi r)}\frac{C\epsilon_F^r\sigma_0^2}{\epsilon_F} \tag{14}$$

from which it is seen explicitly that ϵ_F and σ_0 go to zero together at the transition. For present purposes σ_0^2 can be neglected in Eq. (11) to obtain

$$\frac{CT_0^r}{r}\approx\frac{\pi}{\sin(\pi r)}C\epsilon_F^r. \tag{15}$$

Thus we find

$$\epsilon_F\approx T_0[\sin(\pi r)/\pi r]^{1/r} \tag{16}$$

and

$$\Delta\equiv\pi CT_0^r\sigma_0^2\approx T_0\left(\frac{n_f}{N}\right)\pi r\left(\frac{\sin(\pi r)}{\pi r}\right)^{1/r-1} \tag{17}$$

which should be compared with the standard Kondo results[12]

$$\epsilon_F=T_K\cos(\pi/N) \tag{18}$$

and

$$\pi\rho\sigma_0^2=T_K\sin(\pi/N). \tag{19}$$

In both cases the resonance at ϵ_F is of order T_0 from the Fermi energy, as expected. Note also that the resonance width Δ is smaller than ϵ_F by a factor of $1/N$ and is proportional to the density of states near the resonance.

Magnetic field and chemical potential.—The phase transition discussed here exists only if the zero in the density of states occurs *exactly* at the Fermi energy, since any finite density of states at the Fermi energy will lead to the smooth crossover associated with the ordinary Kondo effect. This rounding of the phase transition can be seen explicitly in the current model by introducing a nonzero chemical potential μ to move the Fermi energy away from the center of the band. The resultant model is probably a more realistic representation of actual materials whenever the density of states at the Fermi energy is small but nonzero.

The chemical potential corresponds to the upper limit of integration in Eqs. (10) and (11), which therefore become

$$\frac{n_F}{N}=\int_{-D}^{\mu}\frac{C|\epsilon|^r\sigma_0^2 d\epsilon}{(\pi C|\epsilon|^r\sigma_0^2)^2+[\epsilon_F-\epsilon-\sigma_0^2C|\epsilon|^r\tan(\pi r/2)\mathrm{sgn}(\epsilon)]^2} \tag{20}$$

and

$$\frac{1}{J}=\int_{-D}^{\mu}\frac{C|\epsilon|^r(\epsilon_F-\epsilon)d\epsilon}{(\pi C|\epsilon|^r\sigma_0^2)^2+[\epsilon_F-\epsilon-\sigma_0^2C|\epsilon|^r\tan(\pi r/2)\mathrm{sgn}(\epsilon)]^2}. \tag{21}$$

When μ is nonzero Eq. (21) has a solution for any positive value of J, and the critical coupling constant is therefore $J=0$ as in the usual Kondo model. If J is small, Eq. (21) implies that σ_0^2 and $\epsilon_F-\mu$ must also be small, which implies that the resonance becomes narrower and follows the Fermi energy when the coupling constant is small.

The chemical potential provides the problem with an additional energy scale, and several possible behaviors might be expected. The effective crossover energy should be determined by an average of the density of states near the energy

scale of interest. For very high energies this average density of states is an increasing function of energy, so the effective crossover energy will also increase and the approach to the high-energy limit should be correspondingly slower. At low energies the average density of states is constant and relatively small, so the model could be well into the high-energy regime before this increase in the effective crossover energy begins. If $J < J_c$, this should always be true, but the slowing of the approach to the high-energy limit might appear earlier if μ is smaller than the effective T_0 at the beginning of the increase.

A magnetic field can be introduced by adding a Zeeman term to the Hamiltonian to scan the energy scales of the model and study the crossover behavior. When $\mu=0$ and $J > J_c$ the magnetization saturates at a finite value of the magnetic field. As an example consider the case in which the magnetic field splits the degeneracy into two $N/2$-fold degenerate levels.[13] Equation (13) then becomes

$$\frac{CT_0^r}{r}=\frac{1}{2}\int_{-D}^{0}d\epsilon\, C|\epsilon|^r\left[\frac{2}{\epsilon}-\frac{\epsilon_F+h-\epsilon}{(\pi C|\epsilon|^r\sigma_0^2)^2+[\epsilon_F+h-\epsilon+\sigma_0^2 C|\epsilon|^r\tan(\pi r/2)]^2}\right.$$
$$\left.-\frac{\epsilon_F-h-\epsilon}{(\pi C|\epsilon|^r\sigma_0^2)^2+[\epsilon_F-h-\epsilon+\sigma_0^2 C|\epsilon|^r\tan(\pi r/2)]^2}\right], \tag{22}$$

which is adequate for $r < \frac{1}{2}$. At the saturation point the lowest-energy level magnetizes completely. This point is signaled here by $\sigma_0^2 \to 0$ and $\epsilon_F \to 0$, and Eq. (22) then becomes

$$CT_0^r/r=\tfrac{1}{2}\int_0^\infty d\epsilon\,\epsilon^{r-1}/(\epsilon+2h_c), \tag{23}$$

which can be solved for

$$h_c=\tfrac{1}{2}T_0[2\sin(\pi r)/\pi r]^{1/r}, \tag{24}$$

where h_c is the field at saturation. Note that the smooth crossover of the usual Kondo model is recovered since $h_c \to \infty$ as $r \to 0$.

If $\mu \neq 0$, it is found numerically that the model magnetizes smoothly in much the same way as the ordinary Kondo model. The size of the field in the crossover region is related to $\epsilon_F-\mu$ at zero field, which plays the role of the Kondo energy scale. When n_F/N is small, σ_0^2 is also small. After a subtraction like that in Eq. (13) we find

$$\frac{CD^r}{r}-\frac{C\mu^r}{r}-\frac{1}{J}=\int_\mu^D\frac{C|\epsilon|^{r-1}d\epsilon}{\epsilon_F+\epsilon}. \tag{25}$$

In the $J \to 0$ limit the logarithmic behavior of the integral in Eq. (25) for ϵ near $-\epsilon_F$ dominates to give

$$T_0\equiv\epsilon_F-\mu\approx\mu\exp\left[\frac{1}{r}\left(\frac{D}{\mu}\right)^r-\frac{1}{r}-\frac{1}{C\mu^r J}\right], \tag{26}$$

which is to be compared with $T_K=De^{-1/\rho J}$ for the ordinary Kondo problem. Note in particular that the crossover temperature contains in both cases the factor $e^{-1/\rho(\mu)J}$, where $\rho(\mu)$ is the density of states at the Fermi energy.

In this paper we have studied the phase transitions at zero temperature of a gapless Fermi system coupled to a single magnetic impurity. We have shown that for systems with a bare density of states of the form $\rho(E)\approx E^r$, with $r>0$, there is no Kondo effect for weak values of the coupling constant J. For $J > J_c$ we find a nonvanishing Kondo temperature T_0 and a singlet ground state. The Kondo temperature T_0 is found to vanish at J_c like $T_0 \approx |J-J_c|^\nu$, with $\nu=1/r$. We also studied the crossovers both in an external magnetic field and in chemical potential. We find a rich spectrum of possible behaviors. Typically, away from the degeneracy points, a standard Kondo effect is seen. However, as the degenerate limit is reached by lowering the chemical potential, the Kondo scale is seen to drop to zero for $J < J_c$ and to reach a limiting nonzero value for $J > J_c$. At J_c we find a critical point with anomalous dimensions. A similar behavior is seen in the presence of external magnetic fields.

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