THE KONDO EFFECT IN A SYSTEM WITH A SINGULAR DENSITY OF STATES

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ABSTRACT

In a number of fermion systems, the quasiparticle density of states varies near the Fermi energy like $|E - E_F|^r$, where $r = 1$ or 2. The effect of magnetic impurities in such systems is studied via a perturbative renormalization-group treatment of the n-channel Kondo model, carried out to third order in the antiferromagnetic exchange coupling J. For $0 < r < 1/2n$, a (multichannel) Kondo effect occurs only if J exceeds a critical value $J_c(r)$; otherwise the impurity moment decouples from the Fermi sea at low temperatures. For $r > 1/2n$, the exchange always renormalizes to zero, whatever the value of J. Strictly, this analysis is valid only in the limits $r \ll 1$ and $n \gg 1$. Extension to the conventional Kondo model ($n = 1$) and larger r is discussed.

1. Introduction

The remarkable properties known as the Kondo effect resulting from an antiferromagnetic exchange interaction between a magnetic impurity and the conduction electrons in a non-magnetic metal depend crucially on the presence of electronic excitations down to arbitrarily small energy scales. Thus, systems with energy gaps cannot exhibit a full Kondo effect. However, there is an interesting marginal case in which the density of states vanishes right at the Fermi energy E_F, but not any other energy in the vicinity of E_F. This situation arises in certain semiconductors in which the valence and conduction bands touch at symmetry points in the Brillouin zone, leading to a density of states varying like $|\epsilon|^{d-1}$ in d spatial dimensions. Examples include $Pb_{1-x}Sn_xTe$ at a suitably chosen composition,[1] and PbTe-SnTe heterojunctions.[2] Gapless excitations can also occur in unconventional superconductors, in which the density of states may vary as $|\epsilon|^{d-2}$ or $|\epsilon|^{d-1}$ near line or point nodes in the gap. Candidates for this behavior are the heavy-fermion superconductors UBe_{13}, UPt_3, URu_2Si_2, and $CeCu_2Si_2$. Finally, a density of states varying as $|\epsilon|$ has been proposed for certain models of strongly correlated electrons.[3]

The properties of magnetic impurities in gapless systems were first studied by Withoff and Fradkin,[4] who considered the density of states

$$\rho(\epsilon) = \begin{cases} C|\epsilon|^r & \text{if } |\epsilon| \le D_0, \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

Here $\epsilon = E - E_F$ is the energy measured from the Fermi level. Using poor-man's scaling for the spin-$\frac{1}{2}$ Kondo model and a large-orbital degeneracy treatment of the Coqblin-Schrieffer model, these authors showed that a novel, unstable fixed point appears at a critical value of the antiferromagnetic exchange coupling between the impurity and the electrons: $J = J_c$. A Kondo effect occurs only for $J > J_c$, while for $J < J_c$, the impurity moment asymptotically decouples from the conduction band. If the zero in the density of states is shifted slightly from the Fermi energy, the system reverts to conventional Kondo physics governed by the small density of states $\rho(0)$.

In this paper I extend the perturbative renormalization-group (RG) treatment to the n-channel Kondo model.[5] At second order in J, Withoff and Fradkin's result is recovered. However, if $2nr$ approaches unity, third-order corrections become significant. Indeed, at $2nr = 1$, the unstable fixed point J_c merges with a stable fixed point J^* which evolves from the overscreened fixed point of the $r = 0$ multichannel Kondo model.[5] For $2nr > 1$, both these fixed points vanish, and the only stable fixed point occurs at $J = 0$. In this case there is complete suppression of the Kondo effect. Although these perturbative results are strictly valid only in the limit of large n and small r, non-perturbative calculations[6] suggest a wider range of applicability.

2. Derivation of the RG Equation

The n-channel Kondo Hamiltonian[5] can be written in the dimensionless form $\tilde{H} = \tilde{H}_0 + \tilde{H}_I$, where

$$\tilde{H}_0 = \sum_{j,\sigma} \int_{-1}^{1} dx\, x\, c^\dagger_{xj\sigma} c_{xj\sigma} \tag{2}$$

and

$$\tilde{H}_I = \sum_{j,\sigma,\sigma'} \tfrac{1}{2} \boldsymbol{\sigma}_{\sigma\sigma'} \cdot \mathbf{S} \int_{-1}^{1} dx \int_{-1}^{1} dx'\, \tilde{J}(x,x') c^\dagger_{xj\sigma} c_{x'j\sigma'}. \tag{3}$$

Here $x = (E - E_F)/D_0$, the reduced energy measured from the Fermi level, falls in the range $-1 \le x \le +1$. The operator $c^\dagger_{xj\sigma}$ $[c_{xj\sigma}]$ creates [annihilates] an s-wave state of reduced energy x and spin z-component σ belonging to channel j $(1 \le j \le n)$; the set of all such operators obeys the standard anticommutation relation $\{c^\dagger_{xj\sigma}, c_{x'j'\sigma'}\} = \delta(x - x')\delta_{jj'}\delta_{\sigma\sigma'}$. The impurity has spin $S = \frac{1}{2}$. The conduction band density of states $\rho(xD_0)$ and the Kondo coupling $J(x,x')$ enter only through the dimensionless combination $\tilde{J}(x,x') = J(x,x')\sqrt{\rho(xD_0)\rho(x'D_0)}$. For simplicity, I shall take $\tilde{J}$ to have the form, derived from Eq. (1),

$$\tilde{J}(x,x') = \begin{cases} \tilde{J}_0\, |xx'|^{r/2} & \text{if } |x|, |x'| \le 1, \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

The RG approach consists of repeated application of the following two-stage transformation: (1) Integrate out all conduction electrons with energies $D < |E - E_F| \le D_0$. Defining $t = \ln(D_0/D)$ — which will be seen to be a natural parameter for the transformation — one obtains an effective Hamiltonian containing only impurity degrees of freedom plus electrons with $|x| \le e^{-t}$. By construction, this Hamiltonian preserves some physical quantity such as the T-matrix,[7] an invariant vertex function[8] or the partition function.[9] (2) Multiply all energies by a factor e^t to restore the conduction band cutoff to ± 1. This transformation produces a new Hamiltonian $\tilde{H}(t) = \tilde{H}_0 + \tilde{H}_I(t)$ in which dimensionless couplings involving impurity degrees of freedom — in this case the $\tilde{J}(x,x')$'s —may acquire renormalized values. In addition, completely new terms may appear in $\tilde{H}(t)$ that have no counterpart in $\tilde{H} \equiv \tilde{H}(0)$. It is known, however, that for the Kondo Hamiltonian such terms are irrelevant (i.e., they decrease in importance upon repeated application of the transformation).

In carrying out step (1) above, I have chosen to follow the thermodynamic scaling procedure of Krishna-murthy and Jayaprakash,[9] in which $\tilde{H}(t)$ and $\tilde{H}(0)$ are related by the requirement

$$\mathrm{Tr}\exp[-\beta\tilde{H}(t)] - \mathrm{Tr}\exp[-\beta\tilde{H}(0)] = \mathcal{O}(e^{-\beta D}).$$

Let us focus on those conduction electrons which determine the low-temperature physics. One finds after considerable algebra that, for $|x|, |x'| \ll 1$, integrating out the high-energy electrons yields an effective impurity Hamiltonian of the same form as $\tilde{H}_I$, but with

$$\tilde{J}_0 \equiv \tilde{J}(x,x')/|xx'|^{r/2} \to \tilde{J}_0 + (e^{-rt}/r)(1-e^{-rt})\tilde{J}_0^2 + \alpha_r(t)\tilde{J}_0^3 + \mathcal{O}(\tilde{J}_0^4), \tag{5}$$

where $\alpha_r(t)$ is a fairly complicated function even for $r = 0$.

In order to complete the RG transformation, the energy scale is multiplied by $e^t = D_0/D$. Thus, one defines

$$\tilde{x} = |E - E_F|/D = e^t x \qquad \text{and} \qquad \tilde{c}_{\tilde{x}\sigma} = e^{-t/2} c_{x\sigma},$$

the normalization of the new operators being chosen so that $\{\tilde{c}^\dagger_{\tilde{x}\sigma}, \tilde{c}_{\tilde{x}'\sigma'}\} = \delta(\tilde{x}-\tilde{x}')\delta_{\sigma\sigma'}$. Substituting these new variables into Eqs. (2) and (3), then multiplying by e^t and reducing the range of all integrals to $-1 \le x \le +1$, one finds that the terms in $\tilde{H}(0)$ for $|\tilde{x}|, |\tilde{x}'| \ll 1$ have precisely the same form as in $\tilde{H}(t)$, provided that a factor of e^{-rt} is absorbed into the dimensionless coupling. Thus, the overall effect of the RG transformation is

$$\tilde{J}_0 \to \tilde{J}(t) = e^{-rt}\left[\tilde{J}_0 + (e^{-rt}/r)(1-e^{-rt})\tilde{J}_0^2 + \alpha_r(t)\tilde{J}_0^3\right] + \mathcal{O}(\tilde{J}_0^4), \tag{6}$$

From Eq. (6), one can obtain a differential equation for $\tilde{J}$. Great care must be taken, though, because the coupling $\tilde{J}$ is just one of an infinite family of coefficients related to the set $\tilde{J}(x,x')$. Equation Eq. (6) indicates that for small r, $\tilde{J}$ is the coefficient of a weakly irrelevant operator (which becomes marginal at $r = 0$). This turns out to be the leading irrelevant operator, meaning that at low temperatures $\tilde{J}$

alone characterizes the physics. Nonetheless, the coefficients of other, more irrelevant operators play an important role in the initial renormalization of $\tilde{J}$. Thus, it is a bad approximation to neglect all other couplings $\tilde{J}(x, x')$ when constructing the differential equation for $\tilde{J}$. The correct procedure was spelled out by Wilson[10]: One starts by differentiating Eq. (6) with respect to t, obtaining

$$\frac{d\tilde{J}}{dt} = -e^{-rt}\left[r\tilde{J}_0 + e^{-rt}(1 - 2e^{-rt})\tilde{J}_0^2 + (r\alpha_r - \alpha_r')\tilde{J}_0^3\right] + \mathcal{O}(\tilde{J}_0^4). \tag{7}$$

Then one inverts Eq. (6) to express $\tilde{J}_0$ in terms of $\tilde{J}$,

$$\tilde{J}_0 = e^{rt}\tilde{J} - (e^{2rt}/r)(1 - e^{-rt})\tilde{J}^2 - e^{3rt}\left[\alpha_r - (2/r^2)(1 - e^{-rt})^2\right]\tilde{J}^3 + \mathcal{O}(\tilde{J}^4), \tag{8}$$

and substitutes for $\tilde{J}_0$ in Eq. (7) to get

$$\frac{d\tilde{J}}{dt} = -r\tilde{J} + \tilde{J}^2 + [e^{2rt}\alpha_r' - (2/r)(e^{rt} - 1)]\tilde{J}^3] + \mathcal{O}(\tilde{J}^4). \tag{9}$$

Finally, one can insert the explicit form for $\alpha_r'(t)$ to obtain

$$\frac{d\tilde{J}}{dt} = -r\tilde{J} + \tilde{J}^2 - \left[n\int_0^1 \frac{y^r dy}{(y+1)^2} - \frac{3}{4}\int_0^{e^t} \frac{y^r dy}{y^2 - 1} - \int_0^{e^t} \frac{y^{r+1} dy}{y^2 - 1} - \frac{1}{r}(e^{rt} - 1)\right]\tilde{J}^3 + \mathcal{O}(\tilde{J}^4). \tag{10}$$

It is to be understood that this RG equation is accurate up to terms of order $e^{-\beta D}$, $e^{-\beta D_0}$ and $e^{-\beta(D_0 - D)}$.

3. Discussion

The first and second order terms on the right-hand side of Eq. (10) are identical to those obtained by Withoff and Fradkin.[4] In the limits $n \gg 1$ and $r \ll 1$, the most important contribution to the somewhat messy third-order term is the same factor $-n/2$ which is found for $r = 0$. One can then approximate Eq. (10) by

$$\frac{d\tilde{J}}{dt} = -r\tilde{J} + \tilde{J}^2 - \frac{n}{2}\tilde{J}^3. \tag{11}$$

The fixed points of this RG equation, satisfying $d\tilde{J}/dt = 0$, occur at $\tilde{J} = 0$ (the decoupled impurity limit), $\tilde{J} = \infty$ (the strong-coupling limit, which clearly lies outside the range of validity of the perturbation theory) and the pair of solutions

$$\tilde{J} = \frac{1}{n}\left(1 \pm \sqrt{1 - 2nr}\right).$$

The locus of the intermediate-coupling fixed-points is shown in Fig. 1, which also indicates the direction of renormalization of $\tilde{J}$ when $\tilde{J}_0$ does not lie at one of the

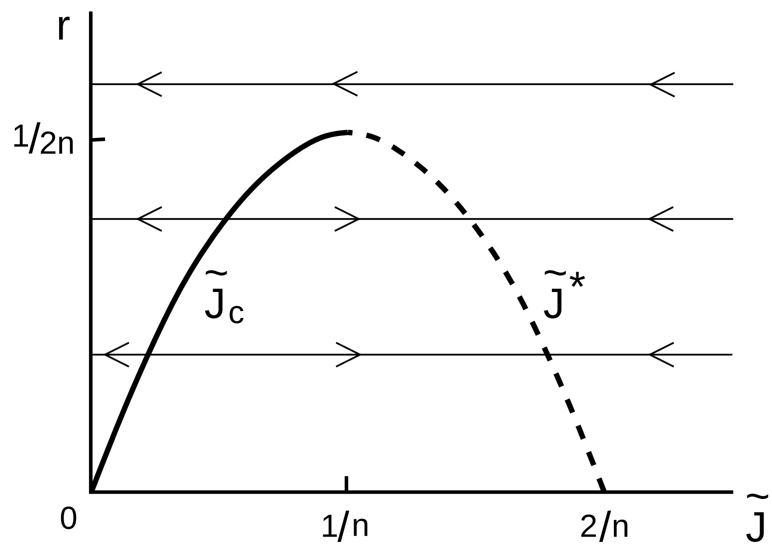

Fig. 1. Renormalization-group flow diagram for the coupling $\tilde{J}$, showing the unstable and stable intermediate-coupling fixed points, $\tilde{J}_c$ and $\tilde{J}^*$, respectively.

fixed points. Two features are noteworthy: First, if $2nr \ll 1$, we can approximate these roots by $\tilde{J}_c = r$, the unstable fixed point found by Withoff and Fradkin,[4] and $\tilde{J}^* = 2/n - r$. The latter fixed point is stable, and is natural to associate it with the overscreened fixed point of the $r = 0$ model. Thus, for $J > J_c$, one expects the model to exhibit anomalous low-temperature properties.

Second, the two solutions $\tilde{J}_c$ and $\tilde{J}^*$ merge at $2nr = 1$. For $r > 1/2n$, the only fixed points obtained from Eq. (11) are $\tilde{J} = 0$ and ∞. The possibility of another fixed point occurring beyond the perturbative regime in $\tilde{J}$ cannot be ruled out. However, the simplest scenario is that $\tilde{J} = 0$ is the only stable fixed point for $r > 1/2n$, i.e., there can be no Kondo effect, however large $\tilde{J}_0$ is made.

Since the Kondo problem with $r > 0$ contains no marginal operator, and for $n \gg 1$ the fixed points J_c and J^* are located at small $\tilde{J}$, it should be possible to calculate the low-temperature properties within perturbation theory. For small r, however, the convergence with increasing order in $\tilde{J}$ will be slow. Moreover, it is desirable to extend the analysis to the cases $n = 1$ and 2 which are of greatest interest. With this motivation, I have extended Wilson's non-perturbative numerical RG method to the density of states given in Eq. (1). Preliminary results[6] indicate that even for $n = 2$, Fig. 1 rather accurately describes the RG behavior: There indeed exist unstable and stable fixed points which merge at around $r = 0.25 = 1/2n$, above which r value there is no Kondo effect. Even more remarkably, the $\tilde{J}_c$ (solid) line in Fig. 1 applies to the conventional Kondo model with $n = 1$: The critical coupling J_c exhibits negative curvature, just as in Fig. 1, and it can be shown analytically[6] that the strong-coupling fixed point becomes unstable for $r > \frac{1}{2}$, leading to a complete suppression of the Kondo effect in this parameter regime. Finally, I note that the numerical RG formulation permits study of more realistic band structures in which the power-law behavior extends only over a small region of the band around the Fermi surface, or in which the zero in the density of states is slightly shifted away from the Fermi level. Work is under way on the determination of the RG flow diagrams for these cases,[6] and on the calculation of physical properties.[11]

In summary, I have extended the perturbative RG analysis of the Kondo effect in a system with a power-law density of states to third order in the exchange coupling and for an arbitrary number of conduction channels. Terms at third order in J are found to have a significant effect on the RG flow diagram. In particular, the existence of a Kondo effect is completely suppressed for densities of states such that $r > 1/2n$.

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