Two-Impurity Kondo Problem

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The two-impurity Kondo problem is studied by use of perturbative scaling techniques. The physics is determined by the interplay between the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction between the two impurity spins and the Kondo effect. In particular, for a strong ferromagnetic RKKY interaction the susceptibility exhibits three structures as the temperature is lowered, corresponding to the ferromagnetic locking together of the two impurity spins followed by a two-stage freezing out of their local moments by the conduction electrons due to the Kondo effect.

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In this Letter we discuss the possible temperature-dependent susceptibilities for two Kondo impurities separated by a distance R imbedded in a metal of noninteracting conduction electrons. The various behaviors depend on the relative magnitude (and sign) of the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction compared with the Kondo temperature of an isolated impurity.

The essential ingredient of this work is the ability to trace the evolution of an *effective Hamiltonian* that describes successively lower energy (and hence temperature) scales. For a given temperature T, the effective Hamiltonian is obtained by integrating out the conduction electrons and holes of energy bigger than a cutoff $D \simeq 10T$. Using a thermodynamic scaling method,[1,2] we are able to describe the variation of the effective Hamiltonian with decreasing cutoff. In this Letter we exhibit only the most important interactions in the effective Hamiltonian. Further, we choose the parameters of the problem so that the relevant energy scales are well separated and can be estimated analytically.

We start with two spin-$\frac{1}{2}$ impurities $\vec{S}_i$ ($i=1,2$) at $\vec{R}_1=\vec{R}/2$ and $\vec{R}_2=-\vec{R}/2$, respectively, and a conduction-electron Hamiltonian $H_{el}(D_0)$ corresponding to a half-filled band of energies $-D_0<\epsilon<D_0$, with a constant density of states ρ. If $\vec{s}_i$ is the conduction-electron spin density at the site $\vec{R}_i$, then the starting Hamiltonian, corresponding to cutoff D_0, is

$$H(D_0)=H_{el}(D_0)-J_0(\vec{s}_1\cdot\vec{S}_1+\vec{s}_2\cdot\vec{S}_2), \quad (1)$$

where J_0 is assumed to be negative (antiferromagnetic).

Two-impurity local moment (2LM) regime $[\max(2|I|, 10T_K)<T]$.—If we integrate out the higher-energy conduction electrons and holes down to a cutoff $D\simeq 10T<D_0$, then we generate an effective Hamiltonian $H_{2LM}(D)$ with a changed value $J(D)$ of the coupling J_0, as well as new interactions not present in (1). Keeping only the most important of these interactions,[3] we have

$$H_{2LM}(D)=H_{el}(D)-I\vec{S}_1\cdot\vec{S}_2-J_s(\vec{s}_1+\vec{s}_2)\cdot(\vec{S}_1+\vec{S}_2)-J_a(\vec{s}_1-\vec{s}_2)\cdot(\vec{S}_1-\vec{S}_2). \quad (2)$$

We can show that $J_s\cong J_a\cong(J_s+J_a)/2\equiv J/2$, where to second order J satisfies the recursion relation [with $J(D_0)\equiv J_0$]

$$d(\rho J)/d\ln(D_0/D)=-(\rho J)^2. \quad (3)$$

Further, I is just the RKKY interaction, given by

$$I\cong(J_0)^2\sum_k n_k \exp(i\vec{k}\cdot\vec{R})\sum_{k'}(1-n_{k'})\exp(-i\vec{k}'\cdot\vec{R})(\epsilon_{k'}-\epsilon_k)^{-1} \quad (4)$$

with the integration range restricted so as to exclude the region where *both* $|\epsilon_k - \epsilon_F|$ and $|\epsilon_{k'} - \epsilon_F|$ lie between 0 and D.

We note that two important characteristic energy scales have naturally arisen in the renormalization process. The first is the Kondo temperature

$$T_K \sim D_0 \exp(1/\rho J_0), \qquad (5)$$

which is the energy scale at which Eq. (3) breaks down.[4] In the absence of any other effect, this is also the temperature at which the local spins would be screened by the conduction electrons (i.e., the Kondo effect).

The second important energy scale is the RKKY interaction I itself. Figure 1 depicts $I(D \simeq 0)$ vs $k_F R$ for two model band structures (see figure caption). For small $k_F R$, I is ferromagnetic as both the local moments then interact with essentially the same conduction electron. For large $k_F R$, I oscillates with an envelope that falls off as $(k_F R)^{-3}$. For $D \ll D_0$, the D dependence of $I(D)$ is quite negligible.[5]

At high temperatures $[D_0 > T \gg \max(2|I|, 10T_K)]$, the 2LM regime is obtained. Then $|I/D|$ and $|\rho J|$ are small compared with unity and thermodynamic properties can be calculated by treating all the interactions in (2) perturbatively. For instance, the susceptibility is given by $T\chi_{imp}/(g\mu_B)^2 \simeq \frac{1}{2}(1 + I/4T + \rho J)$, where the zeroth-order term corresponds to[6] two free local moments.

But as T decreases, and hence D (since we always take $D \simeq 10T$), either $|I/D|$ or $|\rho J|$ will become large, whence there will be a crossover to new regimes of behavior. Two possible characteristic cases are easy to discuss. In case A, $|I| \ll T_K$. Then $|\rho J|$ grows to order unity while $|I/D|$ remains small, whence the Kondo effect suppresses the local moments, and the RKKY interaction plays a very minor role. The temperature dependence of $T\chi$ in this case is shown schematically by curve A of Fig. 2. In case B, I is antiferromagnetic and $-I \gg T_K$. In this case, as T gets small compared with $-I$, the two impurity spins are locked antiferromagnetically into a singlet. Consequently $T\chi$ drops rapidly as depicted schematically in curve B of Fig. 2, and the Kondo effect plays a minor role. Note that in case A $T\chi$ drops slowly, logarithmically, with temperature, whereas in case B it drops quickly, roughly as $1/T$.

Case C, when I is ferromagnetic and $I \gg T_K$, is the most interesting, and will occupy the bulk of the rest of this paper. As T gets small compared with I, the two impurities are locked ferromagnetically into a triplet state described by an ef-

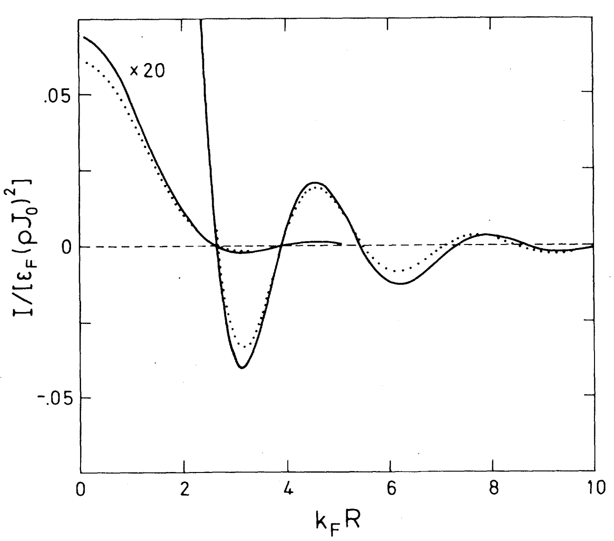

FIG. 1. The RKKY interaction I for two model band structures. The solid curve corresponds to a linear dispersion $\epsilon_k - \epsilon_F = v_F(k - k_F)$ and a constant density of states ρ; the dotted curve corresponds to a free electron band. Both bands are cut off at $D_0 = \epsilon_F = k_F v_F/2$.

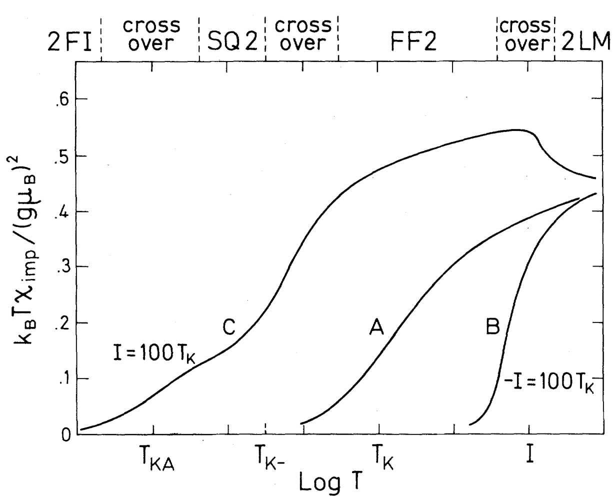

FIG. 2. Schematic plots of $T\chi_{imp}$ for the two-impurity Kondo problem for the three cases considered in the text. In case A, where $T_K \gg |I|$, there is a slow crossover from the 2LM to the two-frozen-impurity (2FI) regime due to the Kondo effect. In case B, there is a rapid crossover from the 2LM to the 2FI regime as the antiferromagnetic RKKY interaction locks the impurity spins into a singlet. In case C, that of ferromagnetic $I \gg T_K$, we have the various regimes indicated at the top of the figure. The temperatures T_{KA} and T_{K-} refer to this case.

fective spin-1 operator $\vec{S}$. Necessarily $T\chi$ rises rapidly (as $1/T$) from a value of $\frac{1}{2}$, characteristic of the 2LM regime, to $\frac{2}{3}$, characteristic of a spin-1 impurity, as depicted in curve C of Fig. 2, but does not reach $\frac{2}{3}$, because the interactions present in (2) generate interactions between $\vec{S}$ and the conduction electrons. Indeed, the effective Hamiltonian for $D \lesssim I$, i.e., *just after* the crossover to the new regime, which we will call the ferromagnetically frozen two-impurity (FF2) regime, is essentially given by[7]

$$H_{\mathrm{FF2}}(I) \cong H_{\mathrm{el}}(I) - J_s^*(\vec{s}_1 + \vec{s}_2)\cdot\vec{S}, \qquad (6)$$

where[8] J_s^* is J_s evaluated at $D \simeq I$.

Ferromagnetically frozen two-impurity (FF2) regime ($10T_{\mathrm{K}} < T < I/2$).— For the purposes of discussing the evolution of $H_{\mathrm{FF2}}(D)$ it is convenient to define two orthogonal conduction-electron channels which are *even* and *odd* with respect to the midpoint between the two impurities; in terms of which[9]

$$(\vec{s}_1 + \vec{s}_2) = 2u_+^2\vec{s}_{\mathrm{even}} + 2u_-^2\vec{s}_{\mathrm{odd}}, \qquad (7)$$

where

$$2u_\pm^2 = 1 \pm \sin(k_{\mathrm{F}}R)/k_{\mathrm{F}}R. \qquad (8)$$

Then the most important terms in $H_{\mathrm{FF2}}(D)$ are given by

$$H_{\mathrm{FF2}}(D) = H_{\mathrm{el}}(D) - J_+(D)\vec{s}_{\mathrm{even}}\cdot\vec{S} - J_-(D)\vec{s}_{\mathrm{odd}}\cdot\vec{S}, \qquad (9)$$

where the "starting" values for $J_+(D)$ and $J_-(D)$, at $D \lesssim I$, are given by [cf. Eqs. (6) and (7)] $J_\pm(I) = 2u_\pm^2 J_s^*$. Furthermore, the recursion relations for $J_\pm(D)$ up to second order are identical to (3). It follows that two new energy scales now arise, namely the even- and the odd-channel Kondo temperatures:

$$T_{K\pm} \sim I\exp[1/(2u_\pm^2\rho J_s^*)]. \qquad (10)$$

Thus in the FF2 regime defined by $\max(10T_{\mathrm{K}\pm}) < T < I/2$, thermodynamic properties can be calculated by treating $J_\pm$ perturbatively. In particular, $T\chi = \frac{2}{3}(1 + \rho J_+ + \rho J_-)$, so that as T decreases $T\chi$ decreases logarithmically.

If I/T_{K} is sufficiently large, then $T_{\mathrm{K}+}$ and $T_{\mathrm{K}-}$ can be well-separated energy scales.[10] In such a case, there will be a *two-stage* Kondo effect. In the first stage, as T approaches $T_{\mathrm{K}-}$, ρJ_- grows to order unity while ρJ_+ is still small. In this crossover $\frac{1}{2}$ unit of the spin-1 impurity will be compensated by the odd-channel conduction electrons, which reduces the impurity degrees of freedom to an effective spin-$\frac{1}{2}$ operator $\vec{\tau}$. Consequently, $T\chi$ drops to $\frac{1}{4}$, as depicted in curve C of Fig. 2. Note that the crossover for $T \sim T_{\mathrm{K}-}$ is a many-body effect, and that $\vec{\tau}$ is a complicated spin-$\frac{1}{2}$ object: the triplet combination of the impurity spins antiferromagnetically clothed by a spin-$\frac{1}{2}$ cloud of odd-channel conduction electrons.

Semiquenched two-impurity (SQ2) regime ($5T_{\mathrm{K}A} < T < T_{\mathrm{K}-}$).— For temperatures well below $T_{\mathrm{K}-}$, we have a new regime, the semiquenched two-impurity (SQ2) regime, in which the effective Hamiltonian corresponds to interactions between $\vec{\tau}$ and the even- and odd-channel conduction electrons given by [compare Eq. (9)]

$$H_{\mathrm{SQ2}}(D) = H_{\mathrm{el}}(D) - J_F\vec{s}_{\mathrm{odd}}\cdot\vec{\tau} - J_A\vec{s}_{\mathrm{even}}\cdot\vec{\tau}. \qquad (11)$$

With use of the same logic as before, just after the crossover into the SQ2 regime, i.e., at $T \lesssim T_{\mathrm{K}-}$, $J_A(T_{\mathrm{K}-})$ is essentially equal to[11] $\frac{4}{3}J_+(T_{\mathrm{K}-})$. However, $J_F(D \lesssim T_{\mathrm{K}-})$ is *ferromagnetic*, since it is the residual coupling of $\vec{S}$ to the odd channel to which it is already strongly bound antiferromagnetically.[12] The recursion relations for $\rho J_A(D)$ and $\rho J_F(D)$ are also identical to (3), but now, as D decreases, while $|\rho J_A|$ increases, ρJ_F decreases. Consequently $T\chi \simeq \frac{1}{4}(1 + \rho J_A + \rho J_F)$ decreases slowly with temperature. When the temperature decreases to[13] $T_{\mathrm{K}A} = T_{\mathrm{K}-}\exp[1/\rho J_A(T_{\mathrm{K}-})]$, $|\rho J_A|$ grows to order unity, and the remaining impurity spin $\vec{\tau}$ is compensated by the even-channel conduction electrons. With decreasing temperature $T\chi$ drops to zero as the system crosses over to the two-frozen-impurity (2FI) regime. See curve C of Fig. 2.

Two-frozen-impurity (2FI) regime [$5T < \min(T_{\mathrm{K}A}, T_{\mathrm{K}}, -I)$].— For all the cases we have considered, in the very low-temperature regime (i.e., for $T \ll T_{\mathrm{K}}$, $-I$, and $T_{\mathrm{K}A}$ in cases A, B, and C, respectively) the impurity degrees of freedom are completely quenched. In this regime, the effective Hamiltonian has only residual self-interactions among the even- and odd-channel conduction electrons. This leads to a constant susceptibility $\chi \sim 1/T^*$, and a linear specific heat $C \sim k_{\mathrm{B}}^2 T/T^*$, where T^* is the final energy scale at which the crossover into the 2FI regime takes place (i.e., T^* is T_{K}, $-I$, or $T_{\mathrm{K}A}$ for the cases A, B, or C).

The above methods may prove useful in studying concentrated systems of local moments such as spin-glasses, valence fluctuators, and magnets.

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[1]H. R. Krishna-murthy and C. Jayaprakash, to be published.

[2]This method is an extension of the "poor man's scaling" approach of P. W. Anderson, J. Phys. C 3, 2436 (1970), made in the light of the later work of K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).

[3]Apart from a constant term, there are eight other interactions not displayed in Eq. (2).

[4]This is seen by integrating Eq. (3) to get $\rho J(D) = \rho J_0/[1+\rho J_0 \ln(D_0/D)]$, and noting that as D approaches T_K, $|\rho J|$ becomes large.

[5]For example, if $RD/v_F \ll 1$, one has $|I(D)-I(0)|/D_0 \cong -(\rho J_0)^2 2\ln 2[\sin(k_F R)/k_F R]^2 (D/D_0)$. Note that in our model $I(D_0)=0$, but we could easily include a direct interaction at the outset.

[6]The various zeroth-order results that we quote for $T\chi$ are easily obtained by calculating $\langle S_z^2\rangle$, where S is the *total effective* impurity spin, for a noninteracting situation.

[7]The result (6) follows from (2) by noting that, *within the triplet subspace of the impurity states*, $(\vec{S}_1+\vec{S}_2)$ is identical to $\vec{S}$, $\vec{S}_1-\vec{S}_2$ is identically zero, and $I\vec{S}_1\cdot\vec{S}_2$ is just a constant, $I/4$, which can be ignored.

[8]Using Ref. 4 and Eq. (5), we can estimate that $\rho J_s^* \cong \rho J(I)/2 \cong -[2\ln(I/T_K)]^{-1}$. In all estimates we omit, for simplicity, all numerical factors multiplying I, etc.

[9]The even- and odd-channel conduction-electron operators to which the impurity couples are defined as $u_+\psi_{\text{even}} \equiv \sum_k \cos(\vec{k}\cdot\vec{R}/2)a_{\vec{k}}$, $u_-\psi_{\text{odd}} \equiv \sum_k \sin(\vec{k}\cdot\vec{R}/2)a_{\vec{k}}$, where $u_\pm$ are normalization factors given by Eq. (8). The conduction-electron operators at sites 1 and 2 are hence $\psi(\pm\vec{R}/2) = u_+\psi_{\text{even}} \pm i u_-\psi_{\text{odd}}$. Equation (7) follows from the definitions $\vec{s}_1 = \frac{1}{2}\psi^+(\vec{R}/2)\vec{\sigma}\psi(\vec{R}/2)$, etc.

[10]From Eqs. (10) and (8) and Ref. 8, we get $T_{K\pm} \sim I(T_K/I)^{1/u_\pm^2}$, so that $T_{K-}/T_{K+} \simeq (I/T_K)^{-4\sin(k_F R)/k_F R}$. The ensuing discussion refers to $k_F R$ near the first maximum in Fig. 1 where $\sin(k_F R)/kR \simeq -0.2$. Near the second maximum, $\sin k_F R > 0$, and hence the roles of + and − channels would be reversed.

[11]The factor of $\frac{4}{3}$ comes from projecting $\vec{S}$ into the subspace of $\vec{\tau}$.

[12]This point has been made in other contexts by D. M. Cragg and P. Lloyd, J. Phys. C 12, L215 (1979), and P. Nozières and A. Blandin, J. Phys. (Paris) 41, 193 (1980).

[13]Using earlier quoted results, we can estimate that $\rho J_+(T_{K-}) \cong -[(u_+^{-2}-u_-^{-2})\ln(I/T_K)]^{-1} \simeq -\{[4\sin(k_F R)/k_F R]\ln(I/T_K)\}^{-1}$. Hence $T_{KA} \sim T_{K-}(I/T_K)^{-3\sin(k_F R)/k_F R}$. Note that T_{KA} is higher than T_{K+}: $T_{KA}/T_{K+} \simeq (I/T_K)^{-\sin(k_F R)/k_F R}$.