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COMPETITION BETWEEN DIRECT INTERACTION AND KONDO EFFECT: RENORMALIZATION-GROUP APPROACH

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ABSTRACT

Via the Wilson renormalization-group approach, the effect of the competition between direct interaction (J_L) and Kondo coupling is studied, in the magnetic susceptibility of a model with two different magnetic impurities. For the ferromagnetic interaction $(J_L > 0)$ between the localized impurities, we find a magnetic ground state and a divergent susceptibility at low temperatures. For $(J_L < 0)$, two different Kondo temperatures and a non-magnetic ground state are distinguished.

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1 INTRODUCTION

In order to understand the different physical processes that can take place in magnetism of transition metals and some rare earth systems ($CeAl_2$, $CeIn_3$, $CeAl_3$, $CeCu_2Si_2$,...), the behavior of two magnetic impurities in a nonmagnetic metal has been viewed as an important problem for the understanding of a wide range of phenomena.[1] More particularly, the question of whether or not the magnetic moment of the impurities persists down to zero temperature.

There has been a considerable amount of theoretical effort in recent years devoted to the understanding of the interplay between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction (K_0).[2-8] One expects that if the Kondo temperature T_K is larger than K_0, the impurity spin never develops significant correlations.[2-5] On the other hand, some authors[6,7] conclude that the RKKY interaction as well as the Kondo effect play an important role at sufficiently low temperatures even for $K_0 << T_K$.

In this paper, we consider the particular problem of the competition between direct interaction and Kondo effect in a model with two different magnetic impurities (for instance Gd and Ce) near to each other in an otherwise completely nonmagnetic material. We wish to report here the results obtained from this model for the temperature dependence of the magnetic susceptibility due to impurities, via Wilson's Renormalization-group (RG) approach[9].

In Sec. 2, we set up a model Hamiltonian. In Sec. 3, we analize some limiting cases of the model and present the numerical results. Finally, we conclude in Sec. 4 with a discussion.

2 THE MODEL

The model Hamiltonian is the Kondo Hamiltonian[9] extended to include the direct interaction between the Kondo impurity and the other local magnetic moment decoupled from the conduction-electron states:

$$H = D[\int_{-1}^{1} k a^{\dagger}_{k\mu} a_{k\mu} dk - J \int_{-1}^{1} dk \int_{-1}^{1} dk' (\frac{1}{2} a^{\dagger}_{k\mu} \vec{\sigma_{\mu\nu}} a_{k'\nu}).(\frac{1}{2}\vec{\tau}) - J_L \ (\frac{1}{2}\vec{\tau}).(\frac{1}{2}\vec{\tau_L})] . \quad (1)$$

In Eq. (1) we use the same notation as in Ref. 10. The first two terms correspond to the spin-$\frac{1}{2}$ Kondo Hamiltonian, and the

last one is the added direct interaction between the two-spin-$\frac{1}{2}$ magnetic moments.

Measuring energies from the Fermi level, and in units of the half-band width D, the Hamiltonian is characterized by only two parameters: J, the coupling strength of the Kondo impurity to the conduction band, and J_L measuring the strength of the direct interaction.

The logarithmic discretization of the conduction band in terms of parameter Λ (> 1), as discussed in Ref. 10, generates a sequence of effective Hamiltonians:

$$H_N = \Lambda^{(N-1)/2}[\sum_{n=0}^{N-1} \Lambda^{-n/2} \xi_n (f^{\dagger}_{n\mu} f_{n+1\mu} + H.c.) - \tilde{J}(f^{\dagger}_{0\mu} \vec{\sigma_{\mu\nu}} f_{0\nu}).\vec{\tau} - \tilde{J}_L \ \vec{\tau}.\vec{\tau_L}] , \quad (2)$$

where

$$\xi_n = (1 - \Lambda^{-n-1})(1 - \Lambda^{-2n-1})^{-1/2}(1 - \Lambda^{-2n-3})^{-1/2} ,$$

$$\tilde{J} = [\frac{2}{(1 + \Lambda^{-1})}][\frac{J}{2}] ,$$

and

$$\tilde{J}_L = [\frac{2}{(1+\Lambda^{-1})}][\frac{J_L}{4}] .$$

In Eq. (2) the operator $f_{n\mu}$ refers to a conduction electron shell state of extent $\sim \Lambda^{n/2}/K_F$ centered at the Kondo impurity site. The evolution of the lowest energy levels of the Hamiltonian H_N, with the number of iterations N, allows us to calculate numerically the temperature-dependent properties of H.

3 RESULTS

In order to analyze the numerical results, at first we study two limiting cases:

a) For $J = 0$, the resulting Hamiltonian (Eq.(2)) is clearly just the free conduction band term plus two impurity orbitals. The band is decoupled from the localized magnetic moments and the magnetic susceptibility due to impurities is given by

$$\chi(T) = \frac{(g\mu_B)^2}{K_B T}\frac{2\exp(\tilde{\beta}J_L/4)}{[3\exp(\tilde{\beta}J_L/4)+\exp(-\tilde{\beta}3J_L/4)]} , \qquad (3)$$

where $\tilde{\beta} = D/K_B T$. Within the context of Renormalization-group theory, three different physical regimes are found in Eq.(3):

(a.1) The Non-interacting impurities (NI) regime corresponds to $J_L = 0$, with

$$\chi(T) = \frac{(g\mu_B)^2}{K_B T}\frac{1}{2} . \qquad (4)$$

(a.2) The Ferromagnetic coupling (FC) regime corresponds to $J_L = \infty$, with

$$\chi(T) = \frac{(g\mu_B)^2}{K_B T}\frac{2}{3} . \qquad (5)$$

(a.3) The Antiferromagnetic coupling (AC) regime corresponds to $J_L = -\infty$, with $T\chi = 0$.

b) For $J_L = 0$, the resulting Hamiltonian is clearly just the Kondo Hamiltonian plus a free-impurity orbital. We here have two independent problems and then, in according with the Kondo problem, the results for the two fixed points ($J = 0, J = -\infty$) are:

(b.1) For $J = 0$, we recover the NI regime and we have $\mu_{eff}^2 = K_B T\chi/(g\mu_B)^2 = \frac{1}{2}$.

(b.2) For $J = -\infty$, the Kondo impurity is strongly coupled to the conduction band. In this regime, one of the two magnetic moments is compensated by a conduction electron spin polarization cloud which forms a singlet with the Kondo impurity. The magnetic susceptibility due to impurities, such as a free impurity case, is given by

$$\chi(T) = \frac{(g\mu_B)^2}{K_B T}\frac{1}{4}. \qquad (6)$$

For general values of J and J_L, we use the numerical diagonalization of H_N in order to calculate $\chi(T)$ follows the procedure of Ref. 10. All results were obtained using $\Lambda = 3$, and a maximum of 1120 states was kept.

The Figure shows the magnetic susceptibility due to impurities as a function of T for a fixed value of $J = -0.24$ and different values of J_L. It can be seen that there is, at low temperatures, a significant difference between the $J_L \geq 0$ and $J_L < 0$ results. For antiferromagnetic coupling ($J_L < 0$) between the two magnetic moments, the magnetic susceptibility saturates at low temperatures. On the other hand, for ferromagnetic coupling we observe a divergent susceptibility a $T = 0$.

4 DISCUSSION

In the same form that the RG calculations for the Kondo problem[9], as $\mid J \mid$ decreases the number of iterations required

before the energy level structure of H_N approaches that of the $T = 0$ structure becomes enormous, due to the presence of the marginal operator generated by $(f^{\dagger}_{0\mu}\vec{\sigma_{\mu\nu}} f_{0\nu})\vec{\tau}$. This makes it hard to compute numerically for small $\mid J \mid$, because numerical errors are accumulated over many iterations and also because too much computer time is required. For this reason, we take $J = -0.24$, through all this calculation.

The numerical results for different values (but small) of J_L show that the NI regime gives a good approximation to the magnetic susceptibility for small N (i.e.,$T \sim D$). As N is increased the deviations from the NI fixed point increased. For $J_L = 0$ (curve D), the energy level structure of H_N changes rapidly over the next few iterations and finally approaches that of the $J = -\infty$ fixed point (b.2). In this case, the numerical Kondo temperature (T_K) gives $T_K \sim 0.004$. *For* $T << T_K$, *no further transitions can occur* and we find a magnetic ground state with a divergent susceptibility (Eq.(6)).

For the ferromagnetic case (curves E and F), we find again that the ground state is degenerate, leading to Curie-type susceptibility at low temperatures. But in this case, as N is increased the deviations from the NI fixed point to the FC regime can occur (curve F). For $J_L >> | J |$, the results can be compared with the spin-1 Kondo problem [11,12]. For $J_L = \infty$ and $J \neq 0$ Eq. 2 reduced to

$$H_N = \Lambda^{(N-1)/2}[\sum_{n=0}^{N-1} \Lambda^{-n/2}\xi_n(f^{\dagger}_{n\mu}f_{n+1\mu} + H.c.) - \tilde{J}(f^{\dagger}_{0\mu}\vec{\sigma_{\mu\nu}}f_{0\nu}).\vec{S}]\,, \tag{7}$$

where $\vec{S}(S_x, S_y, S_z)$ are the spin-1 matrices associated with a spin-1 local moment. For temperatures of the order of the corresponding Kondo temperature μ^2_{eff} falls to $\frac{1}{4}$, i.e., the free spin-$\frac{1}{2}$ value.

For antiferromagnetic coupling (curves A, B, and C) between the localized impurities we find a nonmagnetic ground state and two different Kondo temperatures can appear. Curve A shows the effect of the strong antiferromagnetic coupling; As N is increased, after few iterations, the deviations from the NI fixed point to the AC regime (a.3) occur and μ^2_{eff} falls to zero. This is a stable fixed-point and no further transitions can occur when $N \to \infty$. Finally, curves B and C, after few iterations, show the Kondo effect and a local-moment (b.2) develops before the AC regime. As N is increased, the deviations from the local-moment to AC occur, and we observe that the low temperature shapes also have the

universal shape of the Kondo susceptibility. In conclusion, for the antiferromagnetic case and $| J | >> | J_L |$, the model always gives two different Kondo temperatures.

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FIGURE CAPTION

Magnetic susceptibility due to impurities as a function of the temperature on a logarithmic scale. The parameters measured in units of D are J=-0.24 and J_L ranging from -0.012 to 0.12. The six curves correspond to J_L=-0.012 (A), J_L=-0.0008 (B), J_L=-0.0004 (C), J_L=0 (D), J_L=0.0012 (E), and J_L=0.12 (F).