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Mean-field analysis of two antiferromagnetically coupled Anderson impurities

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We have solved, near $T=0$, a model describing two magnetic impurities coupled to a band of itinerant electrons and also antiferromagnetically to each other, using an auxiliary-boson mean-field theory which is exact in a large-N limit. Depending upon parameters we find two possible ground states: one in which the Kondo effect occurs and one in which it does not. As the direct antiferromagnetic interaction is varied relative to the Kondo coupling at $T=0$, a phase transition occurs which may be of first or second order. We compute the low-temperature behavior of the specific heat and the uniform and staggered susceptibility. The nature of the Kondo phase and of the phase transition differ notably from the results found in a recent numerical renormalization-group calculation of a similar model with $N=2$.

The interplay, in a material with a high density of magnetic moments, between the Kondo effect (which involves quenching of a local moment via coupling to conduction electrons) and magnetic ordering of the moments is a long-standing problem. It is of particular current relevance to the study of heavy-fermion metals, for in the past several years many of these have been shown by neutron scattering[1] or NMR (Ref. 2) to exhibit interesting magnetic behavior. The issue also arises in the theoretical analysis of a class of models[3] intended to describe the high-T_c CuO_2-based superconductors; these models idealize the high-T_c materials as a set of localized spins, residing on the Cu sites, magnetically coupled to each other and to itinerant holes on the O sites.

The interplay between the Kondo effect and magnetic ordering in a lattice is an unsolved problem. As a first step, much attention has been devoted to the problem of two magnetic impurities in a normal metal host. There are two important energy scales: the single-impurity Kondo temperature, T_K, and the magnetic interaction I. In our conventions $I>0$ corresponds to antiferromagnetic coupling of the two spins. It is clear that for $I \gg T_K$ the Kondo effect will be inhibited because the magnetic interaction will tend to bind the spins into a singlet. Until recently it was believed[4] that the $T=0$ physical properties of the two-impurity problem would vary smoothly with I/T_K.

However, a recent numerical renormalization-group (RG) study of the two-impurity Kondo problem found different behavior.[5] As the ratio I/T_K was varied through a critical value $(I/T_K)_c \approx 2.2$, a surprising behavior was found. For $(I/T_K) < (I/T_K)_c$, the ground state was one in which a Kondo effect occurred, while for $(I/T_K) > (I/T_K)_c$ the Kondo effect did not occur. For (I/T_K) near the critical value, the zero temperature values of the staggered susceptibility χ_s and the specific-heat coefficient $\gamma = C/T$ diverged approximately as $|I/T_K - (I/T_K)_c|^{-2}$, while the uniform susceptibility χ did not diverge. The existence of the phase transition raises many questions, including the robustness of these results to effects not included in the idealized model studied numerically and also the generalization to higher spin and to more than two impurities.

As a step towards understanding the issues outlined above we have solved in mean-field theory a model describing two magnetic impurities coupled to a band of itinerant electrons and also antiferromagnetically to each other via an exchange interaction I. The model with $I=0$ has been discussed previously.[6] Our mean-field solution is exact in an $N \rightarrow \infty$ limit where N is the spin degeneracy of the impurity levels and the conduction band. The magnetic coupling I is to be thought of as being mediated by degrees of freedom not explicitly included in the model, for example as a superexchange via filled orbitals. Such a term would also be generated by performing poor-man scaling[4,7] on an Anderson model. The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction mediated by the explicitly included conduction electron degrees of freedom would only appear as fluctuation corrections to the mean-field theory. As is shown below and in Ref. 6, the mean-field theory contains some intersite effects due to multiple scattering of the conduction electrons, but these are not due to the RKKY interaction.

Our results are summarized in Figs. 1 and 2 and discussed in detail below. We find that for typical values of parameters the mean-field equations have several solutions, of which more than one may be locally stable. If we restrict attention to the global minimum of the free energy, then in qualitative agreement with the numerical study of the two-impurity Kondo problem we find at $T=0$ two possible regimes. For $(I/T_K) > (I/T_K)_c \sim 2$ we find a regime in which the Kondo effect does not occur; while

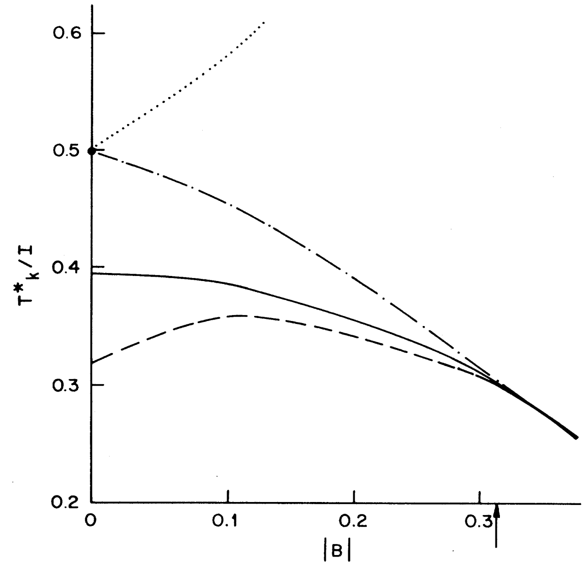

FIG. 1. Phase diagram for mean-field equations [Eqs. (3) in text]. The solid line is the boundary $(T_K^*/I)_c$ between the large (T_K^*/I) regime where the Kondo solution is the global energy minimum and the small T_K^*/I regime where the non-Kondo solution is the global minimum. The arrow marks the point $B=1/\pi$. For $B<1/\pi$ the transition is first order (light solid line); for $B>1/\pi$ the transition is continuous (thick solid line). Below the dashed line the non-Kondo solution is the only minimum, although an unstable solution of Eqs. (3) with $\mathrm{sgn}\delta=-\mathrm{sgn}B$ also exists. The non-Kondo solution is locally stable below the dash-dot line and locally unstable above. The dash and dot-dash lines merge with the solid boundary line for $B\gtrsim 1/\pi$. Above the dotted line Eqs. (3) have only one solution, the Kondo solution described in the text. This solution evolves smoothly and without bifurcation as T_K^*/I is lowered at fixed B. Below the dotted line Eqs. (3) have other unphysical solutions with $\delta\neq\pi/2$.

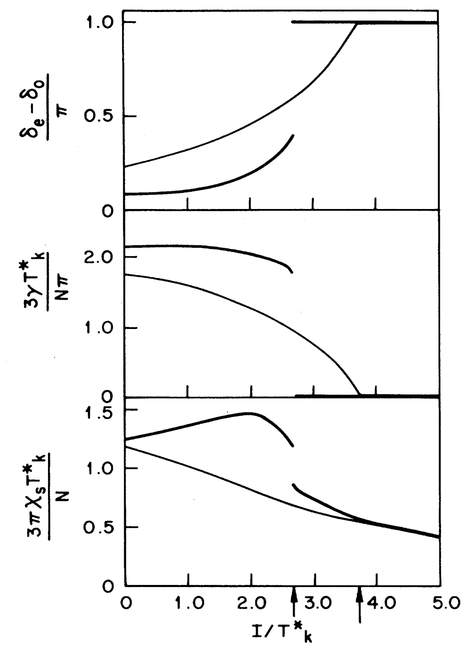

FIG. 2. Behavior of physical quantities as antiferromagnetic interaction I is varied at fixed T_K^*, for two representative values of $|B|$; $|B|=0.1$ (heavier curves), $|B|=0.4$ (lighter curves). The arrows indicate the values of I/T_K^* at which the transition from Kondo-like to non-Kondo-like solution occurs. The upper panel shows the difference of the even (δ_e) and odd (δ_o) channel phase shifts from $\pi/2$ (note $\delta_e+\delta_o=\pi$), the central panel shows the normalized specific-heat coefficient γ, and the lowest curve shows the normalized staggered susceptibility χ_s. For $B=0$ the curves would be independent of I for $I<(T_K^*)_c$.

for $(I/T_K)<(I/T_K)_c$ we find a regime in which the Kondo effect does occur. The Kondo regime may be thought of as a theory of two channels (even and odd parity) of electrons moving in scattering resonances with phase shifts δ_e and δ_o at the Fermi surface. In the numerical RG work, the result $\delta_e=\delta_o=\pi/2$ was found throughout the Kondo regime. In the mean-field theory we find that in general $\delta_e\neq\delta_o$, although $\delta_e+\delta_o=\pi$ as required by the Friedel sum rule. A further difference is that in the mean-field theory the transition between the Kondo and non-Kondo regime may be first or second order; in no case do any of the quantities γ, χ, and χ_s diverge at the transition. At present the reason for the difference between our results and the numerical RG results is not known. One possible explanation is that the RG calculation was performed for a model with $N=2$, while our calculation is valid in an $N\rightarrow\infty$ limit. At finite N, fluctuation corrections to the mean-field theory may become important. We discuss possible effects of such corrections at the end of this paper.

Our formal analysis proceeds from the standard auxiliary boson version of the two impurity $U=\infty$ Anderson model,[6] to which is added an antiferromagnetic interaction $I\mathbf{S}_1\cdot\mathbf{S}_2$ where $\mathbf{S}_{1,2}$ are the usual SU(N) spin operators and $I>0$.

The Hamiltonian is

$$H=\sum_{k,m}\varepsilon_k c_{km}^\dagger c_{km}+\sum_{\substack{\alpha=1,2\\ m}}E_0 f_{\alpha m}^\dagger f_{\alpha m}+\frac{V}{\sqrt{N}}\sum_{\substack{\alpha=1,2\\ m}}b_\alpha^\dagger e^{i\mathbf{k}\cdot\mathbf{r}_\alpha}c_{km}^\dagger f_{\alpha m}+\mathrm{H.c.}+\frac{I}{N}\sum_{m,m'}f_{1m}^\dagger f_{2m}f_{2m'}^\dagger f_{1m'}\,. \qquad (1)$$

Here $\alpha=1,2$ labels spin sites and we enforce the constraint $n_{f\alpha}+n_{b\alpha}=N/2$. Here n_{fi} and n_{bi} are the number of f electrons and auxiliary bosons on site α. In the previous heavy-fermion literature[6,8] a more general constraint $n_{fi}+n_{bi}=q_0N$ $(q_0\leq\frac{1}{2})$ was employed. We must choose $q_0=\frac{1}{2}$ to correctly represent the state where the two impurities are in a singlet.

We write the model as a functional integral, introducing Lagrange multipliers $i\lambda_i$ to enforce the constraints. We decouple the antiferromagnetic interaction via a Hubbard-Stratonovich transformation, introducing a link variable R,[9] integrate out the conduction and f electrons, and make a static approximation for R, $i\lambda_i$, and b_i. Because there are two conservation laws (one for each site) there are two arbitrary phase degrees of freedom, which we choose so that the two auxiliary-boson (b_a) fields are real. The free energy per spin, F/N, may then be written

$$\frac{F}{N}=-\sum_{i,\omega_n}\mathrm{Tr}\ln\underline{M}+\sum_{a=1,2}\left[\frac{\varepsilon_{fa}-E_0}{\pi\rho V^2}\Delta_a+\tfrac{1}{2}(\varepsilon_{fa}-E_0)\right]+R^2/I\,. \tag{2}$$

Here $\varepsilon_{fa}-E_0$ is the mean-field value of $i\lambda_a$; $\Delta_a=\pi\rho V^2|b_a|^2/N$, and now R and b_a denote mean-field values. ρ is the conduction-electron density of states at the Fermi level.

The 2×2 matrix $\underline{M}$ has components $M_{aa}=-i\omega_n+\varepsilon_{fa}-i\Delta_a\mathrm{sgn}\omega_n$,

$$M_{12}=R-(iA\,\mathrm{sgn}\omega_n+B)\sqrt{\Delta_1\Delta_2}\,,$$

$$M_{21}=R^*-(iA\,\mathrm{sgn}\omega_n+B)\sqrt{\Delta_1\Delta_2}\,,$$

and

$$\pi\rho(iA\,\mathrm{sgn}\omega_n+B)=\sum_k\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{-i\omega_n+\varepsilon_k}\,.$$

A and B are numbers of magnitude ≤ 1 determined by the conduction-electron band structure and the impurity separation r. As $r\rightarrow 0$, $A\rightarrow 1$. For $k_F^{-1}\ll r\ll L$ (where L is the Kondo length v_F/T_K) one finds $A\cong\sin k_Fr/k_Fr$ and $B\cong\cos k_Fr/k_Fr$.

The mean-field equations may be derived by varying the free energy with respect to Δ_a, ε_{fa}, R, and R^*. The full mean-field equations are formidable; on the basis of the solution of the $I=0$ case we have assumed $\Delta_1=\Delta_2=\Delta$ and $\varepsilon_{f1}=\varepsilon_{f2}=\varepsilon_f$ and we have checked the local stability of our results against static fluctuations in $\Delta_1-\Delta_2$ and $\varepsilon_{f1}-\varepsilon_{f2}$.

The parameter R is complex; however, for $A<A_c(B)$ [with $A_c(B)\gtrsim 0.7$] we find that the physically relevant free-energy minima have $\mathrm{Im}R=0$. For $A>A_c(B)$, solutions with both Δ and $\mathrm{Im}R\neq 0$ are favored. The case $A>A_c$ is briefly discussed below, and will be analyzed at length in a future paper.[10]

With the notation $E_1=\varepsilon_f+B\Delta+R$, $E_2=\varepsilon_f-(B\Delta+R)$, the mean-field equations are

$$\frac{1}{\pi}\tan^{-1}\frac{E_1}{\Delta(1-A)}+\frac{1}{\pi}\tan^{-1}\frac{E_2}{\Delta(1+A)}-2\frac{\Delta}{\pi\rho V^2}=0\,, \tag{3a}$$

$$\frac{1}{\pi}\tan^{-1}\frac{E_1}{\Delta(1-A)}-\frac{1}{\pi}\tan^{-1}\frac{E_2}{\Delta(1+A)}-\frac{2R}{I}=0\,, \tag{3b}$$

$$\frac{2BR}{I}+\frac{1-A}{2\pi}\ln\frac{E_1^2+\Delta^2(1-A)^2}{D^2}+\frac{1+A}{2\pi}\ln\frac{E_2^2+\Delta^2(1+A)^2}{D^2}+\frac{2(\varepsilon_f-E_0)}{\pi\rho V^2}=0\,. \tag{3c}$$

In the Kondo limit, in which terms proportional to $\Delta/\rho V^2$ and $\varepsilon_f/\rho V^2$ are neglected, the three coupled nonlinear equations may be reduced to one,

$$\left[\frac{T_K^*}{I}\right]e^{B\delta}(\sin\delta-B\cos\delta)=\delta/\pi\,. \tag{4}$$

Here $T_K^*=De^{-1/\pi\rho J^*}$, where D is the conduction bandwidth and the modified Kondo coupling J^* is given by

$$(\rho J^*)^{-1}=-E_0/\rho V^2+\frac{1}{\pi}[(1-A)\ln(1-A)+(1+A)\ln(1+A)]\,.$$

$-\pi/2\leq\delta\leq\pi/2$ is an angle in terms of which the original variables are $\Delta=T_K^*e^{B\delta}\cos\delta$, $R+B\Delta=T_K^*e^{B\delta}\sin\delta$, and $\varepsilon_f=-A(B\Delta+R)$. Equation (4) may easily be solved by graphical or numerical techniques.

A and B express the intersite correlations. A gives the difference in widths of the two resonances in the Kondo limit and enters the theory in an essentially trivial way for $A<A_c(B)$. The parameter B gives the splitting of the resonances, and will be seen to play a more important role. Our results turn out to depend only on $|B|$. We note that J_{RKKY}, the RKKY interaction due to explicitly retained conduction electron degrees of freedom, goes for large k_Fr as

$$\cos(2k_Fr)/(k_Fr)^3\sim(B^2-A^2)/k_Fr\,.$$

Thus $|B|$, on which our results depend crucially, is not directly related to the magnitude or sign of J_{RKKY}.

Depending on the values of (T_K^*/I) and B, Eq. (4) may have 0, 1, 2, or 3 solutions. In addition, the solution $\Delta=0$, $R=I/2$ is always a free-energy extremum. However, if we focus only on global minima of the free energy, then only two solutions are relevant. One is the non-Kondo solution $\Delta=0$, $R=I/2$, which corresponds to decoupling the f electrons from the conduction band, but coupling them to each other, so that the even parity eigenfunctions are filled and lie $I/2$ below the chemical potential; the odd parity solutions are empty and $I/2$ above. This is the fermion representation of a spin singlet. The non-Kondo solution is the global minimum for $(T_K^*/I)<(T_K^*/I)_c$.

To construct the other, Kondo, solution, consider T_K^*/I large. For T_K^*/I sufficiently large, Eq. (4) has only one solution, with $\Delta=T_K^*/\sqrt{1+B^2}$ and $R=aI\,\mathrm{sgn}B$. Here a is a number of order B. The Kondo solution evolves continuously as the ratio T_K^*/I is lowered until at $(T_K^*/I)_c$ the non-Kondo solution becomes favored. The Kondo solution is a theory of two channels of electrons moving in scattering resonances with phase shifts $\pi/2\pm\delta$, where δ is the value of the relevant solution Eq. (4). We have found that for $B\neq 0$ it is not possible to find a stationary point which corresponds to two channels of electrons moving in Lorentzian scattering resonances with the same phase shift in each channel. Note also that the sign of R is found to be such as to *increase* the difference of the phase shifts from $\pi/2$. The various regimes discussed above are shown in Fig. 1.

The specific-heat coefficient γ may be calculated in the standard way, by evaluating the Matsubara sum in Eq. (1) at nonzero temperature. The uniform (χ) staggered (χ_s) susceptibilities may be calculated by adding a term of the form $\sum_m (h/N)m(f_{1m}^\dagger f_{1m} \pm f_{2m}^\dagger f_{2m})$ to the initial Hamiltonian. We find

$$\gamma = \frac{N\pi}{3} \frac{2e^{-B\delta}\cos\delta}{(1-A^2)T_K^*} = \pi^2 \chi \,, \tag{5a}$$

$$\chi_s = \frac{N}{3\pi} \frac{e^{-B\delta}}{T_K^*} \frac{A \ln[(1+A)/(1-A)]\cos\delta + 2\delta \sin\delta}{\sin^2\delta + A^2 \cos^2\delta} \,. \tag{5b}$$

The Wilson ratio $R=1$. The divergence of γ and χ_s for $|A| \rightarrow 1$ occurs because in that limit one of the resonances becomes arbitrarily narrow. The behavior of δ, γ, and χ_s as I is varied for fixed T_K^* is plotted in Fig. 2 for two representative values of B.

The above results have been obtained in the Kondo limit. Away from the Kondo limit the equations must be solved and the energies and stabilities checked numerically. We have verified that the two physically relevant solutions we have identified evolve smoothly as the ratio $\Delta/\rho V^2$ increases. We believe that the phase diagram remains essentially similar to what we have found in the Kondo limit.

In conclusion we speculate briefly upon the likely effect of including fluctuation corrections to the mean-field theory.

In mean-field theory we find a second-order phase transition for $B > 1/\pi$, with Δ vanishing and the physical quantities varying continuously through the transition. In this regime, for any finite N, fluctuation corrections will become comparable to the mean-field values sufficiently near the transition, leading to a breakdown of perturbation theory. We suspect that in this case the fluctuation effects will smooth out the transition, so that the model would exhibit only a smooth crossover as T_K^*/I is varied. In the single impurity Anderson model, an $N=\infty$ second-order phase transition with $\Delta \rightarrow 0$ at $T \sim T_K$ similarly becomes a crossover at any finite N. This argument suggests that in this model at finite N there is no order parameter characterizing the difference between the Kondo and non-Kondo regimes, because it is possible to go smoothly from the Kondo to the non-Kondo regimes by appropriately varying B and T_K^*/I.

For $B < 1/\pi$ the situation could be different. Because the transition is first order, a perturbation expansion in powers of $1/N$ would, we believe, converge at sufficiently large N, say $N > N_c$. Then, in the absence of nonperturbative effects arising for example from tunneling between the two minima, the transition would remain first order for $N > N_c$ so that the point $B = 1/\pi + O(1/N)$ would be a critical point, the end of a line of first-order phase transitions. For $N < N_c$ the transition could become a smooth crossover for all B or a second-order phase transition for some values of B. Nonperturbative effects could lead to $N_c = \infty$.

An important difference between our results and those of Ref. 5 is the value of the Fermi-surface phase shifts δ_e and δ_o. We note that the model of Ref. 5 has a special particle-hole symmetry in which even (odd) parity particles are mapped to even (odd) parity holes. When this symmetry is enforced in our model, $B=0$ implying $\delta_e = \delta_o = \pi/2$ in the Kondo phase. We are currently studying whether at finite N the symmetry is restored. It might be interesting to extend the analysis of Ref. 5 to a model that lacked the above symmetry.

The generalization of the results of this paper to the lattice is in principle straightforward;[10] however, the large variety of possible magnetic behavior (both ordered and resonating-valence-bond-like), will make the analysis much more involved.

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[1]See, e.g., G. Aeppli, E. Bucher, C. Broholm, J. K. Kjems, J. Baumann, and J. Hufnagl, Phys. Rev. Lett. **60**, 615 (1988).

[2]See, e.g., F. Ohkawa *et al.*, J. Magn. Magn. Mater. (to be published).

[3]B. G. Kotliar, P. A. Lee, and N. Read, Physica B&C **153-154**, 538 (1988); C. Castellani and B. G. Kotliar, Phys. Rev. B **39**, 2876 (1989); P. Coleman and N. Andrei (unpublished).

[4]C. Jayaprakash, H. R. Krishna-murthy, and J. W. Wilkins, Phys. Rev. Lett. **47**, 737 (1981).

[5]B. A. Jones and C. M. Varma, Phys. Rev. Lett. **58**, 843 (1987); B. A. Jones, C. M. Varma, and J. W. Wilkins, *ibid.* **61**, 125 (1988).

[6]P. Coleman, Phys. Rev. B **35**, 5072 (1987); D. M. Newns and N. Read, Adv. Phys. **39**, 799 (1987).

[7]P. W. Anderson, J. Phys. C **3**, 2436 (1970).

[8]N. Read, D. M. Newns, and S. Donaich, Phys. Rev. B **30**, 3841 (1984); A. J. Millis and P. A. Lee, *ibid.* **35**, 3394 (1987); A. Auerbach and K. Levin, Phys. Rev. Lett. **57**, 877 (1986).

[9]I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988).

[10]B. A. Jones, B. G. Kotliar, and A. J. Millis (unpublished).