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Study of Two Magnetic Impurities in a Fermi Gas

B. A. Jones

AT&T Bell Laboratories, Murray Hill, New Jersey 07974, and Laboratory for Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853,[a] *and Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, California 93106*

and

C. M. Varma

AT&T Bell Laboratories, Murray Hill, New Jersey 07974

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The problem of two magnetic moments in a Fermi gas is studied with the numerical renormalization group used by Wilson for the Kondo problem. Even when the interaction energy of the moments is much smaller than the Kondo energy, the asymptotic low-temperature behavior is that of a *correlated* Kondo effect. An effective Hamiltonian for the low-temperature properties, which are nonuniversal, is deduced.

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The problem of a magnetic impurity in a metal—the Kondo problem—is now well understood.[1-3] Some conjectures have been made for the two-magnetic-impurities problem. A solution to this problem is important for an understanding of heavy fermions as well. The most popular conjecture is that if the Kondo temperature T_K is larger than the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction K_0 between the magnetic moments, the impurity spin is quenched and the many-body problem is that of two isolated magnetic impurities. On the other hand, Abrahams and Varma[4] have recently discovered that the RKKY interaction itself acquires logarithmic divergences in higher-order perturbation theory. The calculation of Abrahams and Varma shows that impurity interactions cannot be ignored but, as in the case of the one-impurity problem, diagrammatic perturbation analysis does not provide a good picture of the physics at low temperatures. We have therefore resorted to an extension of Wilson's numerical renormalization-group method[1] for the Kondo problem to the two-impurity problem.

Wilson's method generates a sequence of effective Hamiltonians which accurately describe the low-lying many-body states at successively lower temperatures. By examining the flow of these Hamiltonians and by comparing their symmetry with that for special cases, we conclude that the effective RKKY interaction strongly affects the asymptotic low-temperature behavior and that the isolated impurity behavior is not obtained even for $K_0 \ll T_K$. We also generate an effective Hamiltonian for the low-lying eigenstates near the strong-coupling ($T \rightarrow 0$) fixed point and derive the Fermi-liquid parameters for the model.

The model Hamiltonian is a straightforward extension of that of Wilson to the two-impurity case:

$$H = H_K + H_{int}, \tag{1}$$

$$H_K = \sum_{\mathbf{k},\sigma} \varepsilon(\mathbf{k}) a_{k\sigma}^{\dagger} a_{k\sigma}, \tag{2}$$

$$H_{int} = J_0[a^{\dagger}(r_1)\boldsymbol{\sigma} a(r_1)\cdot \mathbf{S}_1 + a^{\dagger}(r_2)\boldsymbol{\sigma} a(r_2)\cdot \mathbf{S}_2] + K_0'\mathbf{S}_1\cdot\mathbf{S}_2, \tag{3}$$

where $a_{\mathbf{k}}$ are conduction-electron operators. As in Wilson $\varepsilon(\mathbf{k})=k$, for $-1<k<1$. $a(r_i)$ is the projection of $a_{\mathbf{k}}$ on the site $i=1,2$ where two-spin $\frac{1}{2}$ magnetic moments $\mathbf{S}_1$ and $\mathbf{S}_2$ reside. For generality, a direct interaction $K_0'\mathbf{S}_1\cdot\mathbf{S}_2$ is allowed. Such a term is also generated (RKKY) by the first part of (3) to second order in J.

Symmetry about the midplane of the two moments is used to construct even- and odd-parity states $a_{\mathbf{k}e}$ and $a_{\mathbf{k}o}$ from $a_{\mathbf{k}}$ in terms of which

$$H_{\text{int}}=J_0\sum_{\mathbf{k},\mathbf{k}'}(\mathbf{S}_1+\mathbf{S}_2)\cdot[g_e(\mathbf{k})g_e(\mathbf{k}')a^\dagger_{\mathbf{k}'e}\sigma a_{\mathbf{k}e}+g_o(\mathbf{k})g_o(\mathbf{k}')a^\dagger_{\mathbf{k}'o}\sigma a_{\mathbf{k}o}]$$
$$+(\mathbf{S}_1-\mathbf{S}_2)\cdot[g_e(\mathbf{k})g_o(\mathbf{k}')a^\dagger_{\mathbf{k}'o}\sigma a_{\mathbf{k}e}+\text{H.c.}]+K_0'\mathbf{S}_1\cdot\mathbf{S}_2, \quad (4)$$

where $g_e(\mathbf{k})=\cos\mathbf{k}\cdot\mathbf{R}$, $g_o(\mathbf{k})=i\sin\mathbf{k}\cdot\mathbf{R}$.

This model is difficult to do calculations with because it has $\mathbf{k}$-dependent coupling constants. In the Kondo problem the $\mathbf{k}$ dependence of the coupling constant is known to be *irrelevant;* we expect the same in the present problem. We take the value of $g_{e,o}$ at $\mathbf{k}=k_\mathrm{F}$ to get (after integration over angles)

$$H_{\text{int}}=\textstyle\sum_{k,k'}(\mathbf{S}_1+\mathbf{S}_2)\cdot(J_e a^\dagger_{k'e}\sigma a_{ke}+J_o a^\dagger_{k'o}\sigma a_{ko})+\mathbf{S}_1-\mathbf{S}_2)(iJ_m a^\dagger_{k'e}\sigma a_{ko}+\text{H.c.})+K_0'\mathbf{S}_1\cdot\mathbf{S}_2. \quad (5)$$

Here

$$J_m=(J_eJ_o)^{1/2},\quad J_{e,o}=(J_0/2)(1\pm\sin k_\mathrm{F}R/k_\mathrm{F}R). \quad (6)$$

The RKKY interaction generated to second order is

$$H_{\text{RKKY}}=(8\ln 2)\rho(J_e-J_o)^2\mathbf{S}_1\cdot\mathbf{S}_2\equiv K_0\mathbf{S}_1\cdot\mathbf{S}_2, \quad (7)$$

which is always ferromagnetic. Antiferromagnetic couplings can be studied by adjustment of K_0' or alternately by the use of general values for J_m/J_e, J_m/J_o with K_0' set to zero.

Wilson's momentum-shell renormalization together with his choice of basis states on the two-channel Hamiltonian gives the recursion relation for the Hamiltonian H_N at the Nth iteration:

$$H_{N+1}=\Lambda^{1/2}H_N+\sum_{p=e,o}(f^\dagger_{Np}f_{N+1p}+f^\dagger_{(N+1)p}f_{Np}), \quad (8)$$

where Λ is the step size for logarithmic discretization, and f_{Ne} and f_{No} are basis operators obtained from a_{ke} and a_{ko} by transformations used by Wilson.[1]

In our calculations, we have kept up to about 1200 states at each iteration and used $\Lambda=2.5$ and 3. For the single-impurity problem about 1200 states and $\Lambda=2$ yielded Wilson an accuracy in the large iteration eigenvalues of $\sim 10^{-6}$. In our two-channel problem the asymptotic accuracy achieved for the coupling constants we use is better than 10^{-3}.

There are three quantum numbers specifying the many-body eigenstates. We have adopted the notation $(Q,2S,P)_n$ for the states, the first number standing for total charge above or below charge neutrality, the second number standing for twice the total spin, and the third for the parity—0 for even and 1 for odd. The subscript labels in sequence of increasing energy the states with the same quantum numbers. To arrive at some qualitative conclusions, we display in Fig. 1 the flow of the energy of the lowest bunch of states which are asymptotically degenerate in the strong-coupling limit for various initial parameters. It should be remembered that an iteration N corresponds roughly to a temperature $\Lambda^{-N/2}$ (in units of the bandwidth).

(a) $J_e=J_o$ *(noninteracting impurities).*—From Eq. (7) or in the first iterations of the renormalization procedure, no RKKY coupling between the two moments is introduced for $J_e/J_o=1$. This is true at any iteration. Figure 1(a) shows the flow of the eigenvalues at odd iterations. We have also separately performed a calculation for a single magnetic impurity. All the eigenvalues shown in Fig. 1(a) are obtained from a combination of appropriate pairs of the single-impurity eigenvalues.

There are two kinds of symmetries in the noninteracting impurity Hamiltonian, which are reflected in the degeneracies in Fig. 1(a). First, there is the parity symmetry, reflected for instance in the degeneracy of the 110_1 and the 111_1 states. Second, there is the simultaneous rotation of spin triplet to spin singlet with a flip of parity. This is reflected, for instance in the degeneracy of the 000_1 and 021_1 states.

(b) $S=1$ *two-channel problem.*—This is calculated by our keeping only the triplet state of $\mathbf{S}_1+\mathbf{S}_2$ in H_0. The second term in H_0 is then effectively zero since it has matrix elements only between the singlet and triplet states of $\mathbf{S}_1+\mathbf{S}_2$. The problem then corresponds to a spin-1 impurity interacting with two conduction-electron channels with coupling constants J_e and J_o, respectively. Let $J_e>J_o$. A two-stage Kondo effect is expected[5] with an intermediate unstable spin-$\frac{1}{2}$ fixed point characterized by a Kondo temperature $T_\mathrm{K}(J_e)$ and a low-temperature spin-0 fixed point characterized by a lower Kondo temperature $T_\mathrm{K}(J_o)$. Figure 1(b) shows the Hamiltonian flows for this case. Both the symmetries mentioned for the noninteracting impurity case are absent. The ground state is 021_1 and the 000_1 state is degenerate with the 000_2 state. Such degeneracies are characteristic of the spin-1 Kondo effect. The intermedi-

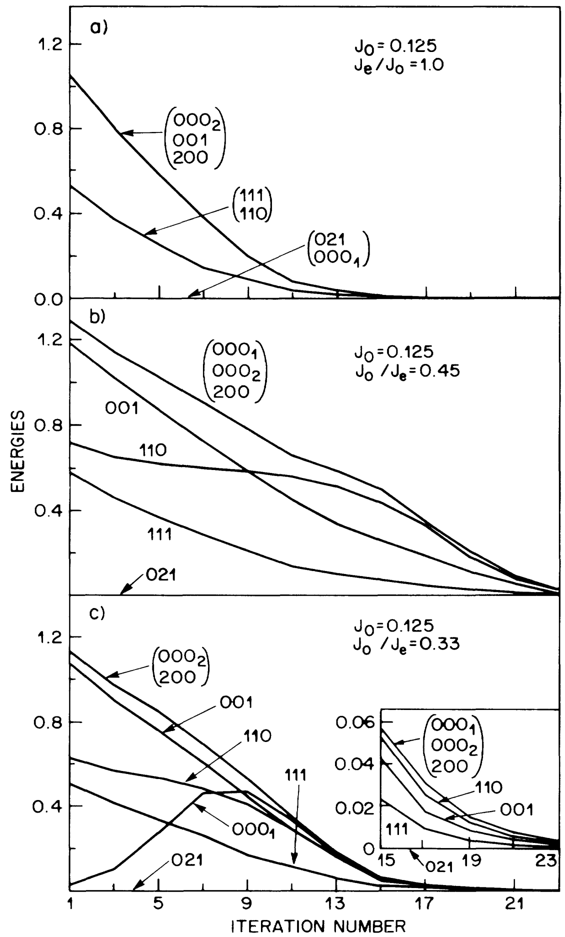

FIG. 1. The eigenvalue flows for H_N [Eq. (8) in the text] for the two-impurity problem for odd iterations. Only the lowest bunch of states which becomes asymptotically degenerate is shown. T_K is defined as $(2\rho J)^{1/2} d \exp(-1/2\rho J)$. (a) Noninteracting impurities; (b) impurities locked in a triplet state at the outset; and (c) impurities interacting ferromagnetically for $K_0 \approx T_K/3$. Inset: Energies for large iterations on an expanded scale.

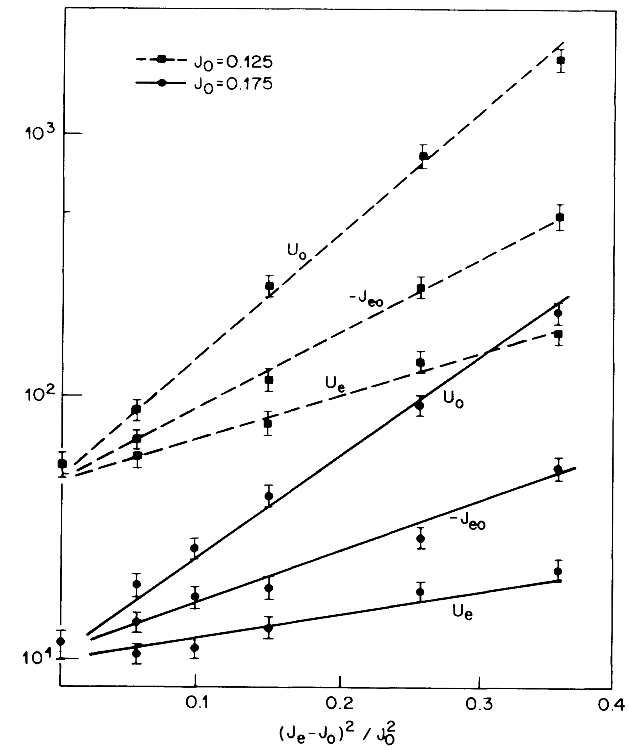

FIG. 2. The values of the coefficients in the asymptotic effective Hamiltonian normalized to the density of states for various values of the initial coupling constants.

ate unstable-fixed-point Hamiltonian of a spin-$\frac{1}{2}$ impurity is also seen in the calculations. If we use $K_0 \gg T_K$ in the general problem, we find that the states lock to the $S=1$ problem at $T \approx K_0 \gg T_K$ and subsequently a two-stage Kondo effect as for the $S=1$ problem follows.[5]

(c) *Kondo energy larger than RKKY energy.* —Finally, we discuss the case $J_e \neq J_o$ and such that $T_K \gg K_0$, which is of great interest for the heavy fermion solids. Figure 1(c) shows the results of odd iteration for parameters such that $T_K \approx 3K_0$. We have checked up to $T_K \approx 10K_0$ to make sure that the results shown are representative of $T_K \gg K_0$.

The large-N (iteration number) eigenvalues (i.e., the large-N fixed-point Hamiltonian) for odd iterations for finite values of J_e and J_o are the same as the small-N eigenvalues for even iterations (not shown) and vice versa. This means that the even- and odd-parity states both acquire a phase shift of $\pi/2$ near the fixed point. Following Wilson's reasoning, this means that the fixed-point Hamiltonian corresponds to strong coupling with both J_e and $J_o \rightarrow \infty$.

Throughout the flows shown in Fig. 1(c) parity degeneracy stays lifted; for instance, 110_1 and 111_1 are nondegenerate. Similarly the lack of the triplet-odd-parity and singlet-even-parity degeneracy at the zeroth iteration continues except asymptotically near the fixed point. The symmetries of the effective Hamiltonians at any finite temperature are thus shown to be unlike those of the noninteracting problem, Fig. 1(a).

On the other hand, the faster than linear rise in Fig. 1(c) of the state 000_1 corresponds to $K_0 \mathbf{S}_1 \cdot \mathbf{S}_2$ being a relevant operator about the weak-coupling fixed point.[4] The degeneracy pattern subsequently of all states becomes close to that of Fig. 1(b) qualitatively displaying a ferromagnetic correlation between the magnetic moments while undergoing a Kondo effect.

These conclusions can be expressed quantitatively by our deducing an effective Hamiltonian to fit the eigenvalues close to the strong-coupling limit. There are in general seven *irrelevant* operators describing the deviation from the strong-coupling fixed point for the two-impurity problem (compared to two for the one-impurity problem). In terms of these such an effective Hamiltonian is

$$H_{12}=\sum_{p,\alpha}t_p(f^\dagger_{0p\alpha}f_{1p\alpha}+\text{c.c.})+\sum_p U_p(n_{0p}-1)^2+U_{eo}\{(n_{0e}-1)(n_{0\alpha}-1)+\sum_\alpha(f^\dagger_{0e\alpha}f^\dagger_{0e-\alpha}f_{0o-\alpha}f_{0o\alpha}+\text{c.c.})\}$$
$$+J_{eo}f^\dagger_{0e}\boldsymbol{\sigma}f_{0e}\cdot f^\dagger_{0o}\boldsymbol{\sigma}f_{0o}, \quad (9)$$

where $\alpha=\uparrow,\downarrow$ and n_{0p} is 0, 1, and 2. The coefficients in H_{12} are extracted from the fits to the asymptotic spectra such as shown in Fig. 1(c). For noninteracting impurities [case (a) above], one must have $U_e=U_o=U_{eo}=-J_{eo}$ and $t_e=t_o$.

The relationship between the parameters is quite different for case (c). In Fig. 2 the numerically determined U_e, U_o and $|J_{eo}|$ normalized to the one-spin density of states ρ are shown for various values of J_0 and K_0. Within our numerical accuracy, we find that they are all given by

$$\{(1.7\pm0.3)\rho J_0\}^{-1/2}(\rho D)^{-1}\exp((2\rho J_0)^{-1}\{1+a_i[\rho K_0/(\rho J_0)^2]\})\simeq(\rho T_\text{K})^{-\{1+a_i[\rho K_0/(\rho J_0)^2]\}}, \quad (10)$$

where D is the bandwidth and a_i are constants whose value is different for the three terms. For $J_e>J_o$, $a_{U_e}=(0.09\pm0.01)/8\ln2$, $a_{U_o}=(0.27\pm0.02)/8\ln2$, and $a_{J_{eo}}=(0.17\pm0.02)/8\ln2$. The ratio $\approx 1{:}3{:}2$ between these quantities is noteworthy. We find U_{eo} decreasing towards 0 as a function of K_0/T_K; it must be 0 for the $S=1$ problem. A linear relationship between t_e and U_e, and t_o and U_o is expected based on Nozières's[3] "weak-universality" argument. Our numerical results give $t_{e,o}=-(1\pm0.3)U_{e,o}$. Note that for K_0 ferromagnetic the resonance width decreases from the Kondo value.

Equation (9) can be reexpressed in terms of sites 1 and 2. One then finds that the Hamiltonian displays ferromagnetic interactions among quasiparticle interactions at sites 1 and 2 for ferromagnetic K_0. Our preliminary calculations for antiferromagnetic K_0 lead to an increased resonance width and antiferromagnetic interactions between such quasiparticles.

Following Nozières and Blandin,[3] we may construct a phase-shift expansion from Eq. (9):

$$\delta_{e\uparrow}(\varepsilon)=\tfrac{1}{2}\pi+\alpha_e\varepsilon+(\phi_{eo}+\psi_{eo})\delta n_{o\uparrow}+(\phi_{eo}-\psi_{io})\delta n_{o\downarrow}+(\phi_{ee}-3\psi_{ee})\delta n_{e\downarrow}, \quad (11)$$

and similar expression for $\delta_{e\downarrow}$, $\delta_{o\uparrow}$, etc. Here α_p is related to t_p, $\phi_{ee}-3\psi_{ee}$ to U_e, ϕ_{eo} to U_{eo}, and ψ_{eo} to J_{eo}. With $\phi_{eo}=0$ for the ferromagnetic case, weak universality gives $\alpha_p=-2\rho(\phi_{pp}-3\psi_{pp})$. Wilson's ratio can be calculated to be

$$(\Delta\chi/\chi)/(\Delta C/C)=2+4\rho(\psi_{eo}+\phi_{eo})/(\alpha_e+\alpha_o),$$

which is thus no longer universal.

We have shown that the Hamiltonian (9) is necessary to describe the low-temperature behavior to two magnetic impurities for $K_0 \ll T_\text{K}$. This has important implications for the heavy-fermion problem. If, as is expected, the characteristic three-particle interaction energies are much smaller than pair interaction energies, the low-temperature behavior of the heavy-fermion lattice may be discussed in terms of a sum of pair Hamiltonians of the form (9).

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[(a)]Present address.

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