

Critical point in the solution of the two magnetic impurity problem

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We discuss in a physical fashion the key results obtained in the solution of the two interacting Kondo impurity problem via the numerical renormalization group. Special emphasis is placed on the nature of the unstable fixed point separating the regimes of flows to the correlated Kondo effect fixed point and the locked-impurity singlet fixed point.

I. INTRODUCTION

Wilson¹ devised a remarkable numerical renormalization-group method to solve the single-impurity Kondo problem given by the Hamiltonian

$$H = -JS_0 \cdot \psi_0^\dagger \sigma \psi_0 + \sum_{i < j} t_{ij} \psi_{i\alpha}^\dagger \psi_{j\alpha} + \text{H.c.}, \quad (1)$$

where an impurity spin at site 0 has a local antiferromagnetic interaction with conduction electrons. The latter have a kinetic energy specified by t_{ij} , and move in a band of width D . Subsequently, the problem was solved² analytically using a generalized Bethe ansatz with the results in agreement with the Wilson solution. In the last few years we^{3,4} have used Wilson's method to solve the problem of two magnetic impurities interacting with conduction electrons and through them with each other [the RKKY (Ruderman-Kittel-Kasuya-Yosida) interaction]. This problem does not appear soluble analytically.

The model Hamiltonian is

$$H = \int d^3k \epsilon_k a_{k\alpha}^\dagger a_{k\alpha} - J[\mathbf{s}(r_1) \cdot \mathbf{S}_1 + \mathbf{s}(r_2) \cdot \mathbf{S}_2]. \quad (2)$$

It is useful to work with states which have even (e) and odd (o) parity about the midplane of the two impurities at sites 1 and 2. With some simplifications, the second term in H is transformed to

$$H = \sum_{k,k'} (\mathbf{S}_1 + \mathbf{S}_2) \cdot \left[J_e a_{k'e}^\dagger \frac{\sigma}{2} a_{ke} + J_o a_{k'o}^\dagger \frac{\sigma}{2} a_{ko} \right] + (\mathbf{S}_1 - \mathbf{S}_2) \cdot \left[J_m a_{k'e}^\dagger \frac{\sigma}{2} a_{ko} + \text{H.c.} \right]. \quad (3)$$

The expressions for J_e , J_o , and J_m in terms of the variables in (2) have been given.³ The relevant energy scale governing interactions on site is the Kondo temperature $T_K \approx \exp(-1/|J|)$, with $J^2 = J_e^2 + J_o^2 + 2J_m^2$. (The half bandwidth has been taken to be unity.) To second order in the J 's an interaction (RKKY) between the two moments is generated,

$$H_{\text{RKKY}} = I_o \mathbf{S}_1 \cdot \mathbf{S}_2, \quad (4)$$

with

$$I_o = 2 \ln 2 (J_e^2 + J_o^2 - 2J_m^2). \quad (5)$$

If we adjust the ratios J_m/J_e and J_m/J_o so that the generated $I_o = 0$ but add a term of the form (4), the renormalization-group results are identical to those for Eq. (3).

We found that the ground state of a pair of spin one-half impurities with nonzero separation is always a singlet. The principal physical results of this solution are the following.

(a) For the initial interaction between the moments I_o , ferromagnetic (>0), or antiferromagnetic (<0), with $I_o > -2.2T_K$, the low-temperature behavior is that of a correlated Kondo effect. The fixed-point Hamiltonian is that for two independent Kondo impurities but the ground-state expectation value $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ is not zero, as for two independent spins, even for $|I_o|/T_K \ll 1$. The quantitative behavior is given in Ref. 4. The low-energy (or low-temperature) properties, determined by the leading irrelevant operators about the fixed point, depend on both I_o and T_K as shown in Fig. 3 of Ref. 4. The universality in the properties characteristic of the single-impurity Kondo problem is lost in the two-impurity problem.

The phase shift of the conduction electrons in this regime is asymptotically $\pi/2$ in both the even and odd parity channels, and not larger than $\pi/2$ in one and less than $\pi/2$ in the other with the sum equal to π as naively expected for interacting resonances (see Fig. 1). At the fixed point there is then particle-hole symmetry in each channel separately. The fixed-point Hamiltonian contains no coupling between the odd and the even channels—the problem asymptotically becomes that of two pointlike orthogonal scatterers.

(b) For larger antiferromagnetic interactions $I_o < -2.2T_K$, no Kondo effect occurs. The asymptotic phase shift is zero. The two magnetic moments are not in a singlet state until $I_o \ll -T_K$ but the total spin including the conduction electrons is zero. The Kondo correlations clearly persist in this regime.

(c) The transition between the regimes described in paragraphs (a) and (b) is marked by an unstable fixed point (a critical point) at which the staggered susceptibility and the specific-heat coefficient γ diverge. The ground-state correlation $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ approaches $-\frac{1}{4}$. The unstable fixed point is a new kind of fixed point at and

around which a local description of the impurity and conduction electron degrees of freedom in terms of a local Fermi-liquid breakdown. [The renormalization group flows are shown in Figs. 2(a)–2(c)].

The behavior in the very strongly ferromagnetic or antiferromagnetic regimes $|I_0| \gg T_K$ is straightforward and was guessed at or supported by earlier calculations.^{5,6} For comparison with earlier results, see Ref. 7. For strong antiferromagnetic I_0 the two moments lock to a singlet at a temperature well above T_K . This singlet is then decoupled from the conduction electrons and may be treated perturbatively. The surprise in the solution is how slowly the behavior approaches this limit as $|I_0|/T_K$ increases. For strong ferromagnetic coupling $I_0 \gg T_K$, the two impurities form an $S=1$ state which undergoes a two-channel Kondo renormalization to ultimately a singlet state for the whole system, but with $\langle S_1 \cdot S_2 \rangle$ close to the triplet value of $\frac{1}{4}$.

Of the new results noted in paragraphs (a), (b), and (c)

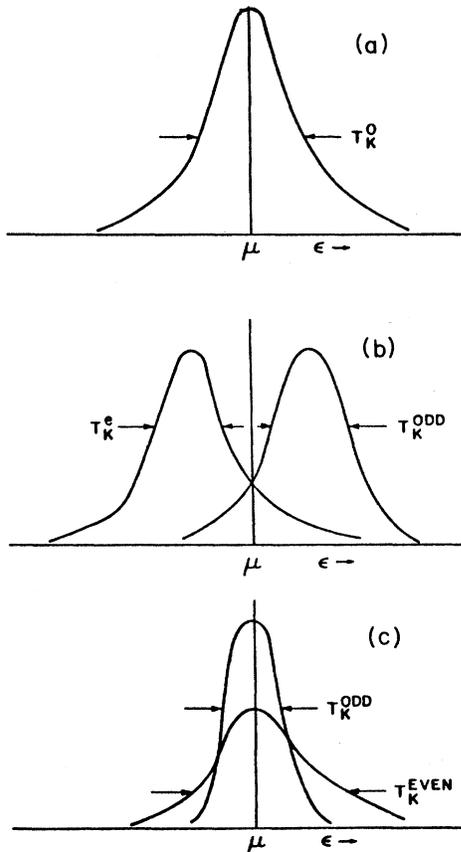


FIG. 1. Energy distribution of (a) the single-impurity Kondo resonance, (b) the resonance behavior naively expected for two interacting Kondo resonances, and (c) the actual resonance behavior found for two coupled Kondo resonances in Refs. 3 and 4.

above, especially interesting is the existence of the critical point at a finite value of a coupling constant, noted in (c). Our principal aim here is to give a physical description of this critical point in terms of the passage between the two radically different fixed points on either side of it.

II. $\pi/2$ PHASE SHIFT IN EACH CHANNEL

One would, of course, like to have a simple physical interpretation of all the results. We have not succeeded in this and must accept them as simply the results of a complicated calculation (just as the $J \rightarrow \infty$ fixed point at $T \rightarrow 0$ is accepted for the single-impurity Kondo problem). We take special note of one of the results which is crucial to the understanding of the “critical point”: The phase shift in both the odd and the even parity channels at $T \rightarrow 0$ is $\pi/2$ for all values of coupling constants in which the Kondo effect occurs (to the right of the critical point in Fig. 2). This is a remarkable result which is worth dwelling on.

Just as for the Kondo problem, the asymptotic low-energy behavior for the two-impurity problem is expressible by an effective Hamiltonian consisting of a fixed-point Hamiltonian H^* and the leading irrelevant operators about it which can be classified into one-electron Hamiltonian $H^{(1)}$ and an interaction Hamiltonian H^{int} ,

$$H_{12}^{\text{eff}}(1, \dots, N) = H^* + (H^{(1)} + H^{\text{int}})T. \quad (6)$$

Consider H^* . Recall that for the single-impurity problem Wilson constructs an effective one-dimensional problem such that H^* is a free-electron Hamiltonian for all odd numbers of lattice sites if the original Hamiltonian has an even number of lattice sites and vice versa. This means an electron is effectively lost as a “bound state” or that the asymptotic phase shift is $\pi/2$, as indeed required by Friedel’s sum rule. Equivalently a resonance appears at the chemical potential which is exactly half occupied [see Fig. 1(a)]. With Wilson’s procedure the two-impurity problem is expressed^{3,4} as two coupled one-dimensional problems, one in the even parity channel and the other in the odd parity channel. By Friedel’s theorem the *sum* of the phase shifts in the two channels must be π or the total number of electrons lost must be two. One would have expected the resonance behavior as in Fig. 1(b) or a phase shift larger than $\pi/2$ in one channel and less than $\pi/2$ in the other. Our result is that starting with an even (odd) lattice, H^* is that of noninteracting electrons for an odd (even) lattice. The resonance behavior is therefore as schematically shown in Fig. 1(c) with phase shift $\pi/2$ in each channel.

The implication of this result is that it is not meaningful to speak of a Kondo effect for individual moments but only of the Kondo effect for appropriate symmetry channels—odd and even parity in this case. The result is equivalent to the statement that the coefficient of all interference terms between the odd and even channels such as the third term in Eq. (3) or any others generated in the intermediate stages of the renormalization group go to zero at the fixed point. Note that since such terms multiply the operator $(S_1 - S_2)$, matrix elements coupling the $S=0$ and $S=1$ states of the two impurities vanish in the

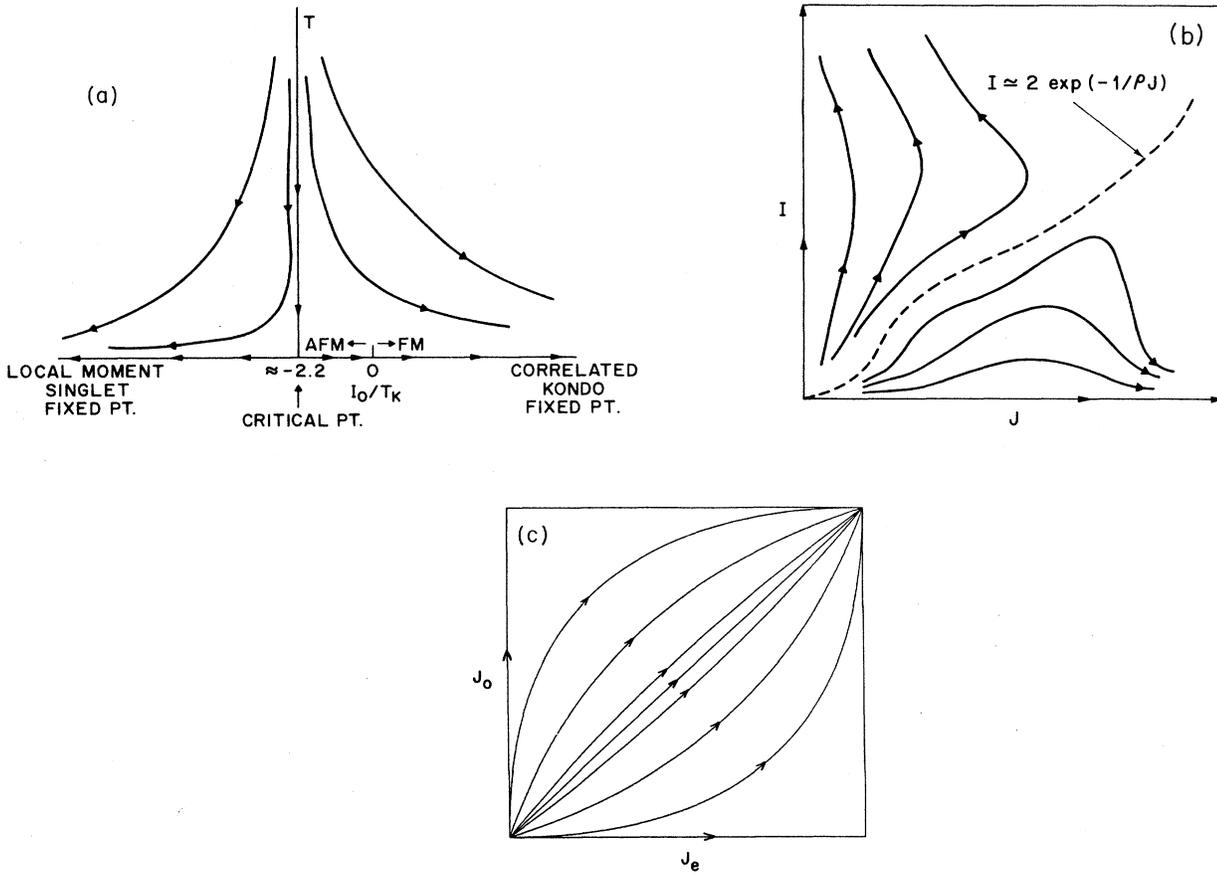


FIG. 2. (a) Schematic renormalization-group flows in the temperature $-I_0/T_K$ plane. (b) Schematic flow diagram in parameter space for the antiferromagnetic regime. The two relevant parameters are the RKKY coupling I and the Kondo coupling J . Here and in (c) the end points represent one or more of the parameters scaling to infinity. The curved line up the center represents the line $I \approx 2.2T_K$, terminating at the unstable fixed point. All flows with initial parameters to one side or the other of this line terminate at either the correlated Kondo effect (strong-coupling) fixed point or the locked-impurity singlet fixed point. (c) Schematic flow diagram for the ferromagnetic regime $J_m = (J_e/J_0)^{1/2}$. The center diagonal is the flow for $J_e = J_0$, the independent impurities case. When $J_e \neq J_0$, the flows deviate toward one of the marginally unstable fixed points. Flows terminate at the stable correlated Kondo effect (strong-coupling) fixed point. As in (b), this diagram is schematic in the sense that it implies $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ is the same for all flows (here, the implication is that it is zero), since all end at the same point. The fixed points are the same, but the correlations are not.

fixed-point Hamiltonian. This means

$$H^* = H_{\text{free}}^{*\text{even}} + H_{\text{free}}^{*\text{odd}}, \quad (7)$$

where H_{free} are free-electron Hamiltonians and the superscripts refer to the parity of the free quasiparticles.⁸

III. CRITICAL POINT

The Hamiltonian of the two-impurity problem including terms generated to any order in the renormalization can be divided into (i) the subspace in which the two impurities are in a singlet state: $H_{S=0}$, $S = S_1 + S_2$; (ii) the subspace in which they are in a triplet state: $H_{S=1}$; and (iii) the subspace connecting the former with the latter: H_{mix} . Both the impurity $S=0$ and $S=1$ subspaces are diagonal in the cumulative parity of the conduction-

electron states, while the mixing term is purely off diagonal in the cumulative parity of such states. Thus, in general, we can write

$$H = \begin{pmatrix} \begin{bmatrix} H_{S=0}^{\text{even}} & 0 \\ 0 & H_{S=0}^{\text{odd}} \end{bmatrix} & \begin{bmatrix} 0 & H_{\text{mix}} \\ H_{\text{mix}} & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & H_{\text{mix}} \\ H_{\text{mix}} & 0 \end{bmatrix} & \begin{bmatrix} H_{S=1}^{\text{even}} & 0 \\ 0 & H_{S=1}^{\text{odd}} \end{bmatrix} \end{pmatrix}, \quad (8)$$

where S refers only to the impurities and the even-odd parity only to the conduction-electron states.

$H_{S=0}$ is just the free-electron Hamiltonian; this sector undergoes no Kondo renormalizations and has a phase shift of zero. We also know that the low-temperature fixed point of $H_{S=1}$ is a free-electron Hamiltonian $H_{S=1}^*$

with a total phase shift π . From the discussion above, we know that a phase shift of $\pi/2$ occurs separately in the even and odd parity channels implying that at the low-temperature fixed point $H_{\text{mix}} \rightarrow H_{\text{mix}}^* = 0$.

For large antiferromagnetic I_o , $-I_o/T_K \gg 1$, the ground state of $H_{S=0}^*$ lies lower than that of $H_{S=1}^*$ and for large ferromagnetic I_o , $I_o/T_K \gg 1$, the ground state of $H_{S=1}^*$ lies lower than that of $H_{S=0}^*$. It follows that there must exist a value of I_o/T_K where the ground state of $H_{S=0}^*$ and $H_{S=1}^*$ are degenerate. The unstable fixed point (the critical point) exists at this special value $(I_o/T_K)_c$. This simple argument implies that at the fixed point, the nondegenerate ground state with zero total axial charge (see below), zero total spin, and even parity has equal admixture of the impurity $S=0$ and $S=1$ states. This leads to $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -\frac{1}{4}$. This is indeed, within numerical accuracy, found in the calculations.

Suppose one measures the *staggered* susceptibility χ_π in the problem by applying a field $|H|$ that is antiparallel at the two sites. χ_π is then the response to $\mathbf{H} \cdot (\mathbf{S}_1 - \mathbf{S}_2)$. This term lifts the degeneracy between $H_{S=0}^*$ and $H_{S=1}^*$ to linear order in $|H|$. It follows that χ_π diverges at the critical point, as calculated.

The calculated divergence in the coefficient γ of the linear specific heat is a more subtle matter. The divergence means that infinitely many degrees of freedom are affected at the critical point, unlike away from it where the low-temperature problem is quite local. Alternatively the degeneracy implies a singular density of states of excitations as $\omega \rightarrow 0$. We believe this is the physical basis for the divergence of the specific heat.

An analytically soluble model which also has a critical point is an $S = \frac{1}{2}$ impurity interacting with two conduction-electron channels with coupling constants J_1 and J_2 . Nozières and Blandin⁹ had conjectured a critical point for $J_1/J_2 = 1$. This critical point was discovered in

a Wilson renormalization-group calculation by Cragg, Lloyd, and Nozières,¹⁰ who also found the even-odd lattice degeneracy. Subsequently, the model was solved¹¹ by the Bethe ansatz. The specific-heat coefficient γ was found to diverge at the critical point.

The divergence of the specific-heat coefficient means that a Fermi-liquid description of the low-temperature properties breaks down near the critical point. In the temperature coupling-constant plane the flows will look as in Fig. 2(a).

IV. EXPANSION ABOUT THE CRITICAL POINT

The breakdown of the Fermi-liquid description is evident in the study of the leading operators about the low-temperature fixed point $H^{(1)}$ and H^{int} . $H^{(1)}$ is written

$$H^{(1)} = t_e (f_{0e}^\dagger f_{1e} + \text{H.c.}) + t_o (f_{0o}^\dagger f_{1o} + \text{H.c.}), \quad (9)$$

where f_{io} and f_{ie} are the annihilation operators in the Wilson representation for the odd and the even conduction-electron channel, respectively. For the single-impurity one-channel problem $t = D/T_K^0$, where T_K^0 is the "zero temperature" Kondo temperature. For $I_o = 0$ one has $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = 0$, $t_e = t_o = t$. For any finite I_o , ferromagnetic or antiferromagnetic, t_e and $t_o > t$ in the "Kondo regime", $I_o/T_K > -2.2$. This reflects the increased matrix element for hopping of the quasiparticles when the spins on the two sites are correlated, i.e., $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle \neq 0$. Near the critical point t_e and t_o diverge. The interesting dependence of $t_{e,o}$ on I_o/T_K has been given.⁴

While the single-impurity Kondo effect has just one interaction term asymptotically, the two-impurity problem has in general five interaction terms. This was also noted by Yamada and Yosida¹² and by Schlottmann,¹³

$$H^{\text{int}} = \sum_{p=e,o} U_p (n_{0p} - 1)^2 + U_{eo} \left[(n_{0e} - 1)(n_{0o} - 1) + \sum_{\sigma} (f_{0e}^\dagger \sigma f_{0e}^\dagger - \sigma f_{0o} - \sigma f_{0o\sigma} + \text{H.c.}) \right] + J_{eo} f_{0e}^\dagger \sigma f_{0e} \cdot f_{0o}^\dagger \sigma f_{0o}. \quad (10)$$

Here $n_{0p} = \sum_{\sigma} f_{0p\sigma}^\dagger f_{0p\sigma}$. The simplifications introduced in the model solved, in which the interaction between the even and odd channel is effectively a δ function in space, induce an additional symmetry, axial charge. Axial charge \mathbf{j} is a three-dimensional axial vector quantity which is conserved in the one-impurity problem.⁴ In particular,

$$\begin{aligned} j^+ &= \sum_n (-1)^n f_{np}^\dagger f_{np}^\dagger, \\ j^- &= (j^+)^\dagger, \\ j^z &= \sum_n \frac{1}{2} (f_{np}^\dagger f_{np}^\dagger + f_{np}^\dagger f_{np}^\dagger - 1). \end{aligned} \quad (11)$$

With this symmetry, the third and fourth terms in (9) are required to have equal coefficients, and H^{int} can be

rewritten as

$$H^{\text{int}} = \sum_{p=e,o} 4U_p j_{0p}^z + 4U_{eo} \mathbf{j}_{0e} \cdot \mathbf{j}_{0o} + 4J_{eo} \mathbf{s}_{0e} \cdot \mathbf{s}_{0o}. \quad (12)$$

As noted earlier,⁴ weak universality provides only two relationships between the seven coefficients required to characterize the low-temperature properties of the two-impurity problem: $U_e/t_e = \text{const} \approx 1$, $U_o/t_o = \text{const} \approx 1$. This means that the universality (all low-temperature properties expressible in terms of a single parameter T_K^0) of the single-impurity Kondo problem has been lost. Near the unstable fixed point $J_{eo} \rightarrow 0$, implying an additional symmetry of the critical point, the conservation of \mathbf{s}_e and \mathbf{s}_o separately, instead of just their sum.

Given $H^{(1)} + H^{\text{int}}$, one can calculate the uniform and the staggered susceptibilities χ_0 and χ_π , respectively, in the mean-field approximation, as was done for the single-impurity problem by Blandin and Nozières.⁹ We find

$$\chi_0 = \chi_0^o [1 - \chi_0^o (U_e + U_o - 2J_{eo})], \quad (13)$$

$$\chi_\pi = \chi_\pi^o [1 - \chi_0^o (3U_{eo} - J_{eo})], \quad (14)$$

where χ_0^o is the susceptibility from the one-electron term alone. Near the unstable fixed point $U_e, U_o \rightarrow -\infty$, $U_{eo} \rightarrow +\infty$ ($|U_e|, |U_o|, |U_{eo}| \sim [(I_o/T_K) - (I_o/T_K)_c]^{-2}$), and $J_{eo} \rightarrow 0$. Here the subscript c stands for the value at the critical point. Equations (12) and (13) are, of course, only valid in the mean-field region. However, they predict behavior consistent with $\chi_\pi \rightarrow \infty$, as found numerically. They also predict $\chi_0 \rightarrow 0$. There are large errors in the determination of χ_0 near the critical point, but $\chi_0 = 0$ is consistent with numerical accuracy.

V. IMPURITY SPIN-SPIN CORRELATION

The renormalization-group equations for the Hamiltonian in the Kondo regime lead to a fixed point which contains no information about $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$, and is, in fact, indistinguishable from the fixed point obtained starting from $I_o = 0$. The effect of I_o is seen in the deviations from the fixed point and thus in all observable properties. In the renormalization-group equation for the correlation function $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ the effect of I_o is seen at the fixed point; its ground-state (fixed-point) value depends on I_o no matter how small I_o/T_K is. Since the fixed point is characterized by J_e, J_o scaling to infinity, a finite ground-state value for $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ is only possible if one thinks of I_o also as scaling to infinity and in the same fashion as J_e and J_o as far as the renormalization-group recursion for $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ is concerned.¹⁴

VI. OTHER METHODS

Much was learned in the Kondo problem by perturbation theory,¹⁵ poor man's scaling,¹⁶ and Gellman-Low renormalization equations about the high-temperature weak-coupling fixed point. Considerable effort with such methods was expended by Abrahams, Varma, and Zawadowski¹⁷ in the two-impurity Kondo problem. These methods, however, flounder. The most interesting difficulty that appears is that in any order of perturbation theory, logarithmically divergent diagrams appear which cannot be generated from any divergent diagrams in the previous order. All such diagrams appear to have the feature that the Kondo effect at one site is interrupted by the spin flip between the two sites induced by their mutual interaction. Two low-order examples of such a diagram are given (Fig. 3).

With this sort of thing it is not clear how to proceed. Perturbation theory, however, provides the answer as to why the scale for the physical behavior in the two-impurity problem is set by I_o/T_K . The crucial point is that around the high-temperature-local-moment fixed point, I_o is the coefficient of a relevant operator; perturbation calculations yield corrections $\rho I_o^2 D / \omega$, where D is the bandwidth and ρ is the density of states. On the other hand J is a marginal operator yielding corrections

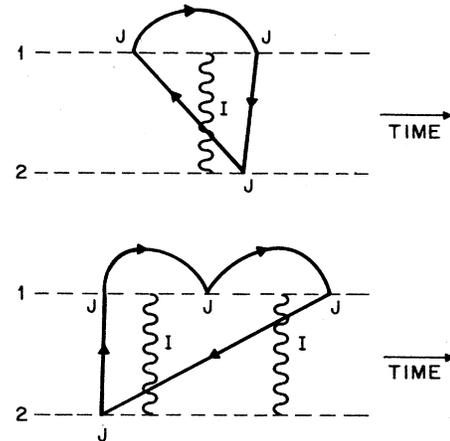


FIG. 3. Low-order diagrams leading to logarithmic corrections to the effective interaction between impurities 1 and 2, which are not generated by previous orders in perturbation theory. The dashed lines are the pseudofermion propagators for the impurities, full lines represent the propagators for the conduction electrons, and the wiggly lines represent the RKKY interaction.

$\rho J^2 \ln D / \omega$. For the two parameters to affect physical quantities comparably, I_o must be compared to a quantity which is exponentially smaller than J . Hence I_o/T_K sets the scale.

Another method which fails for the two-impurity problem for very related reasons is the path-integral representation.^{18,6} The spin flips at successive times at one site $\{t_{1i}\}$ and at the other sites $\{t_{2i}\}$ become interrelated in a manner which has proved impossible to handle mathematically. A phase relationship of the Kondo effect at the two sites is indicated. Such a phase relationship seems to be the essence of the correlated Kondo effect. Bethe ansatz methods also appear inapplicable because of the coupling between channels. At the moment it appears the full low-temperature solution can only be obtained via Wilson's numerical renormalization methods used in Refs. 3 and 4. Mean-field methods of the large- N variety are known to reproduce key features of the correct solution to the single-impurity Kondo problem; when applied to the interacting two-impurity Kondo problem, they give¹⁹ results different from the solutions of Refs. 3 and 4.

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