

1/N expansion for the Kondo lattice

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A diagrammatic expansion is developed for the partition function of a lattice of spin- j local moments interacting with a band via the Coqblin-Schrieffer exchange interaction. By examining the limit of large spin degeneracy, $N=2j+1$, a $1/N$ expansion is obtained for the partition function, which clearly exhibits how local spin fluctuations are enhanced by large spin degeneracy. The competition between the Ruderman-Kittel-Kasuya-Yosida interaction and local Kondo spin fluctuations is examined using scaling theory, and the critical value of the Kondo coupling constant above which a spin-compensated Kondo-lattice ground state is stable is shown to tend to zero as $O(1/N)$, providing new justification for the applicability of the Kondo-lattice model to rare-earth systems. Physical arguments are advanced, based on the nature of the crossover to the strong-coupling regime, which suggest that the low-temperature excitations of the Kondo lattice form a narrow band of heavy fermions.

I. INTRODUCTION

The ground-state properties of a lattice of localized moments interacting with an electron band via a Kondo spin-exchange process are of particular interest to current research on rare-earth "mixed-valence" and "Kondo-lattice" systems.¹⁻³ These systems are believed to be well modeled by the Anderson Hamiltonian, describing a lattice of localized f levels, hybridizing with a delocalized spd electron band. When the atomic f level is well below the Fermi level the rare-earth ion behaves as a localized moment in which the orbital and spin angular momenta are coupled together into a state of definite total angular momentum j . Coqblin and Schrieffer⁴ have shown that for an impurity Anderson model, in this localized moment regime the spin- j moment interacts with the band via a generalized Kondo spin-exchange process. Extending their result to a lattice of rare-earth ions with r sites, in the local-moment regime the system will be described by a Kondo-lattice Hamiltonian

$$H = H_b + \sum_{i=1}^r H_f^i + \sum_{i=1}^r H_K^i, \tag{1}$$

where

$$H_b = \sum_{\vec{k}, \sigma} E(k) c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma}, \tag{2}$$

$$H_f^i = \sum_{m=-j}^j E_f f_m^{i\dagger} f_m^i + U \sum_{m=-j}^j \sum_{\substack{m'=-j \\ m' < m}}^j f_m^{i\dagger} f_m^i f_{m'}^{i\dagger} f_{m'}^i, \tag{3}$$

$$H_K^i = J \sum_{k, k', m, m'} c_{km}^{i\dagger} c_{k'm'}^i \times \left[f_{m'}^{i\dagger} f_m^i - (1/N) \delta_{mm'} \sum_{m''=-j}^j f_{m''}^{i\dagger} f_{m''}^i \right]. \tag{4}$$

Here $c_{\vec{k}\sigma}^\dagger$ creates a band electron of momentum \vec{k} , spin component σ ,

$$c_{km}^{i\dagger} = \sum_{\vec{k}', \sigma'} c_{\vec{k}'\sigma'}^\dagger \langle \vec{k}', \sigma' | R_i; k, j, m \rangle$$

creates a band electron at site i with energy $E(k)$, in the angular momentum state $|j, m\rangle$; $f_m^{i\dagger}$ creates an f electron at site i in the angular momentum state $|j, m\rangle$. $N=2j+1$ is the degeneracy of the f state.

For simplicity the band is taken to be featureless, with a constant density of states ρ , halfwidth D , centered on the Fermi level. The f level is below the Fermi energy and U is taken to be $\gg D - E_f$, so that charge fluctuations from the state of single f occupation are quenched out.

Previous studies of the Kondo lattice have been confined to the spin- $\frac{1}{2}$ case. Doniach^{5,6} treated the Kondo lattice in a mean-field approximation and showed that when the coupling constant $J\rho$ is greater than a critical value $(J\rho)_c$ of order $O(1)$, a spin-compensated ground state is stable relative to a magnetically ordered one. The effects of spin fluctuations were incorporated in later work, using real-space renormalization group^{7,8} and approximate functional-integral techniques.⁹ This work confirmed the essence of the mean-field result, setting a finer value on $(J\rho)_c$ somewhat below one. These values for the critical coupling constant cast doubt on the applicability of the Kondo-lattice model to real systems because such large coupling constants are neither observed in practice, nor are they theoretically feasible for an Anderson lattice in the local-moment regime.¹⁰

For large spin degeneracy $N=2j+1$, a new approach to the Kondo-lattice problem can be taken that was first suggested by Anderson.¹¹ In this case the largeness of degeneracy may be exploited to carry out an expansion of the physical properties in terms of the small parameter $1/N$. The hope is that the large- N limit will bear some resemblance to the behavior of rare-earth systems, which already have a large spin degeneracy. The work reported here is motivated by these considerations. Of particular interest in the results is the N dependence of $(J\rho)_c$, which is found to vanish as $O(1/N)$ providing renewed confi-

dence in the applicability of the Kondo-lattice model to rare-earth systems.

II. DIAGRAMMATIC EXPANSION OF PARTITION FUNCTION

The pseudofermion technique of Abrikosov¹² can be extended to the Kondo lattice. Following Abrikosov it is recognized that the large repulsive Hubbard term projects out the states in which the atomic f states are singly occupied. Rather than use (1), the Hubbard U term is omitted and instead the partition function is calculated for a lattice in which energies λ_i are assigned to the f state at site i as follows:

$$H^A = H_b + \sum \tilde{H}_f^i + \sum H_K^i, \quad (5)$$

$$\tilde{H}_f^i = \lambda_i \sum_m f_m^{i\dagger} f_m^i. \quad (6)$$

Since the f occupations are conserved by (5), its grand partition function $Z^A(\beta)$ can be expanded in terms of canonical partition functions of definite f occupation (n_i)

$$Z^A(\beta) = \sum_{(n_i)} \exp \left[-\beta \sum n_i \lambda_i \right] Z(n_1, n_2, \dots, n_r). \quad (7)$$

All energies are measured relative to the Fermi energy. The Kondo partition function is simply

$$Z^K(\beta) = e^{-\beta r E_f} Z(n_1 = 1, n_2 = 1, \dots, n_r = 1), \quad (8)$$

and it may be projected out from $Z^A(\beta)$ by differentiating with respect to the fugacities $z_i = e^{-\beta \lambda_i}$ of each site:

$$Z^K(\beta) = \left[\prod_{i=1}^r \frac{\partial}{\partial z_i} \right] Z^A(\beta) \Big|_{z_i=0}, \quad (9)$$

where the normalizing prefactor $e^{-\beta r E_f}$ has been left out.

The advantage of this technique is that Z^A can be expressed as a time-ordered exponential of the interaction $H_I = \sum_{i=1}^r H_K^i$, and this can be expanded diagrammatically as a sum of closed-loop Feynman diagrams using finite-temperature perturbation theory,

$$Z^A(\beta) = Z(H_0, \beta) \left\langle T \exp \left[-\int_0^\beta H_I(\tau) d\tau \right] \right\rangle_{H_0}. \quad (10)$$

Here $H_0 = H_b + \sum \tilde{H}_f^i$ and

$$H_I(\tau) = e^{H_0 \tau} \sum_{i=1}^r H_K^i e^{-H_0 \tau}. \quad (11)$$

Figure 1 summarizes the Feynman rules for the expansion of the time-ordered exponential. In the diagrammatic expansion, the standard rules apply concerning closed fermion loops, symmetry factors, and summations over complex frequencies $i\omega_n = i\pi k_B T(2n + 1)$. It is convenient to represent the point interaction vertex f by a squiggly line [Figs. 1(d) and 1(e)] where spins are conserved at each end of the vertex. When counting closed fermion loops these vertices are treated as point vertices. The f -electron line that enters and leaves a vertex will be called "uninterrupted" as it represents one localized moment. The only complication that arises in the diagrammatic expansion is that matrix elements must be introduced for the propagation

of a band electron from one site to another as a result of the mixed local and extended representations used for the band electrons in (1) [Fig. 1(b)].

In a given diagram each uninterrupted f -electron line for site i contributes a factor z_i to the diagram, so that the projection operation projects out a cluster expansion for the Kondo partition function

$$Z^K(\beta) = Z(H_b, \beta) N^r \times \left[1 + \sum_i \frac{Z_i}{N z_i} + \sum_{i>j} \frac{Z_{ij} + Z_i Z_j}{N^2 z_i z_j} \dots \right]_{\{z_i\}=0}. \quad (12)$$

Here Z_i is the sum of all connected closed-loop diagrams containing just one uninterrupted f -electron line for site i , Z_{ij} is the sum of all connected closed-loop diagrams containing only one uninterrupted f -electron line for sites i and j , and so on, as shown in Fig. 2. The factor $1/N^p$ multiplying a p -site cluster is a consequence of factoring p terms of the fugacity from the time-ordered exponential, and corresponds to a normalization factor that must be used when calculating a physical quantity involving p sites.¹²

III. FORMULATION OF 1/N EXPANSION

If every site $i = 1, \dots, r$ were at the same point in space then the matrix-element product for intersite propagation of band electrons would be equal to 1 and diagonal in its spin indices. For a finite separation of lattice sites these terms will be oscillatory functions of site separation that will have moduli less than 1 when diagonalized. For the purposes of developing a $1/N$ expansion of the partition function it is convenient to consider the extreme case of

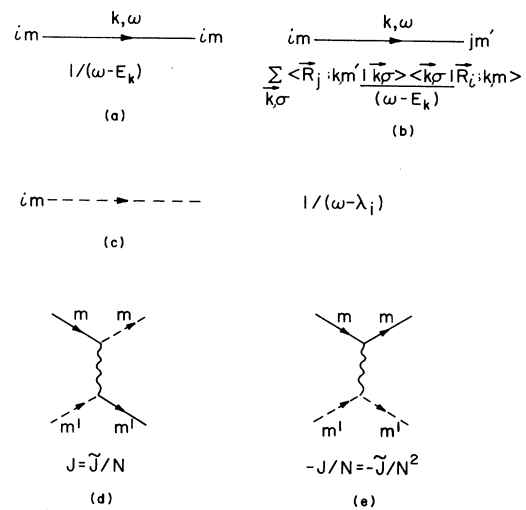


FIG. 1. Diagrams for propagators and vertices used in loop expansion of partition function. (a) Band-electron propagator at one site. (b) Band-electron propagations between sites. (c) f -electron propagator at site i . (d) Spin-exchange interaction. (e) Direct interaction.

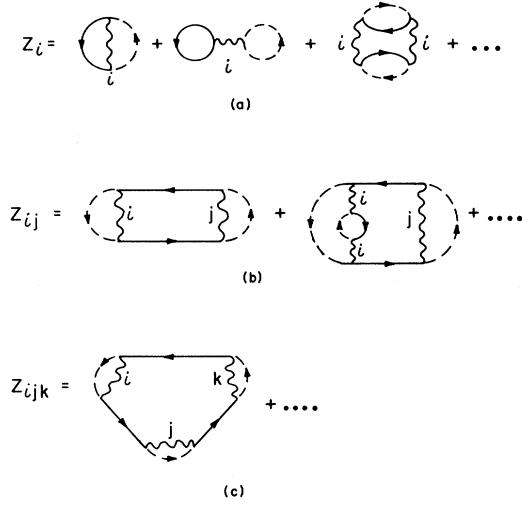


FIG. 2. Examples of connected closed-loop diagrams in the cluster expansion of Z^K . (a) One-site diagrams. (b) Two-site diagrams. (c) Three-site diagrams.

coincident lattice sites in the knowledge that at finite separations the intersite contributions to the partition function will be reduced.

In this extreme case, using the unconventional notation for the interaction vertex, each closed fermion loop that is not interrupted by a squiggly line must be summed over all spin states $m \in [-j, j]$ and thereby contributes a factor N to the diagram. The dominant contribution to the one-site diagrams Z_i comes from multiple spin-flip processes of the type shown in Fig. 3. It is these processes that are responsible for the growth of the effective Kondo coupling constant at low energies. Each loop summation contributes a factor $NJ = \tilde{J}$ to the diagram. In order to have a well-defined large- N limit \tilde{J} must remain fixed as N is increased. Later discussion will explicitly show that the constraint $\tilde{J} = \text{const}$ maintains a finite Kondo temperature.

When the Feynman diagrams for Z^K are expanded in

$$\chi_{11}^{mm'}(\tau) = \frac{1}{Z^K} \frac{\delta^2}{\delta h_1^*(\tau) \delta h_1(0)} Z^K(h_i) = \left[\frac{1}{Z^K N z_1} \right] \frac{\delta^2 (Z_1 + Z_{12}/N z_2)}{\delta h_1^*(\tau) \delta h_1(0)} = O\left(\frac{1}{N}\right), \quad (14)$$

$$\chi_{12}^{mm'}(\tau) = \frac{1}{Z^K} \frac{\delta^2}{\delta h_2^*(\tau) \delta h_1(0)} Z^K(h_i) = \left[\frac{1}{Z^K N^2 z_1 z_2} \right] \frac{\delta^2}{\delta h_2^*(\tau) \delta h_1(0)} Z_{12}(h_i) = O\left(\frac{1}{N^3}\right), \quad (15)$$

and the intersite function is accordingly $O(1/N^2)$ smaller than the one-site correlation function. These arguments automatically extend to the case of finite separation of lattice sites as discussed above, so that in the large- N limit, local spin fluctuations dominate over nonlocal fluctuations.

The perturbation expansion for Z^K is only valid at temperatures above the crossover temperature where the system goes into a strongly coupled low-temperature regime. For the single-site Kondo problem the perturbation expansion is only applicable above the Kondo temperature. For the lattice the crossover could take the form of a phase

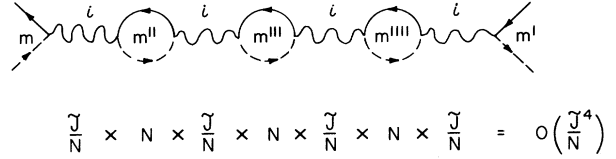


FIG. 3. Multiple local spin-flip process showing how internal loops contribute factors of N .

terms of \tilde{J} , each spin-exchange vertex [Fig. 1(d)] gives a factor \tilde{J}/N while the direct vertices [Fig. 1(e)] give factors of \tilde{J}/N^2 . If there is no closed-loop summation to provide a factor of N to cancel the factors of $1/N$ from the vertices, then the diagram is smaller by orders of $1/N$. This is exactly what happens to the intersite terms.

Figure 4 shows that the single-site terms in the partition function are of leading order $O(1)$, while many-site connected diagrams lack the fermion loops to cancel the vertices so that in general a p -site connected diagram is of leading order $O(1/N^{p-1})$.

Consequently, the amplitude for a correlated spin-flip process is a factor $1/N^{p-1}$ smaller when those spin flips are spread over p sites rather than all occurring at one site. The correlation function measuring the correlation of spins at p sites depends on the square of this amplitude, so the physical meaning of this result is that the correlation of spins at p sites is $O(1/N^{2p-2})$ smaller than the corresponding correlation measured at one site. This can be seen more explicitly by considering the spin-flip correlation function

$$\chi_{ij}^{mm'}(\tau) = \langle T f_m^{i\dagger}(\tau) f_{m'}^i(\tau) f_m^{j\dagger}(0) f_m^j(0) \rangle. \quad (13)$$

This can be calculated using the diagrammatic technique by adding the additional interaction term $-\sum_i [h_i(\tau) f_m^{i\dagger} f_m^i + \text{H.c.}]$ to H_I and then calculating Z^K as a functional of the applied fields $h_i(\tau)$. Consider a lattice of just two sites. The correlation functions $\chi_{11}^{mm'}(\tau)$ and $\chi_{12}^{mm'}(\tau)$ are given as functional derivatives of $Z^K(h_i)$:

transition to a state of long-range magnetic order. However, if local spin correlations dominate over nonlocal correlations at all temperatures above the crossover, then the above results suggest that in the large- N limit, long-range magnetic order cannot occur before reaching a strongly-coupled Kondo ground state. Scaling arguments can be used to confirm this argument.

IV. SCALING THEORY FOR THE KONDO LATTICE

As in the impurity Kondo problem, the crossover to the strongly coupled low-temperature regime can be studied

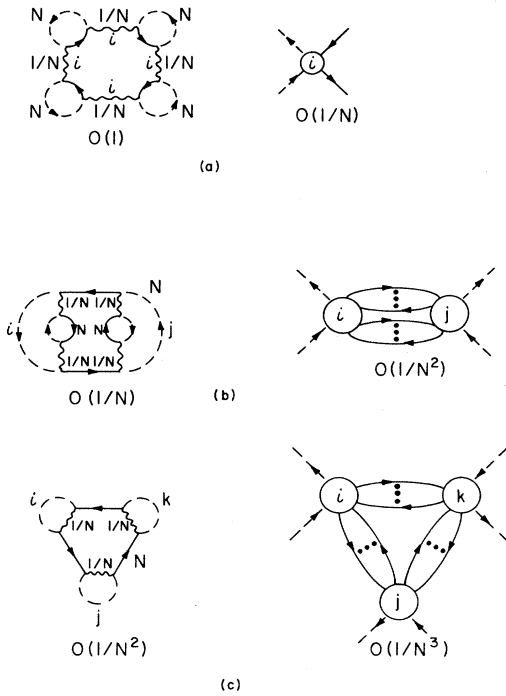


FIG. 4. $1/N$ dependence of closed-loop diagrams and pseudofermion interaction vertices. (a) One site. (b) Two site. (c) Three site.

using Anderson's scaling technique.¹³ The system is mapped onto one with a smaller bandwidth D' , introducing additional interaction terms to the Hamiltonian H so that the partition function is unchanged by the scaling:

$$Z^K(H, D_0, T) = Z(H'(D'), D', T). \quad (16)$$

Scaling corresponds to integrating out the high-energy excitations at the band edge. D' is reduced until $D' \sim T$ at which point the remaining incoherent excitations can be treated by high-temperature perturbation theory, providing that the interaction energies are not of order D' . The process of scaling is thereby equivalent to examining how the interactions scale with the temperature scale $T \sim D'$. A crossover to a strongly coupled regime occurs when one interaction energy becomes of order D' . By identifying the interaction energies that first grow to this size the qualitative nature of the low-temperature ground state can be determined and the parameter ranges for different ground states can be identified.

Anderson's scaling technique is carried out using the diagrammatic expansion for the partition function. Scattering through intermediate states at the band edge renormalizes the f -electron propagator $1/(\omega - \lambda)$ to $d(\omega - \lambda)/(\omega - \lambda)$ and introduces new interaction vertices Γ_{ij} between the f and band-electron lines. The scattering matrix element T_{ij} induced by an interaction vertex Γ_{ij} is given by

$$T_{ij}(D) = \left[\prod_{\text{in}} d(\omega_{\text{in}}) \prod_{\text{out}} d(\omega_{\text{out}}) \right]^{1/2} \Gamma_{ij}(D; \omega_{\text{in}}, \omega_{\text{out}}), \quad (17)$$

where ω_{in} and ω_{out} are the frequencies of ingoing and out-

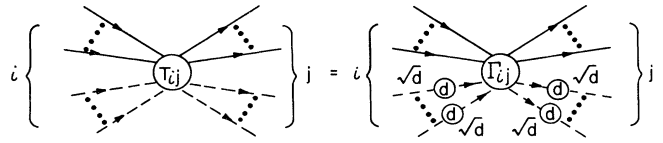


FIG. 5. Expansion of scattering matrix element in terms of vertex function and f -electron legs.

going particles and the prefactor arises from the renormalization of external pseudofermion legs (Fig. 5). When the bandwidth D' is reduced, the $T_{ij}(D)$ will change and additional interaction terms,

$$\delta H = \sum_{i,j} |i\rangle \delta H_{ij} \langle j| = - \sum_{i,j} |i\rangle \delta T_{ij}(D) \langle j|, \quad (18)$$

must be introduced to the Hamiltonian $H(D')$ to compensate. The scaling equation for these interaction terms is accordingly

$$\frac{\partial H_{ij}(D')}{\partial D} = - \frac{\partial}{\partial D'} \left[\prod_{\text{in}} d(\omega_{\text{in}}) \prod_{\text{out}} d(\omega_{\text{out}}) \right]^{1/2} \times \Gamma_{ij}(D'; \omega_{\text{in}}, \omega_{\text{out}}) \Big|_{H(D') = \text{const}}. \quad (19)$$

The right-hand side of this expression can now be calculated using the perturbation theory developed here.

For the single-site terms the scaling procedure renormalizes the Kondo coupling constant \tilde{J} . To lowest order, the Kondo spin-exchange vertex and the pseudofermion propagator are given by (Fig. 6)

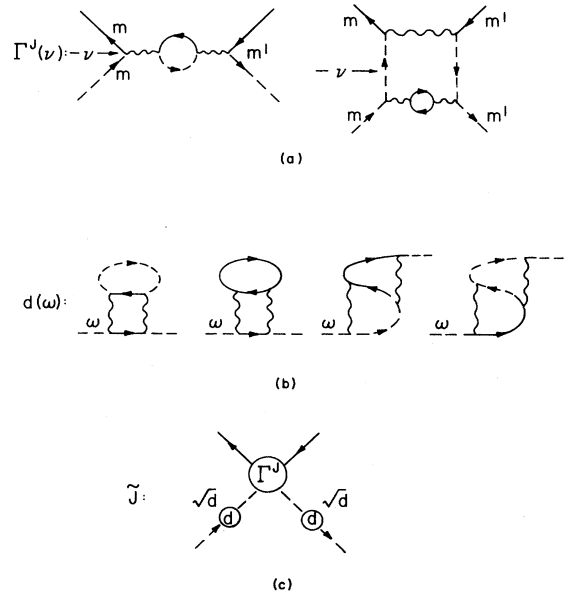


FIG. 6. Lowest-order leading-logarithm diagrams contributing to the renormalization of \tilde{J} . (a) Vertex Γ^J . (b) Renormalization of f -electron propagator. (c) Combination of vertex and external legs in spin-flip scattering matrix.

$$\Gamma^J(k\omega m, k'\omega' m'; (\omega + \nu)m_f, (\omega' + \nu)m_{f'}) = (\tilde{J}/N) \tilde{\Gamma}^J(\omega - \lambda) [\delta_{mm'} \delta_{m'm'} - (1/N) \delta_{mm'} \delta_{m_f m'_f}], \quad (20)$$

$$\tilde{\Gamma}^J(\nu) = 1 + \tilde{J}\rho \ln(D/\nu) - [(\tilde{J}\rho)^3/N^2] \ln(D/\nu) + O((\tilde{J}\rho)^3), \quad (21)$$

$$G_f(\omega) = d(\omega - \lambda)/(\omega - \lambda), \quad (22)$$

$$d(\omega) = 1 - [(\tilde{J}\rho)^2/N] \ln(D/\omega) + [(\tilde{J}\rho)^2/N^3] \ln(D/\omega) + O((\tilde{J}\rho)^3). \quad (23)$$

The scaling equation for \tilde{J} is then

$$\begin{aligned} \frac{\partial \tilde{J}(D)}{\partial \ln D} &= -\tilde{J} \frac{\partial}{\partial \ln D} (d(\omega) \Gamma^J(\nu)) \\ &= -\tilde{J} [(\tilde{J}\rho)^2 - (\tilde{J}\rho)^3/N] + O\left(\frac{1}{N^3}\right) \end{aligned} \quad (24)$$

or

$$\frac{\partial \Phi^N}{\partial \ln D'} (\tilde{J}\rho) = 1, \quad (25)$$

where

$$\Phi^N(g) = \frac{1}{g} - \frac{1}{N} \ln g + O\left(\frac{1}{N^2}\right) \quad (26)$$

is the generalization of Wilson's scaling function $\Phi(x)$.¹⁴ Integrating (26), the dimensionless coupling constant becomes of order unity at $D' \sim T_K$, the Kondo temperature

$$\begin{aligned} T_K &= D_0 \exp[\Phi^N(1) - \Phi^N(\tilde{J}_0\rho)] \\ &= D_0 e^{(\tilde{J}_0\rho)^{1/N}} \exp(-1/\tilde{J}_0\rho). \end{aligned} \quad (27)$$

Now for the lattice, the intersite terms in the partition function cannot be ignored, but they will not affect the renormalization of the Kondo coupling constant. This can be seen by considering a general p -site connected diagram (Fig. 7), which contains p vertices that describe multiple scattering of band electrons at each site. Each vertex contains only one uninterrupted f -electron line and can always be divided into the product of a renormalized f -electron line and an interaction vertex between the f and band electrons. The effect of intersite interactions may be completely incorporated into interaction terms between f electrons at different sites. In particular, the Kondo temperature T_K is unchanged.

In the large- N limit the dominant intersite interaction between f electrons will be the two-site interaction and p -site vertices will be $O(1/N^{p-2})$ smaller. Particle-hole symmetry demands that the general form for the two-site interaction is

$$\begin{aligned} H_{ij} &= \sum_{m, m'} T_{mm'}^{ij}(D) [f_m^{i\dagger} f_{m'}^i - (1/N) \delta_{mm'} n_f^i] \\ &\quad \times [f_{m'}^{j\dagger} f_m^j - (1/N) \delta_{mm'} n_f^j], \end{aligned} \quad (28)$$

where the spin components are measured along the axis between sites. Using (19) the scaling equation for $T_{mm'}^{ij}(D')$ is

$$\frac{\partial}{\partial D'} T_{mm'}^{ij}(D') = -\frac{\partial}{\partial D'} [d^2(\omega) \Gamma_{mm'}^{ij}(\nu)], \quad (29)$$

where $\Gamma_{mm'}^{ij}$ is the intersite scattering vertex and four external f -electron legs introduce the factor d^2 into the T matrix.

When i and j are coincident the lowest-order Ruderman-Kittel-Kasuya-Yosida (RKKY) diagram for $\Gamma_{mm'}^{ij}(D)$ [Fig. 7(b)] gives

$$\Gamma_{mm'}^{ij}(D) = -\delta_{mm'} (4 \ln 2) D (\tilde{J}\rho)^2 / N^2,$$

while for finite separations,

$$\Gamma_{mm'}^{ij}(D) = -\lambda_{mm'}(K_F R_{ij}) D (\tilde{J}\rho)^2 / N^2, \quad (30)$$

where $\lambda_{mm'}(K_F R_{ij})$ is the generalization of the Ruderman-Kittel function to the spin- j case. K_F is the Fermi momentum of the electron band. $\lambda_{mm'}(x)$ has been calculated by Schrieffer and Coqblin,⁴ and it is an oscillatory function of x which is $O(1/x^3)$ at large x . Since it is only weakly dependent on D , this dependence is neglected in further discussion, enabling $\lambda_{mm'}(x)$ to be factored out from the scaling equations. Making the substitution

$$T_{mm'}^{ij}(D') = -\lambda_{mm'}(K_F R_{ij}) t(D'), \quad (31)$$

then $t(D')$ will be positive and by expanding (30), it is governed by the scaling equation

$$\frac{\partial t(D')}{\partial D'} = -\frac{(\tilde{J}\rho)^2}{N^2} + \frac{(\tilde{J}\rho)^2}{ND'} t(D'). \quad (32)$$

The first term simply gives rise to the growth of the

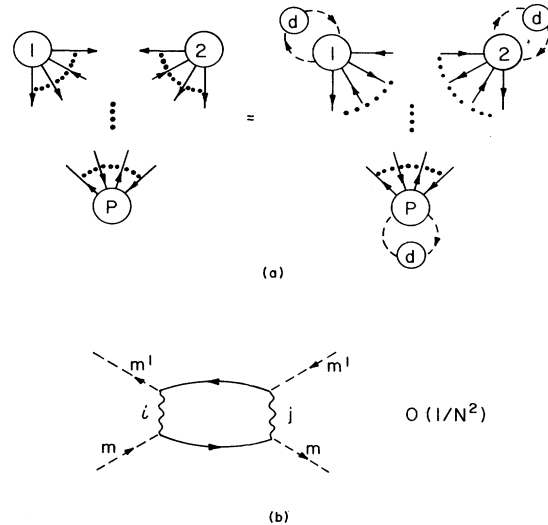


FIG. 7. (a) Showing how interaction between sites does not renormalize f -electron lines. (b) Lowest-order RKKY diagram.

RKKY interaction as D' is increased. The second term (which is of opposite sign) corresponds to the quenching of the RKKY interaction by local spin fluctuations. For $T \gg T_K$, $(\tilde{J}\rho) \simeq (\tilde{J}_0\rho)$ and the second term can be neglected. In this case

$$t(D') = (\tilde{J}_0\rho)^2 (D_0 - D') / N^2. \quad (33)$$

The energy scale of this interaction is given approximately by the product of $t(D')$ with the number of nearest neighbors in the lattice n , and a typical nearest-neighbor value for $\lambda_{mm}(K_F R_{ij})$. It is here that the dimensional dependence will enter the problem. Taking $n\lambda_{mm}(K_F R_{ij}) \simeq 1$ as rough approximation (which is probably an overestimate for a typical three-dimensional lattice), then in the absence of Kondo fluctuations when D' is of order T_m , where $T_m = t(T_m)$ and

$$T_m \simeq T_m^{(0)} = (\tilde{J}_0\rho)^2 D_0 / N^2, \quad (34)$$

there would be a crossover (phase transition) to a state of long-range magnetic order. In the large- N limit this temperature tends to zero and will mean that Kondo local-spin fluctuations can no longer be neglected.

From (32), the inclusion of local-spin fluctuations has two effects. For $D' \sim T_K$ the coupling constant $(\tilde{J}\rho)$ grows to 1, significantly enhancing the growth of the RKKY interaction. When D' is less than the critical value $D_c = t(D_c) \geq NT_m$, the magnetic interaction no longer grows, due to the quenching effect of spin fluctuations. Equation (5) may be used to examine how t scales with the Kondo coupling constant $\tilde{J}\rho = g$. Using (25) in (32) the scaling equation for $t(g)$ is

$$\frac{\partial t(g)}{\partial g} + \frac{t}{N} = \frac{T_K e^{1/g}}{N^2 e} + O\left[\frac{1}{N^3}\right], \quad (35)$$

where the substitution

$$D(g) = (T_K/e) \exp \Phi(g) \quad (36)$$

has been made using (26). The integral of (35) is

$$t(g) = T_K / N^2 e \int_{(\tilde{J}_0\rho)}^g e^{1/x} dx + O\left[\frac{1}{N^3}\right], \quad (37)$$

so that

$$\frac{t(g)}{D'(g)} = \frac{e^{-1/g}}{N^2} \int_{(\tilde{J}_0\rho)}^g e^{1/x} dx + O\left[\frac{1}{N^3}\right]. \quad (38)$$

In the weak-coupling regime $g \leq 1$, $t(g)/D'(g)$ is a monotonically increasing function. Thus if $\tilde{J}_0\rho > (\tilde{J}\rho)_c$ given by

$$\int_{(\tilde{J}\rho)_c}^1 e^{1/x} dx = N^2 e, \quad (39)$$

$t(g)/D'(g) < 1$ for $g \leq 1$, and hence the magnetic crossover will not be reached before the system goes into a strongly coupled Kondo regime. An upper limit for $(\tilde{J}\rho)_c$ is

$$(\tilde{J}\rho)_c = \frac{1}{\ln(N^2 e) + \ln[\ln(N^2 e + \dots)]}, \quad (40)$$

or in terms of the unscaled parameter $J = \tilde{J}/N$,

$$(J\rho)_c = \frac{1}{N\{\ln(N^2 e) + \ln[\ln(N^2 e + \dots)]\}}. \quad (41)$$

This corresponds to the condition $T_m < T_K$.

When $(J\rho)$ is greater than this critical value a crossover occurs to a strongly coupled Kondo regime with strong local-spin correlations and no long-range magnetic order.

Two important features of the scaling theory presented in this section must be emphasized: (a) There is a crucial $1/N$ dependence of $(J\rho)_c$ showing that large spin degeneracy enhances the stability of the Kondo-lattice ground state. (b) In the large- N limit intersite spin correlations vanish and this is true *even at the crossover*. The explicit treatment of the two-site interaction shows that the two-site correlation function is well behaved at the crossover and vanishes as $1/N^2$. The $1/N$ arguments of the previous section enable this result to be generalized to p -site correlation functions which must vanish as $1/N^{2p-2}$ even at the crossover. This result plays a vital role in the discussion of the next section.

V. DISCUSSION: THE APPLICABILITY OF THE KONDO-LATTICE MODEL AND THE NATURE OF ITS LOW-TEMPERATURE EXCITATIONS

A rough calculation is sufficient to indicate that in highly degenerate spin systems, such as the rare-earth compounds, the coupling constant may become large enough to stabilize a Kondo-lattice ground state. Naturally, the expression (33) only sets the approximate N dependence of $(J\rho)_c$. However, the corrections that arise will enter into the logarithms, and they will be independent of N and small in the large- N limit. Taking the expression literally, then for the case of cerium, where $N = 6$, $(J\rho)$ is $\sim \frac{1}{36}$. This is already smaller than values of the coupling constant determined for cerium impurities in lanthanum and ytterbium, typically of order 0.05–0.1.^{4,15,16} Similar values are expected in the lattice, providing important new motivation for the application of the Kondo-lattice model to rare-earth systems.

What then is the nature of the strongly-coupled ground state? Clearly, the diagrammatic approach cannot be extended into the strongly-coupled regime, and other techniques are needed to quantitatively study this regime. However, just as in the Kondo impurity problem the qualitative nature of the crossover into this regime is revealed by the scaling and this enables conclusions to be drawn about its properties. Broadly speaking, these conclusions support the picture proposed by Martin¹⁷ in which the excitations of the Kondo-lattice ground state form a coherent Fermi liquid of extended, heavy quasiparticles.

In the impurity problem the crossover is characterized by an increasing coherence of local spin fluctuations, signaled in scaling by the growth of the coupling constant to 1. Since the coupling constant is antiferromagnetic this indicates that the impurity ground state is a singlet and Nozières was able to elucidate the nature of the low-temperature excitations^{18,19} via simple physical arguments.

From this work a similar growth of the effective coupling constant is seen to occur in the lattice and as

remarked above, the importance of the large- N arguments is to show that all nonlocal spin correlations vanish in the large- N limit. It can hence be argued that to order $1/N$ the Kondo-lattice ground state will be approximated by a lattice of *uncorrelated* Kondo singlet states and the interference between these states will be a $1/N$ effect. A simple picture of the ground state emerges in this large N limit.

Below the Kondo temperature, a band electron that is excited from the Fermi sea will experience potential scattering due to the slow flipping of the local moments inside the Kondo singlets. This scattering is entirely due to spin fluctuations. The flipping rate is given by the Kondo temperature and excitations of this energy will experience resonant scattering. Ignoring the effects of crystal symmetry on the scattering phase shifts, then the phase shifts in each of the N scattering channels will be equal. By the Freidel sum rule their sum must be π so a band electron at the Fermi surface will experience a scattering phase shift of $\delta = \pi/N$ in the f channel at each site. Thus an electron excited from the Fermi sea will see a narrow Suhl resonance of width $\sim T_K$ positioned just above the Fermi energy. The periodic array of f -channel scatterers will create a narrow band of f quasiparticles, with a Fermi surface characteristic of scattering in the f channel. This band will possess structure in its density of states, as suggested by Martin,¹⁷ because of the lattice periodicity.

There is a subtlety connected with the Kondo lattice which does not arise for the impurity problem and deserves mention because it provides a link between the Kondo- and Anderson-lattice models. The field theoretic treatment carried out here is at a constant chemical potential, and implicit in the treatment is the need to determine the final chemical potential self-consistently so as to conserve the number of band electrons. The development of Kondo singlets implies that band states are pulled down below the chemical potential to provide the additional electrons that screen the local moments. The number of bound states per moment is given approximately by the Freidel sum rule,

$$n_b = \frac{N\delta(\mu, T)}{\pi}, \quad (42)$$

where $\delta(\mu, T)$ is the f -channel phase shift at temperature T . Above the Kondo temperature, scattering is small and there are few band states pulled down below the chemical potential. However, below the Kondo temperature the phase shifts rise to a maximum value of π/N , and as this occurs the chemical potential must drop by an amount $\Delta\mu$ given by

$$\Delta\mu = -\frac{N\delta(\mu, T)}{\pi\rho}. \quad (43)$$

Now ρ is the density of band states per local moment. For the lattice this is finite, but for the impurity this is infinite and there is no corresponding renormalization of the chemical potential.

The renormalization of the chemical potential has important consequences. If $\Delta\mu$ is small enough that f level is still well below the Fermi level, then the Kondo-lattice model remains valid. However, if $\Delta\mu$ is comparable with

the initial separation between the f level and the chemical potential, then a mixed-valent regime will be reached and *the full Anderson-lattice model becomes necessary*. In general, provided that the density of states per local moment is large, as in say CeB_6 or CeAl_3 , then the Kondo-lattice model is likely to be still applicable.

The picture of the large- N Kondo lattice as a lattice of uncorrelated Kondo singlets enables the low-temperature thermodynamic properties to be approximated to order $1/N$ by the impurity results. Thus the linear coefficient of the specific heat γ must take the form

$$\gamma = \frac{k_B^2\pi^2}{3} \times \frac{\text{const}}{T_K} + O\left(\frac{1}{N}\right). \quad (44)$$

A clearer picture of the situation can be obtained by relating the Kondo-lattice model back to the Anderson-lattice model from which it is derived. The f electrons in the highly renormalized Fermi liquid of an Anderson lattice in the local-moment regime are expected to have a sharp quasiparticle pole in their propagators of strength $z < 1$ near the Fermi surface and it is this pole that is responsible for the narrow band above the Fermi level. Since the quasiparticle bandwidth W^* is very narrow we may approximate the thermodynamic behavior by that of a resonant level of width Δ^* , where $N\Delta^* = W^*$ and $\Delta^* = z\Delta$. Δ is the bare resonant width of an impurity f level. For such a resonant level, γ is given by²⁰

$$\gamma = N \frac{k_B^2\pi^2}{3} \frac{\sin^2(\delta/\pi)}{\Delta^*} \simeq \frac{k_B^2\pi^2}{3} \frac{1}{N\Delta^*}, \quad (45)$$

and comparing these two expressions the renormalized bandwidth $N\Delta^*$ is seen to be given by the Kondo temperature. The quasiparticle band will exist at temperatures below $\Delta^* = T_K/N$. Because the energy scale of this renormalized band is compressed by a factor z , the effective masses of these quasiparticles will be $z^{-1} = N\Delta/T_K$ larger than that of an unrenormalized f electron. Above $T \sim T_K/N$, excitations of the Kondo singlets will destroy the coherence of the quasiparticle band and susceptibility will fall rapidly. Below $T \sim T_K/N$ there is the interesting possibility of phase transitions in the heavy f -electron system.^{21,22}

In summary, it has been shown how high-spin degeneracy enhances local spin fluctuations in the Kondo lattice and, most important of all, that due to this enhancement a much lower Kondo coupling constant of order $O(1/2j+1)$ is required to stabilize a Kondo-lattice ground state with respect to a magnetically-ordered ground state. Physical arguments based on the nature of the crossover to a Kondo-lattice regime have been advanced to support Martin's picture of heavy quasiparticle excitations at low temperatures.

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