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Scaling approach to the mixed-valence system with large N

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Abstract. We study the ground state of the mixed-valence system by renormalization group theory and numerical exact diagonalizations. A $1/N$ expansion is applied to examine the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction effects. We show that the antiferromagnetic RKKY interaction J_{ij} grows as scaling proceeds and reduces the strength of s–d coupling J. This property clarifies the competition between the local Kondo effect and intersite RKKY interactions. Scaling theory predicts that for small $J_{ij} \ll T_K$ the low-energy scale is given by $\Delta E \approx T_K e^{-\alpha J_{ij}}$, and for large J_{ij}, $\Delta E \approx (1/J_{ij})^{\alpha'}$, which agree well with our numerical diagonalizations. In the intermediate regime where the Kondo and RKKY effects cancel each other, we discuss whether our results support the existence of a zero of $\beta_J = dJ/d\ln D$.

1. Introduction

There has been recent interest in the competition between the Ruderman–Kittel–Kasuya–Yosida (RKKY) interactions and the local Kondo effects in order to understand the formation of the heavy-fermion state [1–7]. This problem is important since it may have some relevance to the oxide superconductors as well as heavy fermions. It is generally agreed that heavy fermions are classified into three groups according to their ground-state properties: superconducting, magnetically ordered, or paramagnetic with an enhanced specific heat coefficient. The rich magnetic structures found in the latter two cases are often explained as being due to competition between the local Kondo effect and the RKKY intersite interactions. Many heavy-fermion samples show antiferromagnetic ordering at low temperatures [8, 9]. Even in the cases categorized as non-magnetic Fermi liquids such as $CeAl_3$, the small magnetic moments involved are observed [10]. Another simple question arising from a large number of experiments is why ferromagnetic short- or long-range orderings in heavy fermions are hardly observed in zero magnetic field. These issues may be explained by clarifying the properties of RKKY interactions.

There are apparently two energy scales J_{ij} and T_K where J_{ij} is the RKKY exchange energy and T_K is the Kondo temperature. We can easily identify two regimes. (i) The Kondo regime when the Kondo temperature T_K is much larger than the RKKY coupling J_{ij}; in this regime the Kondo effect takes place in each individual site with quenching of each local spin. (ii) The RKKY regime when T_K is much smaller than J_{ij}; here a collective state of impurities is formed and localized spins are ordered ferromagnetically or antiferromagnetically. Our understanding is still qualitative because there is no existing theory capable of treating the local Kondo fluctuations and the intersite couplings.

The purpose of this paper is to investigate the ground state of mixed-valence systems by the renormalization group theory [11–18] and the numerical exact diagonalization method. A combination of analytic and numerical methods will provide us with useful information on the heavy fermions. Applying perturbation theory in terms of hybridization in the atomic limit [19, 20], it appears that the energy shows logarithmic dependence on the high-energy cutoff D of the conduction band. Logarithmic dependence is a characteristic of a renormalizable theory, suggesting a scaling property of the model. In the original 'poor man's' derivation of the scaling equation [11], we integrate out the high-energy region $D - \Delta D < |\omega| < D$ and renormalize parameters to include its effects. Scaling equations are defined by

$$\beta_J = \mathrm{d}J/\mathrm{d}\ln D \qquad \beta_{ij} = \mathrm{d}J_{ij}/\mathrm{d}\ln D \tag{1.1}$$

where J is the s–d exchange coupling. A zero of both β_J and β_{ij} shows the existence of a phase transition. A zero of just one of them indicates a crossover phenomenon. Note that we can set up the simplified model such that no new RKKY couplings are generated by scaling, i.e. $\beta_{ij} = 0$. For example, the model proposed by Jones *et al* [1] contains no intersite interactions except the one introduced to the Hamiltonian by hand. For a model of this kind, a zero of β_J shows the existence of a phase transition. Thus one can say that in the language of scaling theory, Jones *et al* have demonstrated that β_J has a zero. In this paper we examine the renormalization of both J and J_{ij}. Since this approach uses formulation in the language of perturbation theory, our equations work well in the weak-coupling region. The numerical calculations may make up for any shortcomings.

We show that scaling properties of J_{ij} sensitively depend on whether the RKKY interactions are ferromagnetic or antiferromagnetic. We insist that the ferromagnetic state is unstable relative to the momentum-quenched state. This may be an important result for us in considering the magnetic orderings in heavy fermions. In fact, the above properties tell us why we rarely observe ferromagnetic orderings in heavy-fermion materials. In contrast, the antiferromagnetic RKKY interactions grow in the scaling processes and produce effects to reduce J. A crossover between the Kondo and RKKY regime is described as the RKKY coupling J_{ij} changes by integrating β-functions $\beta_J = \mathrm{d}J/\mathrm{d}\ln D$ and $\beta_{ij} = \mathrm{d}J_{ij}/\mathrm{d}\ln D$. By comparing the scaling theory with numerical diagonalizations, we show that for small $J_{ij} \ll T_{\mathrm{K}}$, the spin-excitation energy is given by $\Delta E \approx T_{\mathrm{K}}\exp(-\alpha J_{ij})$ where α is a constant, and for large J_{ij} in the antiferromagnetic RKKY regime we find a power law $\Delta E \approx (1/J_{ij})^{\alpha'}$. In the intermediate regime, the exponential law ceases to apply and ΔE assumes power-law behaviour.

This paper is arranged as follows. In section 2, we present a scaling theory by a diagrammatic method. In section 3, we compare the numerical diagonalizations with the scaling properties in section 2 and discuss their relevance. The last section is devoted to a discussion and a summary.

2. Scaling properties

2.1. Perturbation expansions

The model Hamiltonian of interest to us is the two-impurity Anderson model,

$$H = \sum_{k\sigma}\epsilon_k c_{k\sigma}^+ c_{k\sigma} + \epsilon_{\mathrm{f}}\sum_{i\sigma m} f_{i\sigma m}^+ f_{i\sigma m} + V\sum_{ki\sigma m}(\mathrm{e}^{\mathrm{i}k\cdot R_i} c_{k\sigma}^+ f_{i\sigma m} + \mathrm{HC})$$
$$+ U\sum_i f_{i\sigma m}^+ f_{i\sigma m} f_{i\sigma' m'}^+ f_{i\sigma' m'}. \qquad (m,\sigma) \neq (m',\sigma'). \tag{2.1}$$

The subscript i labels the impurity situated at $\boldsymbol{R}_i$ ($i = 1, 2$). The conduction-electron operators are represented by cs and local f electron operators by fs. We shall restrict ourselves to the case where $U = \infty$, i.e. the doubly occupied sites are excluded. The local level ϵ_f will be assumed to lie well below the Fermi level of the conduction-electron band. Note furthermore that we assume the spin–orbit degeneracy N to be large so $1/N$ is a good expansion parameter. We believe that the two-impurity Kondo system is a good starting point from which to investigate heavy fermions when N is large.

The perturbation expansions of the Anderson model in atomic limit have been extensively investigated by many authors [19–29]. It is known that each term in the perturbation series shows logarithmic divergence. Logarithmic dependence on a high-energy cutoff is the characteristic property of a renormalizable theory, where the cutoff dependence tells us how the parameters change when the cutoff D is reduced to $D - \mathrm{d}D$ by integrating out states with energies $D - \mathrm{d}D < |\omega| < D$. One may derive the scaling equation by retaining the divergent terms in each order of hybridization. In the process of truncation of the cutoff new couplings are generated. However, new couplings that vanish in the limit $D \to \infty$ are irrelevant in the sense that we can safely neglect them. In deriving the scaling equation, it is important to note that the hybridization strength Δ ($= N\pi\rho V^2$) is unrenormalized by scaling; more exactly renormalization of Δ vanishes in the limit $D \to \infty$ [15].

The perturbation theory in strongly correlated electron systems has some difficulties since the electron operators obey neither boson nor fermion commutation relations. However, the generalization of Wick's theorem enables us to reduce the expectation values into a sum of graph terms [20, 21]. Some formulae are shown in appendix A.

In the leading order of $1/N$, the RKKY interactions do not affect processes of the scaling theory. We can easily evaluate the energy levels of the vacuum and occupied states, E_0 and E_f, for the single-impurity Anderson model [20]:

$$E_0 = -\frac{\Delta}{\pi}\ln\left|\frac{D}{\epsilon_f - \Sigma_0}\right| + \frac{1}{N}J\frac{\Delta}{\pi}\ln\left|\frac{D}{\epsilon_f - \Sigma_0}\right| + \mathrm{O}(J^2, 1/N^2) \tag{2.2a}$$

$$E_f = \epsilon_f - \frac{1}{N}\frac{\Delta}{\pi}\ln\left|\frac{D}{\epsilon_f - \Sigma_0}\right| + \mathrm{O}(J, 1/N^2) \tag{2.2b}$$

where Σ_0 denotes the self-energy of the f-state Green function of the order of $(1/N)^0$. In figure 1 we show the diagrams contributing to E_0, where the full curves and broken curves denote f-state and conduction-electron Green functions, respectively. The wavy line represents the $|0\rangle$-state propagator defined by $D^{(0)}(\nu) = -1/(\nu + \mathrm{i}\delta)$. (See appendix A.) Both E_0 and ϵ_f are reduced, but the shift of ϵ_f is smaller by an order of $1/N$. Thus the effective level of f electrons rises as scaling proceeds. Following the usual definition of the s–d coupling $J = -\Delta/\pi(E_f - E_0)$, we obtain easily $\beta_J = \mathrm{d}J/\mathrm{d}\ln D = -J^2 + J^3/N$, which is known to be correct up to $\mathrm{O}(J^3)$ [30].

Now let us consider the RKKY interaction effects. In figures 2(a)–(d) we show the processes of order V^4 considered:

$$\sum_{i\neq j} V^2 \sum_{km\sigma}\frac{f_k}{(\epsilon_k - \epsilon_f)^2} V^2 \sum_{km'\sigma'}\frac{f_{k'}}{\epsilon_{k'} - \epsilon_f} \tag{2.3a}$$

$$-\sum_{i\neq j} V^4 \sum_{kk'm\sigma}\frac{f_k f_{k'}}{(\epsilon_k - \epsilon_f)^2(\epsilon_{k'} - \epsilon_f)}\mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} \tag{2.3b}$$

$$\sum_{i\neq j} V^4 \sum_{kk'm\sigma} \frac{f_k(1-f_{k'})}{(\epsilon_k-\epsilon_f)^2(\epsilon_k-\epsilon_{k'})} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}_i-\boldsymbol{R}_j)} \tag{2.3c}$$

$$-\sum_i V^2 \sum_{km\sigma} \frac{f_k}{(\epsilon_k-\epsilon_f)^2} \sum_j V^2 \sum_{k'm'\sigma'} \frac{f_{k'}}{\epsilon_{k'}-\epsilon_f}. \tag{2.3d}$$

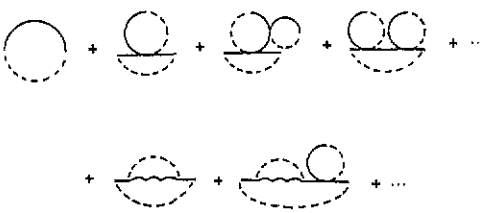

Figure 1. Diagrams contributing to E_0. The full curves denote the f-state Green function and the broken curves represent the conduction-electron Green function. The wavy lines show the propagator $D^{(0)}(\nu) = -1/(\nu + \mathrm{i}\delta)$.

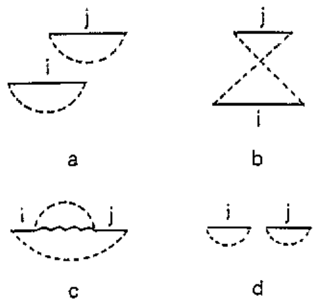

Figure 2. Intersite contributions of the order of V^4. i and j denote the site indices.

A sum of these contributions in figures 2(a)–(d) are shown by Feynman diagrams in figures 3(a) and 3(b). We can identify the terms in figure 3(a) as arising from single-site processes. Figure 3(b) represents an intersite term which is evaluated as

$$\begin{aligned} E_0^{\mathrm{RKKY}} &= V^4 \frac{1}{2} \sum_{kk'm\sigma} \int \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} (G_{m\sigma}^{(0)}(\omega))^2 G_{k\sigma}(\omega) G_{k'\sigma}(\omega) \mathrm{e}^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}_i-\boldsymbol{R}_j)} \\ &= \frac{1}{N}\left(\frac{\Delta}{\pi\epsilon_f}\right)^2 \frac{\pi}{2} D \frac{\cos(2k_F R)}{(k_F R)^3} \equiv \frac{1}{N} J_0^2 D F(R) \end{aligned} \tag{2.4}$$

where $J_0 = -\Delta/\pi\epsilon_f$ and R is the distance between two localized spins situated at $\boldsymbol{R}_i$ and $\boldsymbol{R}_j$: $R = |\boldsymbol{R}_i - \boldsymbol{R}_j|$. This formula is derived in the $k_F R \gg D/|\epsilon_f|$ region. For $k_F R \ll D/|\epsilon_f|$, the RKKY term follows a $1/R^2$ law

$$E_0^{\mathrm{RKKY}} = \frac{1}{N^2} J_0^2 |\epsilon_f| \frac{\pi}{2} \frac{\sin(2k_F R)}{(k_F R)^2}. \tag{2.5}$$

$G_{m\sigma}^{(0)}(\omega)$ and $G_{k\sigma}(\omega)$ denote the unperturbed Green functions of f electrons and conduction electrons respectively,

$$G_m^{(0)}(\omega) = \frac{1}{\omega - \epsilon_f + \mathrm{i}\delta} \tag{2.6a}$$

$$G_{km}(\omega) = \frac{1 - f_k}{\omega - \epsilon_k + \mathrm{i}\delta} + \frac{f_k}{\omega - \epsilon_k - \mathrm{i}\delta}. \tag{2.6b}$$

Thus E_0 rises when $F(R) > 0$ and is reduced when $F(R) < 0$. It is an easy way to include excitations due to mixing processes, which we show in figures 4(a) and (b); figure 4(a) shows explicit $\ln D$ dependence:

$$V^6 \sum_{kk'm\sigma} \int \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} (G^{(0)}_{m\sigma}(\omega))^3 G_{k\sigma}(\omega) G_{k'\sigma}(\omega) \mathrm{e}^{\mathrm{i}(k-k')\cdot(R_i-R_j)}(-1) \sum_{k''m'\sigma'} \frac{f_{k''}}{\epsilon_{k''}-\epsilon_{\mathrm{f}}}$$

$$= \frac{2}{N} J_0^3 \frac{\pi}{2} D \frac{\cos(2k_{\mathrm{F}}R)}{(k_{\mathrm{F}}R)^3} \ln\left|\frac{D}{\epsilon_{\mathrm{f}}}\right|. \tag{2.7}$$

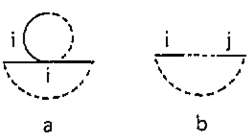

Figure 3. Diagrams responsible for intersite interactions up to the order of V^4.

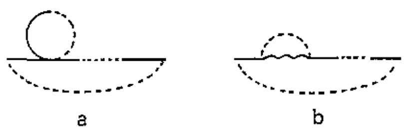

Figure 4. Higher-order diagrams contributing to E_0.

The contribution in figure 4(b), which is the electron–hole excitation above the Fermi level, is smaller by an order of $1/N$. In a similar way, we can take into account the intersite corrections to ϵ_{f}. We have only to notice that we have a negative sign when two spins separated by a distance R are antiparallel and a positive sign when two spins are parallel. The process corresponding to figure 3(b) gives

$$E_{\mathrm{f}}^{\mathrm{RKKY}} = S_{0R} \frac{1}{N} J_0^2 D F(R) \tag{2.8}$$

where S_{0R} is $+1$ for parallel spins and -1 for antiparallel spins. Then the effective levels read

$$E_0 = -\frac{\Delta}{\pi} \ln\left|\frac{D}{\epsilon_{\mathrm{f}} - \Sigma_0}\right| + \frac{1}{N} J \frac{\Delta}{\pi} \ln\left|\frac{D}{\epsilon_{\mathrm{f}} - \Sigma_0}\right| + \frac{1}{N} J^2 \frac{\pi}{2} D \frac{\cos(2k_{\mathrm{F}}R)}{(k_{\mathrm{F}}R)^3} \tag{2.9a}$$

$$E_{\mathrm{f}} = \epsilon_{\mathrm{f}} - \frac{1}{N}\frac{\Delta}{\pi} \ln\left|\frac{D}{\epsilon_{\mathrm{f}} - \Sigma_0}\right| + \frac{1}{N^2} J \frac{\Delta}{\pi} \ln\left|\frac{D}{\epsilon_{\mathrm{f}} - \Sigma_0}\right| + S_{0R} \frac{1}{N^2} J^2 \frac{\pi}{2} D \frac{\cos(2k_{\mathrm{F}}R)}{(k_{\mathrm{F}}R)^3}. \tag{2.9b}$$

When $\cos(2k_{\mathrm{F}}R) > 0$, two spins a distance R apart form an antiferromagnetic state. The condition $\cos(2k_{\mathrm{F}}R) > 0$ shows that the vacuum energy E_0 is pushed up due to intersite-interaction effects, which stabilizes the antiferromagnetic state. In the other case where $\cos(2k_{\mathrm{F}}R) < 0$, the pair spins form a ferromagnetic state. This state is, however, unstable relative to the Kondo-spin-quenched state because E_0 acquires the energy gain being proportional to $J^2\cos(2k_{\mathrm{F}}R)/N$. Thus it follows that the ferromagnetic ordering is unstable in heavy-fermion systems. This observation predicts that ferromagnetic heavy-fermion materials are difficult to observe in zero magnetic field. In figure 5 we show schematic drawings of energy levels to help our understanding.

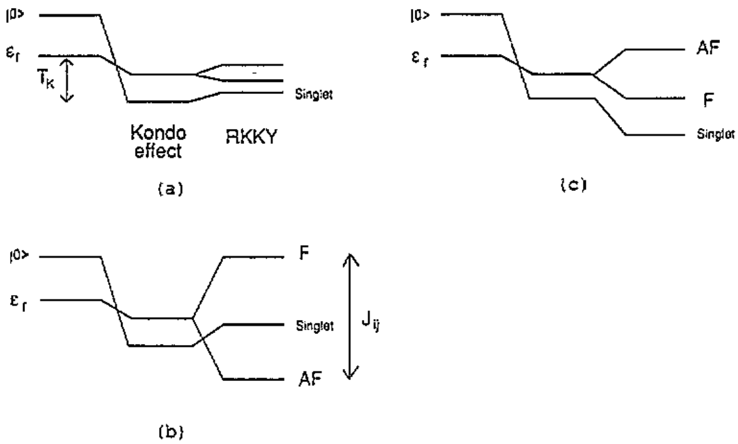

Figure 5. Schematic drawings of energy levels. (a) and (b) are for the antiferromagnetic intersite couplings and (c) is for the ferromagnetic case. In (a), for $T_K > J_{ij}$, the ground state is a Kondo singlet and in (b), for $T_K < J_{ij}$, local spins are antiferromagnetic in the ground state.

2.2. Scaling equations

In the following we pay attention to the antiferromagnetic case because as seen from figure 5(c) there is some ambiguity in defining the intersite coupling J_{ij} for the ferromagnetic case. Here we define J_{ij} by $J_{ij} = (1/N^2)J^2DF(R)$ where $F(R) = (\pi/2)\cos(2k_F R)/(k_F R)^3$. Then the β functions read

$$\beta_J = -J^2[1 - (1/N)J - (\pi N/\Delta)J_{ij}] \tag{2.10a}$$

$$\beta_{ij} = -(1 + 2J)J_{ij}. \tag{2.10b}$$

J_{ij} works to reduce β_J since J_{ij} (> 0) increases as the high-energy cutoff D is reduced. It is natural to expect that J_{ij} decreases due to local spin fluctuations, which are, however, smaller by an order of $1/N$. Since we obtain $J_{ij}D = J_{ij}^0 D_0$ according to (2.10b), J in the weak-coupling limit is expressed as follows:

$$J = J_0/[1 - J_0 \ln(J_{ij}/J_{ij}^0)]. \tag{2.11}$$

We denote the critical coupling of J_0 by J_0^c such that both J and J_{ij} go into the strong-coupling regions simultaneously. Since from (2.11) we easily obtain $J_0^c \approx 1/\{\ln N^2 + \ln[1/(J_0^c)^2]\}$, the following relation holds:

$$(1/N)^2(J_0^c)^2 D_0 \approx D_0 \exp(-1/J_0^c) \tag{2.12}$$

i.e. $J_{ij}^0 \approx T_K$ for $J_0 = J_0^c$. If $J_0 < J_0^c$ the magnetic state will be reached before the system goes into the strongly coupled Kondo regime.

Now we consider the low-energy scale of heavy fermions and try to characterize the Kondo and RKKY regimes quantitatively. Let us denote a scaling invariant by M_{inv}. M_{inv} satisfies the scaling equation $dM_{inv}/d\ln D = 0$, or

$$(\partial/\partial \ln D + \beta_J \partial/\partial J + \beta_{ij}\partial/\partial J_{ij})M_{inv} = 0. \tag{2.13}$$

In the scaling limit the physical properties are expected to depend on the scaling invariant M_{inv}. Thus it is important to explore the behaviour of M_{inv}. Some limiting cases are easily examined. In the limit where J_{ij} is small and $\beta_{ij} \approx 0$, M_{inv} is given by $M_{\mathrm{inv}} \approx D^{-1}\mathrm{e}^{1/J}\exp(-\pi N J_{ij}/\Delta)$. M_{inv} shows an exponential behaviour in the Kondo regime. The local spin fluctuations work to increase J while the RKKY interactions produce effects to reduce J. At the point where the two effects offset each other, β_J should vanish. At the zero of β_J,

$$(\partial/\partial \ln D - J_{ij}\partial/\partial J_{ij})M_{\mathrm{inv}} = 0. \tag{2.14}$$

Then it turns out that M_{inv} obeys a power law $M_{\mathrm{inv}} \propto 1/J_{ij}$. In the next section, by exact diagonalization, we show that the spin excitation gap follows the power behaviour. This observation supports the existence of a zero of β_J. The zero of β_J indicates a crossover phenomenon around this critical point. Our model shows no phase transition because there is almost no chance that β_{ij} vanishes at the same time. Note that the zero of β_J is not a fixed point of J since the other parameter J_{ij} is moving. If we set up the Hamiltonian for which we have $\beta_{ij} = 0$, this model may show conformal invariance and we may observe a phase transition [1]. The conformal properties in this case have been investigated by Affleck and Ludwig [31].

3. Numerical diagonalizations

It is constructive to compare these predictions with exact diagonalizations in small systems. Our model contains the two impurity sites and an L-site conduction-electron ring. We have $L+2$ sites in total. The transfer parameter t is set to unity: $\epsilon_k = -2\cos k$. We consider the half-filled case and with a periodic (or antiperiodic) boundary condition for $L = 4n$ (or $L = 4n+2$). The magnetic spins are set at nearest-neighbour sites and system sizes are $L = 4, 6, 8$, and 10. We employ the Lanczos method [32] to obtain eigenvalues of the lower excited states accurately even for matrices of large size. The conjugate gradient method is used to obtain the eigenvectors.

We show in figures 6(a) and (b) the lowest excitation energy ΔE versus J_{12} for the Anderson model with two local spins where we have added an exchange term to the Hamiltonian H. For small J_{12}, ΔE clearly shows exponential behaviour, and for large J_{12}, ΔE decreases in an algebraic manner $\ln\Delta E \propto -\ln J_{12}$. These exact calculations are consistent with the results of the scaling theory. Thus we can identify the Kondo regime by the exponential law $\Delta E \propto \exp(-\alpha J_{ij})$, and the RKKY regime by the power law. We estimate α through an extrapolation in terms of the system size in diagonalizations. In figure 7, we show α versus $1/L$ for several values of V. Extrapolated values of α in the limit $L = \infty$ are presented in table 1 with the scaling value π/Δ for comparison. $\alpha_{L=\infty}$ values are evaluated by the least-squares method with the form $\alpha = \alpha_{L=\infty} + \alpha_1/L + \alpha_2/L^2$. It is evident that α is proportional to $1/\Delta$ and numerical values agree well with scaling theory. Next we show the spin-correlation function $-\langle S_1^z S_2^z\rangle$ in figure 8. In the Kondo regime it is greatly suppressed, indicating that the ground state is approximated by uncorrelated Kondo singlet states, while in the RKKY regime we find strong spin correlations. In the intermediate region the spin correlations grow rapidly.

4. Summary

We have derived the β functions of J and J_{ij} by the perturbation theory in terms of hybridization. In the large-N limit all non-local spin correlations vanish. Thus it can be

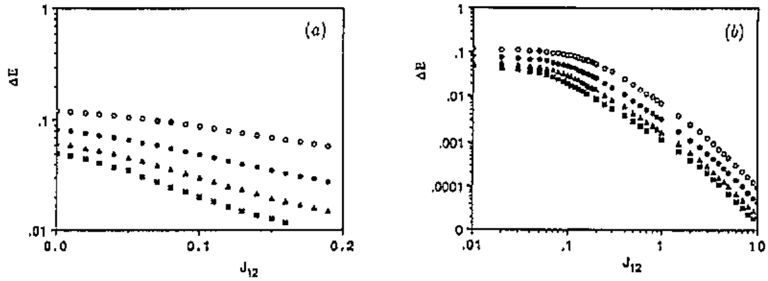

Figure 6. Spin-excitation energy ΔE versus J_{12} for the Anderson model with two local spins and L conduction-electron sites. (a) is for small J_{12} and (b) is for large J_{12}. Parameters are $L = 4$ (open circles), 6 (filled circles), 8 (triangles), and 10 (squares). We set $V = 0.5$ and $\epsilon_f = -2$.

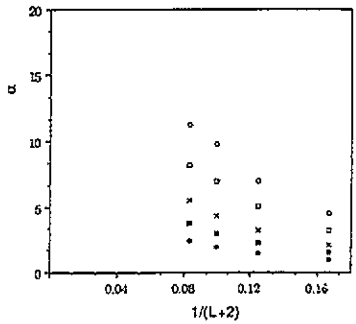

Figure 7. α versus $1/(L+2)$. From the top, $V^2 = 1/8$, 1/6, 1/4, 1/3, and 1/2.

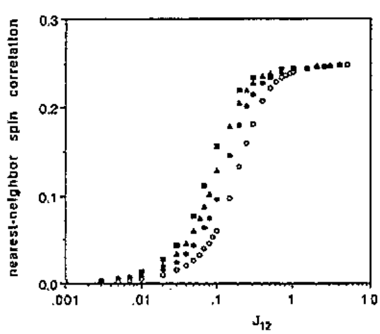

Figure 8. Spin correlation function $-\langle S_1^z S_2^z \rangle$ versus J_{12}.

argued that the Anderson lattice state will be approximated by the independent Kondo singlet states and the intersite interference of order $1/N$. This picture shows a similarity with the two-impurity Anderson model.

In the case without RKKY interactions, our method produces the well known formula of $\mathrm{d}J/\mathrm{d}\ln D$ to the order of J^3 well. We have shown that the ferromagnetic ordering

Table 1. Extrapolated values of α and π/Δ for several values of V.

V^2	$\alpha_{L=\infty}$	π/Δ
1/8	24.6	25.1
1/6	18.1	18.8
1/4	14.0	12.6
1/3	9.30	9.42
1/2	5.93	6.29

is unstable compared to the Kondo state, which indicates that we can hardly observe the ferromagnetic ordering in heavy-fermion compounds in zero magnetic field. On the other hand, the antiferromagnetic intersite interactions emphasize competition with the Kondo effect. As scaling proceeds both J and J_{ij} increase. When $J_{ij}^0 \approx T_{\rm K}$, the crossover regime is reached where both J and J_{ij} go into the strong-coupling regions simultaneously. If $T_{\rm K} > J_{ij}^0$, J goes into the strong-coupling region first and thus only weak magnetic correlations are observed in the ground state. For $T_{\rm K} \gg J_{ij}^0$, the Kondo effect dominates over the RKKY effects.

We have shown that the intersite interactions produce effects which reduce J. When the effects of RKKY interactions and local spin fluctuations cancel each other, J neither increases nor decreases; this indicates the existence of a zero of β_J. At the zero of β_J or beyond this point, the scaling invariant $M_{\rm inv}$ obeys a power law $\ln M_{\rm inv} \propto -\ln J_{ij}$. In fact, we have shown by numerical diagonalization that the spin-excitation gap shows power-law behaviour in the RKKY regime, supporting the existence of β_J. Since a zero of both J and J_{ij} indicates the existence of a phase transition and a zero of just one β shows a crossover phenomenon, our model shows a crossover without singularities in the intermediate regime. In our opinion, the model of Jones *et al* [1] shows singularities because of the condition that $\beta_{ij} = 0$.

In the weak-coupling limit, the scaling theory agrees well with the numerical diagonalizations for the two-impurity Anderson model. We have characterized the Kondo regime by exponential behaviour such that $\Delta E \approx T_{\rm K} \exp(-\alpha J_{ij})$, while in the RKKY regime we obtain the power law $\Delta E \propto 1/J_{ij}^{\alpha'}$. The constant α, evaluated by diagonalizations and scaling, gives consistent results. The above classification of RKKY and Kondo regimes has been justified by calculating the spin correlation functions. In fact in the Kondo regime the moments are quenched and we have a set of uncorrelated Kondo singlet states, and in the RKKY regime a collective state is formed.

Acknowledgments

The author expresses his sincere thanks to Dr K Yamaji, Dr S Abe, Dr Y Asai, and Dr K Harigaya for discussions.

Appendix A. Formulae for Hubbard operators

We show the basic relations in this appendix. According to Hubbard [33], X_{pq} is defined by

$$X_{pq} = |p\rangle\langle q|. \tag{A.1}$$

Here $|m\rangle = f_m^+|0\rangle$, $|mm'\rangle = f_m^+ f_{m'}^+|0\rangle$ and $|0\rangle$ is the vacuum, where f_m^+ is a creation operator of an f electron with orbital-angular momentum m. X operators obey (anti)commutative relations,

$$[X_{pq}, X_{rs}]_\pm = \delta_{qr} X_{ps} \pm \delta_{ps} X_{rq} \tag{A.2}$$

where + should be used only in the case where both operators are fermionic. From now on we use abbreviations $X_\lambda = |0\rangle\langle\lambda|$ and $X_\lambda^+ = |\lambda\rangle\langle 0|$. We define the contraction of X_λ and X_μ^+ as

$$X_\lambda(t)^{\cdot} X_\mu^+(t')^{\cdot} = \mathrm{i}G_\lambda^{(0)}(t-t')\Delta_{\mu\lambda}(t') \tag{A.3}$$

where

$$X_\lambda(t) = \mathrm{e}^{-\mathrm{i}\epsilon_\lambda t} X_\lambda \tag{A.4}$$

$$\mathrm{i}G_\lambda^{(0)}(t-t') = \theta(t-t')\mathrm{e}^{-\mathrm{i}\epsilon_\lambda(t-t')} \tag{A.5}$$

$$\Delta_{\mu\lambda} = [X_\lambda, X_\mu^+]_+ = \delta_{\lambda\mu} X_{00} + X_{\mu\lambda} \tag{A.6}$$

and

$$\Delta_{\mu\lambda}(t) = \mathrm{e}^{-\mathrm{i}(\epsilon_\lambda - \epsilon_\mu)(t-t')}\Delta_{\mu\lambda}. \tag{A.7}$$

In a similar manner we define

$$X_\lambda(t)^{\cdot} \Delta_{\mu\nu}(t')^{\cdot} = \delta_{\lambda\mu}\mathrm{i}G_\lambda^{(0)}(t-t')X_\nu(t') - \delta_{\mu\nu}\mathrm{i}G_\lambda^{(0)}(t-t')X_\lambda(t'). \tag{A.8}$$

Then we obtain the following relations:

$$\begin{aligned}
&\langle 0|TX_{\lambda_1}(t_1)\ldots X_{\lambda_n}(t_n)X_{\mu_1}^+(t_{n+1})\ldots X_{\mu_n}^+(t_{2n})|0\rangle \\
&\quad= \langle 0|TX_{\lambda_1}(t_1)^{\cdot} X_{\mu_n}^+(t_{2n})^{\cdot} X_{\lambda_2}(t_2)\ldots X_{\mu_{n-1}}^+(t_{2n-1})|0\rangle \\
&\qquad - \langle 0|TX_{\lambda_1}(t_1)^{\cdot} X_{\mu_{n-1}}^+(t_{2n-1})^{\cdot} X_{\lambda_2}(t_2)\ldots X_{\mu_{n-2}}^+(t_{2n-2})X_{\mu_n}^+(t_{2n})|0\rangle \\
&\qquad + \cdots + (-1)^{n-1}\langle 0|TX_{\lambda_1}(t_1)^{\cdot} X_{\mu_1}^+(t_{n+1})^{\cdot} X_{\lambda_2}(t_2) \\
&\qquad \ldots X_{\lambda_n}(t_n)X_{\mu_2}^+(t_{n+2})\ldots X_{\mu_n}^+(t_{2n})|0\rangle
\end{aligned} \tag{A.9}$$

and

$$\begin{aligned}
&\langle 0|TX_{\lambda_1}(t_1)\ldots X_{\lambda_n}(t_n)X_{\mu_1}^+(t_{n+1})\ldots X_{\mu_n}^+(t_{2n})\Delta_{\nu\kappa}(t')|0\rangle \\
&\quad= \langle 0|TX_{\lambda_1}(t_1)^{\cdot} X_{\mu_n}^+(t_{2n})^{\cdot} X_{\lambda_2}(t_1)\ldots X_{\mu_{n-1}}^+(t_{2n-1})\Delta_{\nu\kappa}(t')|0\rangle \\
&\qquad - \langle 0|TX_{\lambda_1}(t_1)^{\cdot} X_{\mu_{n-1}}^+(t_{2n-1})^{\cdot} X_{\lambda_2}(t_2)\ldots X_{\mu_{n-2}}^+(t_{2n-2})X_{\mu_n}^+(t_{2n})\Delta_{\nu\kappa}(t')|0\rangle \\
&\qquad + \cdots + \langle 0|TX_{\lambda_1}(t_1)^{\cdot}\Delta_{\nu\kappa}(t')^{\cdot} X_{\lambda_2}(t_2)\ldots X_{\mu_n}^+(t_{2n})|0\rangle.
\end{aligned} \tag{A.10}$$

The generalization of these formulae to a finite-U model is straightforward.

In the following we show the expectation value of an evolution operator U to the order V^4, where unperturbed state ψ_0 is the Fermi sea occupied by the conduction electrons. The evolution operator is defined by

$$U(t_f, t_i) = T \exp\left(-\mathrm{i} \int_{t_i}^{t_f} H_1(t)\,\mathrm{d}t \right) \tag{A.11}$$

where the interaction part of the Hamiltonian is

$$H_1 = V \sum_{k\sigma} (f_\sigma^+ c_{k\sigma} + \mathrm{HC}). \tag{A.12}$$

T denotes the time-ordering operator and $H_1(t) = \mathrm{e}^{\mathrm{i}H_0 t} H_1 \mathrm{e}^{-\mathrm{i}H_0 t}$. The f-electron operator is written as $f_\sigma^+ = X_{\sigma 0} + \sigma X_{d,-\sigma}$ ($N = 2$ for simplicity).

The ground-state energy is given by the formula

$$\Delta E = \frac{\mathrm{i}}{T} \langle \psi_0 | U(\infty, -\infty) | \psi_0 \rangle_c \text{ with } T = \int_{-\infty}^{\infty} \mathrm{d}t. \tag{A.13}$$

The lowest contribution $\langle \psi_0 | U | \psi_0 \rangle^{(2)}$ is given by

$$\begin{aligned} \langle \psi_0 | U | \psi_0 \rangle^{(2)} &= -\frac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2 \langle \psi_0 | T H_1(t_1) H_1(t_2) | \psi_0 \rangle \\ &= \int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2 V^2 \sum_{km} \mathrm{i} G_m^{(0)}(t_1 - t_2) \mathrm{i} G_{km}(t_2 - t_1). \end{aligned} \tag{A.14}$$

Here we have defined G_{km} by

$$G_{km}(t_1 - t_2) = -\mathrm{i} \langle \psi_0 | T c_{km}(t_1) c_{km}^+(t_2) | \psi_0 \rangle. \tag{A.15}$$

Now we denote the singly occupied states as f^1-states and the doubly occupied states as f^2-states $|d\rangle$. Then the fourth-order term $\langle \psi_0 | U | \psi_0 \rangle^{(4)}$ is written as

$$\begin{aligned} \langle \psi_0 | U(\infty, -\infty) | \psi_0 \rangle^{(4)} &= \frac{(-\mathrm{i})^4}{4!} \int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,\mathrm{d}t_4 \langle \psi_0 | T H_1(t_1) H_1(t_2) H_1(t_3) H_1(t_4) | \psi_0 \rangle \\ &= \frac{(-\mathrm{i})^4}{4!} \frac{4}{2} \frac{3}{1} \int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,\mathrm{d}t_4 V^4 \\ &\quad \times \sum_{k_i} \sum_{\sigma_i} [\langle 0 | T X_{\sigma_1 0}(t_1) X_{\sigma_2 0}(t_2) X_{0\sigma_3}(t_3) X_{0\sigma_4}(t_4) | 0 \rangle \\ &\quad + \sigma_2 \sigma_4 \langle 0 | T X_{\sigma_1 0}(t_1) X_{d,-\sigma_2}(t_2) X_{0\sigma_3}(t_3) X_{-\sigma_4,d}(t_4) | 0 \rangle \\ &\quad + \sigma_1 \sigma_4 \langle 0 | T X_{d,-\sigma_1}(t_1) X_{\sigma_2 0}(t_2) X_{0\sigma_3}(t_3) X_{-\sigma_4,d}(t_4) | 0 \rangle \\ &\quad + \sigma_2 \sigma_3 \langle 0 | T X_{\sigma_1 0}(t_1) X_{d,-\sigma_2}(t_2) X_{-\sigma_3,d}(t_3) X_{\sigma_4 0}(t_4) | 0 \rangle \\ &\quad + \sigma_1 \sigma_3 \langle 0 | T X_{d,-\sigma_1}(t_1) X_{\sigma_2 0}(t_2) X_{-\sigma_3,d}(t_3) X_{\sigma_4 0}(t_4) | 0 \rangle \\ &\quad + \sigma_1 \sigma_2 \sigma_3 \sigma_4 \langle 0 | T X_{d,-\sigma_1}(t_1) X_{d,-\sigma_2}(t_2) X_{-\sigma_3,d}(t_3) X_{-\sigma_4,d}(t_4) | 0 \rangle] \\ &\quad \times \langle \psi_0 | T c_{k_1\sigma_1}(t_1) c_{k_2\sigma_2}(t_2) c_{k_3\sigma_3}^+(t_3) c_{k_4\sigma_4}^+(t_4) | \psi_0 \rangle. \end{aligned} \tag{A.16}$$

The first term consists of the f^1-states only. The contribution is written as

$$\frac{1}{2}\left\{\int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,V^2 \sum_{k\sigma} \mathrm{i}G_\sigma^{(0)}(t_1-t_2)\mathrm{i}G_{k\sigma}(t_2-t_1)\right\}^2 - \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,\mathrm{d}t_4\,V^4$$
$$\times \sum_{k_1k_2\sigma} \mathrm{i}G_\sigma^{(0)}(t_1-t_4)\mathrm{i}G_{k_2\sigma}(t_4-t_2)\mathrm{i}G_\sigma^{(0)}(t_2-t_3)\mathrm{i}G_{k_1\sigma}(t_3-t_1)$$
$$+\int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,\mathrm{d}t_4\,V^4$$
$$\times \sum_{k_1k_2\sigma} \mathrm{i}G_\sigma^{(0)}(t_1-t_4)\mathrm{i}G_\sigma^{(0)}(t_4-t_3)\mathrm{i}G_{k_1\sigma}(t_3-t_1)\mathrm{i}G_\sigma^{(0)}(t_2-t_4)\mathrm{i}G_{k_2\sigma}(t_4-t_2)$$
$$-\int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,\mathrm{d}t_4\,V^4 \sum_{k_1\sigma_1} \mathrm{i}G_{\sigma_1}^{(0)}(t_1-t_4)\mathrm{i}G_{\sigma_1}^{(0)}(t_4-t_3)\mathrm{i}G_{k_1\sigma_1}(t_3-t_1)$$
$$\times \sum_{k_2\sigma_2} \mathrm{i}G_{\sigma_2}^{(0)}(t_2-t_4)\mathrm{i}G_{k_2\sigma_2}(t_4-t_2). \tag{A.17}$$

The first term in (A.17) is a disconnected contribution while the others are connected ones. The second term in (A.17) also emerges in the non-interacting case and thus contains contributions from the doubly occupied processes. One can easily be convinced that these doubly occupied states are cancelled out by the third term in (A.17). Inserting $1=\theta(t_4-t_3)+\theta(t_3-t_4)$ in the second term in (A.17), we obtain

$$-\frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,\mathrm{d}t_4\,V^4 \sum_{k_1k_2\sigma} \mathrm{i}G_\sigma^{(0)}(t_1-t_4)\mathrm{i}G_{k_2\sigma}(t_4-t_2)\mathrm{i}G_\sigma^{(0)}(t_2-t_3)\mathrm{i}G_{k_1\sigma}(t_3-t_1)$$
$$\times\{\theta(t_4-t_3)+\theta(t_3-t_4)\}$$
$$= -\int_{-\infty}^{\infty} \mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\,\mathrm{d}t_4\,V^4 \sum_{k_1k_2\sigma} \mathrm{i}G_\sigma^{(0)}(t_1-t_4)\mathrm{i}G_{k_2\sigma}(t_4-t_2)$$
$$\times \mathrm{i}G_\sigma^{(0)}(t_2-t_3)\mathrm{i}G_{k_1\sigma}(t_3-t_1)\theta(t_4-t_3). \tag{A.18}$$

Then according to (A.5), a sum of integrands in the second and third terms in (A.17) is proportional to

$$\theta(t_1-t_4)\theta(t_2-t_3)\theta(t_4-t_3)-\theta(t_1-t_4)\theta(t_2-t_4)\theta(t_4-t_3)$$
$$=\theta(t_1-t_4)\theta(t_2-t_3)\theta(t_4-t_3)-\theta(t_1-t_4)\theta(t_2-t_4)\theta(t_4-t_3)\theta(t_2-t_3)$$
$$=\theta(t_1-t_4)[1-\theta(t_2-t_4)]\theta(t_2-t_3)\theta(t_4-t_3)$$
$$=\theta(t_1-t_4)\theta(t_4-t_2)\theta(t_2-t_3) \tag{A.19}$$

which shows the repulsive effect of correlated electrons, because the propagation of localized electrons, $G_\sigma^{(0)}(t_1-t_4)$ and $G_\sigma^{(0)}(t_2-t_3)$, cannot overlap due to a factor $\theta(t_4-t_2)$. Therefore after cancellation of the doubly occupied states we obtain a simple form. Introducing the Fourier transform of the step function

$$D^{(0)}(\nu)=\mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}t\mathrm{e}^{\mathrm{i}\nu t}\theta(t)=\frac{-1}{\nu+\mathrm{i}\delta} \tag{A.20}$$

the energy shift in the limit $U = \infty$ reads

$$\Delta E^{(4)} = V^4 \sum_{k_1 k_2 m} \int \frac{d\omega\, d\nu}{(2\pi i)^2} (G_m^{(0)}(\omega))^2 G_{k_1 m}(\omega) D^{(0)}(\nu) G_{k_2 m}(\omega - \nu)$$
$$+ \Delta E^{(2)} V^2 \sum_{km} \int \frac{d\omega}{2\pi i} (G_m^{(0)}(\omega))^2 G_{km}(\omega). \tag{A.21}$$

Now let us turn to other contributions in (A.16). The last term in (A.16) vanishes since $X_{d,\sigma}|0\rangle = 0$ and $X_{\sigma,d}|0\rangle = 0$. The second term is given by

$$\begin{aligned}
&\langle 0|T X_{\sigma_1,0}(t_1) X_{d,-\sigma_2}(t_2) X_{0,\sigma_3}(t_3) X_{-\sigma_4,d}(t_4)|0\rangle \\
&\quad = iG_{\sigma_3}^{(0)}(t_3 - t_1)\langle 0|T \Delta_{\sigma_1\sigma_3}(t_1) X_{d,-\sigma_2}(t_2) X_{-\sigma_4,d}(t_4)|0\rangle \\
&\qquad + iG_{\sigma_3}^{(0)}(t_3 - t_4)\delta_{\sigma_3,-\sigma_4}\langle 0|T X_{\sigma_1 0}(t_1) X_{d,-\sigma_2}(t_2) X_{0d}(t_4)|0\rangle \\
&\quad = iG_{\sigma_3}^{(0)}(t_3 - t_4)\delta_{\sigma_3,-\sigma_4}[ig_d^{(0)}(t_4 - t_1)\langle 0|T(-X_{\sigma_1 d}(t_1)) X_{d,-\sigma_2}(t_2)|0\rangle \\
&\qquad + ig_d^{(0)}(t_4 - t_2)\langle 0|T X_{\sigma_1 0}(t_1) X_{0,-\sigma_2}(t_2)|0\rangle] \\
&\quad = -\delta_{\sigma_3,-\sigma_4} iG_{\sigma_3}^{(0)}(t_3 - t_4) ig_d^{(0)}(t_4 - t_2)\langle 0|T X_{0,-\sigma_2}(t_2) X_{\sigma_1 0}(t_1)|0\rangle \\
&\quad = -\delta_{\sigma_3,-\sigma_4}\delta_{\sigma_1,-\sigma_2} iG_{\sigma_3}^{(0)}(t_3 - t_4) ig_d^{(0)}(t_4 - t_2) iG_{-\sigma_2}^{(0)}(t_2 - t_1)
\end{aligned} \tag{A.22}$$

where $g_d^{(0)}(t - t')$ is the f^2-state Green function defined by [20]

$$ig_d^{(0)}(t - t') = \langle 0|T X_{0d}(t) X_{d0}(t')|0\rangle = \theta(t - t') e^{-i(2\epsilon_f + U)(t - t')}. \tag{A.23}$$

Then the last five terms in (A.16) lead to

$$\int_{-\infty}^{\infty} dt_1\, dt_2\, dt_3\, dt_4\, V^4 \sum_{k_1 k_2 \sigma} iG_\sigma^{(0)}(t_3 - t_4) ig_d^{(0)}(t_4 - t_2) iG_\sigma^{(0)}(t_2 - t_1)$$
$$\times [iG_{k_1\sigma}(t_1 - t_3) iG_{k_2,-\sigma}(t_1 - t_3) + iG_{k_1\sigma}(t_1 - t_4) iG_{k_2,-\sigma}(t_2 - t_3)]. \tag{A.24}$$

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