Phase diagram for the Anderson lattice model

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(Received 16 July 1999)

We study the competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida interaction in the framework of the Anderson lattice model with an extra intersite exchange term. By using an approximation based on an atomic expansion, we obtain, for the symmetric half-filled case, a phase diagram analog to the Doniach diagram for the Kondo lattice. The qualitative and quantitative progress in the description of experimental results for the cerium Kondo compounds with respect to previous approaches is discussed. We also calculate the specific heat which exhibits a two-peak structure as a function of temperature.

I. INTRODUCTION

It is well established that there exists, in cerium compounds at low temperatures, a strong competition between the Kondo effect, which is characterized by a heavy-fermion behavior and tends to demagnetize the system, and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, which tends to yield a magnetic ordering. It results that some cerium Kondo compounds are nonmagnetic and exhibit a heavy-fermion behavior, while other ones order magnetically and have a smaller heavy-fermion character.

The competition between the Kondo effect and the RKKY interaction has been described by the Doniach diagram, which gives the Néel and Kondo temperatures as a function of the intrasite exchange constant \( J_K \): the Néel temperature is first increasing with \( |J_K| \), then passing through a maximum and reaching zero at a quantum critical point, while the Kondo temperature \( T_K \) is exponentially increasing in the single impurity Kondo model. The parameter \( |J_K| \) increases with applied pressure or varies with the relative concentration in ternary systems. Such behavior of the Néel temperature has been experimentally observed with increasing pressure in several cerium Kondo compounds, but the Kondo temperature of a compound can be smaller than that predicted by the Doniach diagram.

The Kondo lattice has been studied in a model with both intrasite \( (J_K) \) and intersite magnetic exchange interaction (characterized by a nearest-neighbor exchange constant \( J_H \)) by means of a mean-field approximation. For sufficiently large intersite antiferromagnetic correlations, this model yields a decrease of the Kondo temperature as compared to the one-impurity value, giving, therefore, a “revisited” version of the Doniach diagram with a rather flat Kondo temperature \( T_K \) in the nonmagnetic case, as observed in several cerium compounds. But the two parameters \( J_K \) and \( J_H \) cannot be considered as independent from each other and it is necessary to take into account the relationship between them to obtain the real dependence of \( T_K \) versus \( J_K \). Since the intersite \( f-f \) interaction term \( J_H \) comes mostly from the indirect RKKY interaction, the value of \( J_H \) has been taken proportional to \( J_K^2 \). Strong antiferromagnetic short-range correlations decrease drastically the Kondo temperature with respect to that defined for one impurity and can yield roughly constant values of \( T_K \) versus \( J_K \). This point is in good agreement with experimental results in CeRh\(_2\)Si\(_2\) (Ref. 4) where the Kondo temperature \( T_K \) is roughly constant with pressure up to 17 kbar and in CeRu\(_2\)Ge\(_2\) (Refs. 5, 6) where \( T_K \) increases much less rapidly with pressure than the single impurity Kondo temperature \( T_{K0} \) above the critical pressure of supression of the magnetic order. A similar behavior can be found when the relative concentration is varied in a ternary alloy such as Ce(Ru\(_{1-x}\)Rh\(_x\))\(_2\)Si\(_2\). Such drastic reduction of the Kondo temperature in a lattice with respect to the one-impurity value has been also obtained by considering the “exhaustion” problem due to the fact that only the conduction electrons within an energy range of order \( T_{K0} \) from the Fermi energy are able to screen the localized electrons in the Kondo lattice.

In the present paper, we adopt an alternative point of view and, instead of the Kondo Hamiltonian, we consider the periodic Anderson model (PAM), which can describe both Kondo and intermediate valence Cerium compounds. Then, we perform the exact diagonalization of the on-site Hamiltonian, as previously used for the Anderson lattice and the Hubbard Hamiltonians, and we treat the intersite terms within the same preceding diagrammatic approximation. The parameters of this PAM Hamiltonian include the hybridization \( V \), the \( f \)-electron energy \( E_f \), and the local Coulomb repulsion \( U \) between the \( f \) electrons. It corresponds to the Kondo lattice model in the limit \( V/|E_f| \rightarrow 0 \), where the physics is well described by an intrasite exchange constant \( J_K \):

\[
J_K = \frac{2V^2 U}{E_f(E_f+U)}. \tag{1}
\]
Thus, based on the results of Ref. 3, we include an extra nearest-neighbor Heisenberg term in order to see the effect of intersite magnetic correlations. In the next section, we present our model Hamiltonian and the approximation adopted that takes into account the strong local correlation between the \( f \) electrons in a simplified way. In the third section, we present the theoretical results and the comparison with experiments. Then, in the last section, we present some comments and the conclusion.

### II. Theoretical Model

The periodic Anderson model (PAM) including nearest-neighbor exchange interactions is described by the following Hamiltonian:

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2,
\]

where

\[
\mathcal{H}_0 = \sum_{i\sigma} \left( E_i n_{i\sigma}^+ + \frac{1}{2} U n_{i\sigma}^+ n_{i\sigma}^- + V(f_{i\sigma}^+ d_{i\sigma}^+ + \text{H.c.}) \right),
\]

\[
\mathcal{H}_1 = -\sum_{i\sigma} t_{ij} d_{i\sigma}^+ d_{j\sigma},
\]

\[
\mathcal{H}_2 = -\sum_{ij} J_{ij} S_i^+ \cdot S_j^+,
\]

where \( a_{i\sigma}^+ (a_{i\sigma}) \) is the operator that creates (annihilates) one electron of spin \( \sigma \) in the \( a = d \) or \( f \) orbital at the \( i \)th site, \( n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma} \) is the number operator in that orbital, and \( S_i^+ \) is the \( f \)-electron spin at that site. The parameters included in the first term are the energy \( E_i \) of the \( 4f \) electrons, the Coulomb repulsion \( U \) between two \( f \) electrons of opposite spin on the same site, and the local hybridization \( V \) between \( f \) and \( d \) electrons. The conduction-electron hopping \( t_{ij} \) and the intersite exchange \( J_{ij} \) between \( f \)-electron spins have been considered only for nearest-neighbor sites, in which case they assume the values \( t \) and \( J_H \), respectively. Here we consider the symmetric case \( (2E_f + U = 0) \) at half-filling (two electrons per site), where the chemical potential is equal to zero.

The approximation that we adopt consists of two steps. First, we transform the exchange term \( \mathcal{H}_2 \) into a one-particle term by applying a mean-field approximation

\[
S_i^+ \cdot S_j^+ \approx -\frac{1}{2} \sum_{\sigma} \left( f_{i\sigma}^+ f_{j\sigma} + f_{j\sigma}^+ f_{i\sigma} \right) f_{i\sigma}^+ f_{j\sigma} + \frac{1}{4} m_i m_j + \frac{1}{4} \{ m_i (n_{i1}^f - n_{j1}^f) + m_j (n_{i1}^f - n_{j1}^f) \},
\]

where \( m_i = \langle n_{i1}^f \rangle - \langle n_{j1}^f \rangle \) is the magnetization at the \( i \)th site. In this paper we will be restricted to the nonmagnetic phase, where \( m_i = 0 \) and \( \langle f_{i\sigma}^+ f_{j\sigma} \rangle = \langle f_{i\sigma} f_{j\sigma} \rangle = \langle f_{i\sigma}^+ f_{j\sigma} \rangle \). In this case, we have

\[
\mathcal{H}_2' = -t' \sum_{i\sigma} \left( f_{i\sigma}^+ f_{j\sigma} + \text{H.c.} \right) - J_H \sum_{i\sigma} \langle f_{i\sigma}^+ f_{j\sigma} \rangle^2,
\]

where

\[
t' = -J_H (f_{i\sigma}^+ f_{j\sigma}).
\]

Second, we make the approximation of Refs. 10 and 11 to treat the intersite part of the Hamiltonian \( \mathcal{H}_1 + \mathcal{H}_2' \). By grouping the lattice Green functions in matrix form

\[
G_{ij}(\omega) = \begin{pmatrix} G_{dd}(\omega) & G_{df}(\omega) \\ G_{fd}(\omega) & G_{ff}(\omega) \end{pmatrix},
\]

and defining the hopping matrices

\[
T_{ij} = \begin{pmatrix} t & 0 \\ 0 & t' \end{pmatrix}
\]

for \( i, j \) nearest neighbors,\( \) we obtain the following Dyson-like equation:

\[
G_{ij}(\omega) = g(\omega) \delta_{ij} - g(\omega) \sum_k T_{ik} G_{kj}(\omega).
\]

The matrix elements of \( g(\omega) \) are the atomic Green functions at zero temperature which have the form

\[
g_{ab}(\omega) = \sum_{i=1}^{4} \frac{A_i}{\omega - p_i}.
\]

The poles \( p_i \) and the residues \( A_i \) are determined from the eigenvalues and eigenvectors of \( \mathcal{H}_0 \) which are given in Table I of Ref. 10. In a brief preliminary account of this work,\( \) we have included in the unperturbed Green functions all the temperature excitations present in the exact atomic solution of the Hamiltonian. In the present version of the approximation, the lattice Green functions are built from the zero temperature atomic Green functions, and their temperature dependence will be described uniquely via the Matsubara frequencies. We have also improved the numerical precision to allow for the computation of the specific heat.

Equation (11) can be solved by Fourier transformation

\[
G(\mathbf{q}, \omega) = [1 - g(\omega) E(\mathbf{q})]^{-1},
\]

where

\[
E(\mathbf{q}) = -\frac{1}{N} \sum_{ij} T_{ij} e^{-i \mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)} = \epsilon(\mathbf{q}) T/t.
\]

The matrix elements are

\[
G_{dd}(\mathbf{q}, \omega) = \frac{g_{dd}(\omega) + t' \gamma(\omega) \epsilon(\mathbf{q}) / t}{\Delta(\mathbf{q}, \omega)},
\]

\[
G_{ff}(\mathbf{q}, \omega) = \frac{g_{ff} + \gamma(\omega) \epsilon(\mathbf{q})}{\Delta(\mathbf{q}, \omega)},
\]

\[
G_{df}(\mathbf{q}, \omega) = \frac{g_{df}}{\Delta(\mathbf{q}, \omega)},
\]

where

\[
\gamma(\omega) = g_{df}(\omega) - g_{dd}(\omega) g_{ff}(\omega),
\]
\[ \Delta(\mathbf{q}, \omega) = 1 - A(\omega) \epsilon(\mathbf{q})/t - B(\omega)[\epsilon(\mathbf{q})/t]^2, \]

\[ A(\omega) = t g_{dd}(\omega) + t' g_{ff}(\omega), \]

\[ B(\omega) = tt' \gamma(\omega). \]

The lattice Green functions are obtained from the inverse Fourier transformation

\[ G_{ij}(\omega) = \frac{1}{N} \sum_{\mathbf{q}} G(\mathbf{q}, \omega)e^{-i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)}. \]

For \( i = j \) they can be calculated as

\[ G_{ii}(\omega) = \frac{1}{N} \sum_{\mathbf{q}} G(\mathbf{q}, \omega) = \frac{1}{N} \sum_{\mathbf{q}} F(\epsilon(\mathbf{q})/t) \]

\[ = \int dx \rho_0(x) F(x), \]

where \( \rho_0(x) \) is the tight-binding density of states of the simple cubic lattice. For the nearest-neighbor Green functions, the corresponding expression is

\[ G_{(ij)}(\omega) = \frac{1}{N} \sum_{\mathbf{q}} G(\mathbf{q}, \omega)e^{i\mathbf{q} \cdot \mathbf{r}} = -\frac{1}{6} \int dx \rho_0(x) F(x) x. \]

As the kernel function above has the general form

\[ F(x) = \frac{C + Dx}{1 \pm Ax - Bx^2}, \]

with \( C \) and \( D \) defined from Eqs. (15)–(17), the different Green functions can be expressed in terms of the integral transform

\[ H(z) = \int dx \rho_0(x) \frac{1}{x - z}. \]

Thus, for the general case \( J_H \neq 0 \) we obtain

\[ G_{ii}^{ab}(\omega) = K_+ H(Z_+) - K_- H(Z_-), \]

\[ G_{(ij)}^{ab}(\omega) = \frac{1}{6} \{ Z_- K_+ H(Z_-) - Z_+ K_- H(Z_+) \}, \]

where

\[ Z_\pm = -\frac{A \pm \sqrt{A^2 + 4B}}{2B}, \]

\[ K_\pm = \frac{C + DX_\pm}{B(Z_\pm - Z_\pm)}. \]

The solution for the particular case \( J_H = 0 \) is

\[ G_{ii}^{ab}(\omega) = -\frac{D}{A} - \frac{1}{A} \left( C + \frac{D}{A} \right) H(\frac{1}{A}), \]

\[ G_{(ij)}^{ab}(\omega) = -\frac{1}{A} \left( C + \frac{D}{A} \right) \left\{ 1 + \frac{1}{A} H(\frac{1}{A}) \right\}. \]

The two-operator averages of the model are directly evaluated as a sum over Matsubara frequencies \( \omega_n = (2n + 1)\pi/\beta \):

\[ \langle b_{j \alpha}^\dagger a_{i \sigma} \rangle = \lim_{\tau \to 0^+} \frac{1}{\beta} \sum_\omega G_{ij}^{ab}(i \omega_n) e^{i\omega_n \tau}. \]

At low temperatures the asymptotic part of the series has to be evaluated as an integral, by considering \( \omega_n \) as a continuous variable. The average \( \langle f_{i \alpha}^\dagger f_{j \sigma} \rangle \) appearing in Eq. (8) defines a self-consistent evaluation of the lattice Green functions, which always converges, provided that \( J_H \) is negative.

The specific heat can be calculated directly from the derivative of the internal energy

\[ C = \frac{dE}{dT}. \]

The internal energy per site is given by

\[ E = \langle d_{i \alpha}^\dagger [d_{i \alpha}, \mathcal{H}] \rangle + \langle f_{i \alpha}^\dagger [f_{i \alpha}, \mathcal{H}] \rangle + 2V(d_{i \alpha}^\dagger f_{i \alpha}) \]

\[ - 6t'(d_{i \alpha}^\dagger d_{j \alpha}) - 6t'(f_{i \alpha}^\dagger f_{j \alpha}) - 3J_H(f_{i \alpha}^\dagger f_{j \alpha})^2 + \frac{1}{2} E_{ij} n_f, \]

where \( n_f \) is the \( f \)-electron concentration. The first two terms are calculated by

\[ \langle a_{i \alpha}^\dagger [a_{i \sigma}, \mathcal{H}] \rangle = \lim_{\tau \to 0^+} \frac{1}{\beta} \sum_N [i \omega_n G_{ij}^{aa}(i \omega_n) - 1] e^{i\omega_n \tau}. \]

In the next section, we will present first the averages \( \langle d_{i \alpha}^\dagger f_{j \sigma} \rangle \) and \( \langle f_{i \alpha}^\dagger f_{j \sigma} \rangle \) for different values of the parameters. Within the approximation that we have adopted here, these two averages provide a good account for the intrasite \( d-f \) correlation and the intersite \( f-f \) correlation functions. Finally, Eqs. (34)–(36) will give the specific heat curves versus temperature for the same values of the parameters.

### III. RESULTS

First of all, we plot in Fig. 1 the averages \( \langle d_{i \alpha}^\dagger f_{j \sigma} \rangle \) and \( \langle f_{i \alpha}^\dagger f_{j \sigma} \rangle \) (where \( i \) and \( j \) are nearest neighbors) as a function of temperature for different values of the parameters \( E_f, V, \) and \( J_H \). We choose \( E_f = -3t \) and \( V = t \). For these values of the parameters, the Anderson Hamiltonian is equivalent to a Kondo exchange Hamiltonian with \( J_K = -4t/3 \), which is much smaller than the width \( W = 12t \) of the conduction band. We take several values of \( J_H = 0, -3t, -6t, \) and \( -12t \) in order to study the effect of antiferromagnetic intersite correlations. Each curve is a smooth and monotonically increasing function whose derivative exhibits a well marked maximum, which corresponds to a kind of crossover temperature. We define the Kondo temperature \( T_K \) as the crossover temperature determined from the average \( \langle d_{i \alpha}^\dagger f_{j \sigma} \rangle \). The correlation temperature \( T_{\text{cor}} \), below which short-range magnetic correlations arise, is defined in a similar way with respect to \( \langle f_{i \alpha}^\dagger f_{j \sigma} \rangle \). More precisely, \( T_K \) and \( T_{\text{cor}} \) are taken here equal to the temperatures of the maxima of the derivatives of the curves of Fig. 1 with respect to temperature. From the curves...
in Fig. 1, one can remark that $T_{\text{cor}}$ increases rapidly with $|J_H|$, while $T_K$ seems to saturate to a constant value. Here, in contrast with the preceding Kondo lattice treatment in Ref. 3, the curves giving $\langle d_{i\sigma}^\dagger f_{i\sigma} \rangle$ and $\langle f_{i\sigma}^\dagger f_{j\sigma} \rangle$ do not present any phase transition but are rather smooth. This indicates that the corresponding definition of $T_K$ provides an improved description of the Kondo effect.

Figure 2 gives a plot of the two temperatures $T_K$ and $T_{\text{cor}}$ versus the intersite antiferromagnetic correlation parameter $J_H$ for $V=t$ and $E_f=-3t$. We see that there is a crossing between the two curves at a value $|J_H|=2.57t$ and that the Kondo temperature $T_K$ remains roughly constant, while the short-range correlation temperature $T_{\text{cor}}$ increases very rapidly with $|J_H|$.

Figure 3 shows the temperature dependence of the specific heat for the same values of the parameters as those used in Fig. 1. The specific heat curves show a clear peak near $T_{\text{cor}}$ and another one at $T=0$. As expected, the low temperature peak increases with $|J_H|$, approaches first the high-temperature peak and becomes even larger for the highest value $|J_H|=12t$.

So far, we have studied $T_K$ and $T_{\text{cor}}$ as a function of $J_H$ for constant $E_f/t$ and $V/t$ values. The corresponding value of the $d$-$f$ exchange parameter $J_K$ has also been considered as a constant. In particular, the adopted value $|J_K|=4t/3$ is quite small. Thus, it is interesting to deduce the diagram of $T_K$ and $T_{\text{cor}}$ as a function of $|J_K|$, to see what happens when this parameter increases. As previously established for the Kondo lattice, in cerium compounds, the intersite Heisenberg exchange between localized spins originates mainly from the RKKY interaction which is mediated by the conduction electrons via the hybridization. In Ref. 3, $J_H/t$ has been taken

![FIG. 1. The averages $\langle d_{i\sigma}^\dagger f_{i\sigma} \rangle$ (lower curves) and $\langle f_{i\sigma}^\dagger f_{j\sigma} \rangle$ (upper curves) as a function of temperature for $E_f=-3t$, $V=t$, and different values of $J_H$.](image1)

![FIG. 2. Crossover temperatures $T_K$ and $T_{\text{cor}}$ as a function of $J_H/t$ for $V=t$ and $E_f=-3t$.](image2)

![FIG. 3. Specific heat as a function of temperature for the same parameters as in Fig. 1.](image3)

![FIG. 4. Crossover temperatures $T_K$ and $T_{\text{cor}}$ as a function of the ratio $|V/E_f|$ for $V=0.5t$ and $J_H$ given by Eq. (38).](image4)
proportional to \((J_K/t)^2\). We take here the same relation between \(J_H\) and the \(J_K\) value given by the Schrieffer-Wolff transformation.\(^\text{12}\) We obtain a good description of the physical situation of Cerium Kondo compounds if we choose here

\[
\frac{J_H}{t} = -0.5 \left(\frac{J_K}{t}\right)^2
\]

(37)

or, equivalently, by using Eq. (1),

\[
\frac{J_H}{t} = -8 \frac{V^4}{(E_f t)^2}
\]

(38)

Figure 4 shows the plot of the two crossover temperatures \(T_K\) and \(T_{\text{cor}}\) versus \(|V/E_f|\) for \(V=0.5t\) and \(J_H\) given by Eq. (38). We see that \(T_{\text{cor}}\) increases rapidly and \(T_K\) remains roughly constant versus \(|V/E_f|\) above a value roughly equal to 1, which corresponds to \(J_K/J_H \approx -2t\), which is much smaller than the width \(W=12t\) of the conduction band. Thus, Fig. 4 represents the diagram giving \(T_K\) and \(T_{\text{cor}}\) within the periodic Anderson Hamiltonian and the parameter \(|V/E_f|\) is expected to be proportional to the pressure.

Finally, we show in Fig. 5 the specific heat for the same parameters as those in Fig. 4 and for different values of \(V/|E_f|\). We see that there are also two peaks, the first one corresponding to \(T_{\text{cor}}\) and the second one to roughly \(t\).

**IV. CONCLUDING REMARKS**

The present approach provides a phase diagram for the Anderson lattice described by both the Anderson Hamiltonian and an additional Heisenberg-type exchange interaction between the 4f spins on nearest neighbors. The calculation has been performed here in the nonmagnetic case, as previously for the Kondo lattice.\(^\text{3}\) The magnetic phases of the Anderson lattice have been recently studied through a related approximation developed in Ref. 14.

The present treatment of the Anderson lattice is similar to the “revisited” Doniach diagram for the Kondo lattice\(^\text{3}\) and gives both the Kondo temperature \(T_K\) and the short-range correlation temperature \(T_{\text{cor}}\). The Kondo temperature increases firstly and then remains constant as a function of \(|J_H|\) in Fig. 2 or \(|V/E_f|\) in Fig. 4. Thus, this result gives also a revisited version of the Doniach diagram and shows that \(T_K\) remains roughly constant with \(|V/E_f|\) or \(|J_K|\) and then under pressure in the nonmagnetic region above the quantum critical point where the Néel temperature \(T_N\) disappears. Our calculation can also account for the occurrence of antiferromagneticlike short-range correlations in some Cerium compounds at a temperature \(T_{\text{cor}}\) much larger than \(T_K\), such as in CeRu_2Si_2 where \(T_{\text{cor}}\approx 60–70\) K and \(T_K\approx 14–23\) K (Refs. 7 and 15) and in CeCu_6 where \(T_{\text{cor}}\approx 10\) K and \(T_K\approx 5\) K.\(^\text{15}\)

We obtain two improvements with respect to the preceding Kondo lattice mean-field calculation:\(^\text{3}\) The curves giving \(\langle d_{\varphi f_{\varphi\varphi}}\rangle\) and \(\langle f_{\varphi f_{\varphi\varphi}}\rangle\) are smooth and do not present any phase transition, implying that \(T_K\) and \(T_{\text{cor}}\) correspond to crossover temperatures. This point is well known for the Kondo effect, and it has also been established for \(T_{\text{cor}}\) by neutron scattering experiments.\(^\text{15}\) The values obtained here for \(T_K\) and \(T_{\text{cor}}\) are smaller, and consequently in better agreement with the experimental values. As shown in Figs. 2 and 4, \(T_K/t\) is typically of order 0.3–0.4 and, since the conduction bandwidth is \(W=12t\), \(T_K\) is much smaller here than in Ref. 3.

We have also derived the specific heat \(C\) which exhibits two maxima at temperatures roughly equal to \(T_{\text{cor}}\) and \(t\). Further experiments would be interesting to check this form of the specific heat curves. Finally, the inclusion of the extra intersite exchange term in the nonmagnetic phase is necessary to obtain a good description of cerium Kondo compounds and further theoretical work will be still important to better understand this point.

**ACKNOWLEDGMENT**

We acknowledge the support of the Brazil-France cooperation agreement Capes-Cofecub, Project No. 196/96.

\*On leave from Universidade do Estado de Santa Catarina, Joinville, Brazil.


