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Phase diagram of the Kondo lattice

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We discuss the phase diagram of the Kondo lattice: we generalize to the lattice a method proposed by Yoshimori and Sakurai for the single-impurity Kondo problem; this method transforms the Kondo exchange interaction into a fictitious s-f hybridization, and gives a resonance of width T_K at the Fermi level. We study the Kondo phase and compare its energy with the energy of the magnetic phase. The Kondo state is stable when the exchange interaction is larger than a critical value; this state is insulating when the conduction band is half filled.

I. INTRODUCTION

Some rare-earth compounds show anomalous magnetic properties. For the "normal" rare-earth compounds, the $4f$ level is far below the Fermi surface and these compounds have an integer number of $4f$ electrons with a well-defined magnetic moment, and a positive exchange interaction with the conduction electrons. In the "anomalous" rare-earth compounds the $4f$ level is close to the Fermi surface; thus a large resonant scattering can occur. This scattering is responsible for the Kondo effect occurring in many rare-earth alloys and in some compounds. The anomalous rare-earth compounds can also show a mixed-valence behavior.

Among these materials, compounds with cerium, samarium, and thulium are the most studied: for example, $CeAl_2$ (Refs. 1 and 2) and TmSe (Ref. 3) exhibit magnetic ordering at low temperature and above the Néel temperature, they behave like Kondo compounds; $CeAl_3$ (Refs. 4 and 5) and SmB_6 (Ref. 6) are nonmagnetic down to zero temperature.

Several theoretical works have been done in order to explain these anomalous behaviors. Phenomenological models have been investigated by Benoit *et al.*[7,8] and Barbara *et al.*[9] which describe the properties of $CeAl_2$ in terms of a competition on each cerium ion between the Kondo effect and an effective field due to the other ions.

Doniach[10] introduced the Kondo-lattice model, which is a generalization of the Kondo Hamiltonian to the concentrated case. On each site of the lattice there is one rare-earth ion interacting with the conduction electrons. In this model the exchange interaction between the conduction and $4f$ electrons is responsible both for the Kondo effect and the magnetism through RKKY (Ruderman-Kittel-Kasuya-Yosida) interactions. The three parameters of this problem are (i) the width of the conduction band which will be equal to $2D$ in this paper, (ii) the exchange parameter, J, between $4f$ and conduction electrons; J is negative in the case of Kondo compounds, and (iii) the number of conduction electrons per site, n.

In order to solve this problem, Doniach[10] considered a one-dimensional analog, the Kondo necklace. In the mean-field approximation he found that the ground state is antiferromagnetic for low $|J|/D$ and it is a nonmagnetic Kondo singlet for large $|J|/D$. These results were confirmed by Jullien *et al.*[11,12] using a renormalization-group treatment.

Recently Jullien *et al.*[13] considered the three-dimensional Kondo-lattice Hamiltonian in a mean-field approach. They found that, for $n=1$, the Kondo state can be either metallic or insulating depending on the value of J/D; for $n \neq 1$, the Kondo state is always metallic. However their method does not allow them to investigate a magnetic ground state; in fact such a magnetic ground state is expected for low values of J/D.

In this paper, we start from the Anderson-lattice model, which seems a more physical approach to the problem. This model has been considered by several authors, either for the study of the magnetic phases[14,15] or for the mixed-valence problem.[16,17] However the methods used in all these papers are not appropriate to the study of the Kondo effect; though the purpose of all these calculations are not the same, the results are very similar: a gap is opened in the density of states, of the order of $|V_{kf}|^2/D$, around the energy of the impurity level (V_{kf} being the Anderson mixing parameter); the width of the resonance is also of this order. Thus the resonance is fairly wide and the number of electrons on the impurity can vary easily. In the Kondo problem the resonance must be much narrower, i.e., of the order of the Kondo temperature T_K, and the number of f electrons is a constant.

In Sec. II we introduce the model and develop the approximations. We generalize a method due to Yoshimori and Sakurai[18] for the single impurity case. These authors transformed the initial Kondo interaction into a fictitious s-f hybridization and this hybridization gives a resonance of width T_K at the Fermi level. Then we discuss the phase diagram obtained from this model. We compare the energies of the

Kondo and magnetic states, as a function of the conduction-band filling and the parameter $|J|/D$; for low values of $|J|/D$ the system is magnetic, ferromagnetic for small value of n and antiferromagnetic for n of the order of one. For larger values of $|J|/D$, we obtain a "Kondo state". We finally discuss the validity of the Kondo Hamiltonian for the rare-earth compounds.

II. HAMILTONIAN AND APPROXIMATIONS

A. The Hamiltonian

Let us consider the system of conduction electrons interacting with periodically arranged magnetic ions, described by an Anderson Hamiltonian

$$H=\sum_{k,\sigma}\epsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\sum_{i\sigma}E_0 d_{i\sigma}^{\dagger}d_{i\sigma}+U\sum_i d_{i\uparrow}^{\dagger}d_{i\uparrow}d_{i\downarrow}^{\dagger}d_{i\downarrow}+\sum_{k,\sigma,i}V_{kf}(c_{k\sigma}^{\dagger}d_{i\sigma}e^{ikR_i}+d_{i\sigma}^{\dagger}c_{k\sigma}e^{-ikR_i}) \quad . \tag{1}$$

$c_k^{\dagger}$ and $d_i^{\dagger}$ are the creation operators, respectively, for an s electron of wave vector k and an f electron on site i. We neglect the orbital degeneracy of the f electrons and E_0 is the energy of the f level. We are interested in the case of a large value of the Coulomb interaction between f electrons, U, and a small value of the mixing between s and f electrons, V_{kf}. In this case, for the single impurity problem, Schrieffer and Wolff[19] have shown that the Anderson model is equivalent to the s-f Hamiltonian

$$H=\sum_{k,\sigma}\epsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}-\sum_{k,k'}\tfrac{1}{2}J_{kk'}[S_i^z(c_{k\uparrow}^{\dagger}c_{k'\uparrow}-c_{k\downarrow}^{\dagger}c_{k'\downarrow})+S_i^{+}c_{k\downarrow}^{\dagger}c_{k'\uparrow}+S_i^{-}c_{k\uparrow}^{\dagger}c_{k'\downarrow}]+\sum_{kk'}\tfrac{1}{4}J_{kk'}(d_{i\uparrow}^{\dagger}d_{i\uparrow}+d_{i\downarrow}^{\dagger}d_{i\downarrow})(c_{k\uparrow}^{\dagger}c_{k'\uparrow}+c_{k\downarrow}^{\dagger}c_{k'\downarrow}) \quad , \tag{2}$$

with

$$J_{kk'}=\frac{2V_{kf}V_{k'f}^{*}}{(E_0-E_F)} \quad , \tag{3}$$

E_F being the Fermi level, and S_i is defined by

$$S_i^z=\tfrac{1}{2}(d_{i\uparrow}^{\dagger}d_{i\uparrow}-d_{i\downarrow}^{\dagger}d_{i\downarrow}), \quad S_i^{+}=d_{i\uparrow}^{\dagger}d_{i\downarrow}, \quad S_i^{-}=d_{i\downarrow}^{\dagger}d_{i\uparrow} \quad .$$

We use the same transformation to our Hamiltonian and obtain

$$H=H_0+H_1+H_2 \quad ,$$

where

$$H_0=\sum_{k,\sigma}\epsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\sum_{i,\sigma}E_0 d_{i\sigma}^{\dagger}d_{i\sigma} \quad , \tag{4}$$

$$H_1=-\sum_{k,k'}\tfrac{1}{2}J_{kk'}(c_{k'\uparrow}^{\dagger}c_{k\downarrow}d_{i\downarrow}^{\dagger}d_{i\uparrow}e^{i(k-k')R_i}+c_{k\downarrow}^{\dagger}c_{k'\uparrow}d_{i\uparrow}^{\dagger}d_{i\downarrow}e^{i(k'-k)R_i}) \quad , \tag{5}$$

$$H_2=\sum_{\substack{k,k'\\ \sigma}}\tfrac{1}{2}J_{k,k'}d_{i-\sigma}^{\dagger}d_{i-\sigma}c_{k'\sigma}^{\dagger}c_{k\sigma}e^{i(k-k')R_i} \quad . \tag{6}$$

It is important to remark that this expression is obtained only in the case $\langle\sum_\sigma d_{i\sigma}^{\dagger}d_{i\sigma}\rangle=1$, i.e., this Hamiltonian can not describe mixed-valence properties.

In the following we assume that V_k, and then $J_{k,k'}$, are independent of k; (however in some cases it is important to consider the k dependence of V_k[20]). In this case H_1 and H_2 can be replaced by

$$H_1=-\tfrac{1}{2}J\sum_i c_{i\uparrow}^{\dagger}c_{i\downarrow}d_{i\downarrow}^{\dagger}d_{i\uparrow}+c_{i\downarrow}^{\dagger}c_{i\uparrow}d_{i\uparrow}^{\dagger}d_{i\downarrow}$$

$$=\tfrac{1}{4}J\sum_i(d_{i\uparrow}^{\dagger}c_{i\uparrow}+c_{i\downarrow}^{\dagger}d_{i\downarrow})^2+(d_{i\downarrow}^{\dagger}c_{i\downarrow}+c_{i\uparrow}^{\dagger}d_{i\uparrow})^2 \quad , \tag{7}$$

$$H_2=\tfrac{1}{2}J\sum_{i,\sigma}d_{i-\sigma}^{\dagger}d_{i-\sigma}c_{i\sigma}^{\dagger}c_{i\sigma} \quad . \tag{8}$$

The term H_1 describes the scattering of the conduction electrons by the impurity and is responsible for the Kondo effect; H_2 describes the polarization of the conduction electrons by the impurity spin and gives the usual RKKY interaction.

B. Functional integration method

In the following H_2 is simply treated in Hartree-Fock approximation

$$H_2=\tfrac{1}{2}J\sum_{i,\sigma}\langle d_{i-\sigma}^{\dagger}d_{i-\sigma}\rangle c_{i\sigma}^{\dagger}c_{i\sigma}+\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle d_{i-\sigma}^{\dagger}d_{i-\sigma}$$

$$-\tfrac{1}{2}J\sum_{i,\sigma}\langle d_{i-\sigma}^{\dagger}d_{i-\sigma}\rangle\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle \quad . \tag{9}$$

The problem is to approximate the term H_1 and obtain a correct description of the Kondo effect. For this purpose we use a functional integration approach similar to that introduced by Yoshimori and Sakurai[18] for the single impurity case. The partition function is

$$Z=\mathrm{Tr}\exp[-\beta(H_0+H_1+H_2)] \quad .$$

We can apply to Z the Stratanovitch-Hubbard transformation, valid for any bound operator A,

$$\exp\alpha A^2=\left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{+\infty}dx\exp(\alpha x^2+2\alpha Ax) \quad .$$

This transformation can be done on the two terms of H_1 given by Eq. (7) and we obtain

$$Z=\int dx_i(\tau)\,dy_i(\tau)\,Z(x_i,y_i)\exp\int_0^{\beta}\tfrac{1}{4}J(x_i^2+y_i^2)\,d\tau \quad , \tag{10}$$

where

$$Z(x_i,y_i) = \mathrm{Tr}\, T_\tau \exp\left[-\int_0^\beta H(\tau)\, d\tau\right] ,$$

$$H(\tau) = H_0(\tau) + H_2(\tau) + \sum_i \tfrac{1}{2} J x_i(\tau)[d_{i\uparrow}^\dagger(\tau)\, c_{i\uparrow}(\tau) + c_{i\downarrow}^\dagger(\tau)\, d_{i\downarrow}(\tau)] + \tfrac{1}{2} J y_i(\tau)[d_{i\downarrow}^\dagger(\tau)\, c_{i\uparrow}(\tau) + c_{i\uparrow}^\dagger(\tau)\, d_{i\uparrow}(\tau)] \quad . \quad (11)$$

$x_i(\tau)$ and $y_i(\tau)$ are fictitious time-dependent s-f mixing matrix elements coming from the transformation of H_1 and T_τ is the time-ordering operator.

Now the problem is to solve the Hamiltonian $H(\tau)$ with time-dependent parameters $x_i(\tau)$ and $y_i(\tau)$ and then to make the functional average over all possible functions x_i and y_i. It seems that the initial problem has been replaced by a more complicated one, however, it turns out that the usual static approximation which restricts to functions x_i and y_i independent of τ is a good approximation: for the single impurity case the results are qualitatively correct, though the static approximation is a very crude one; the ground-state energy of the Kondo state has the correct behavior for small values of ρJ, $\Delta E \simeq D e^{1/\rho J}$; the static susceptibility is finite and proportional to $1/T_K$; the low-temperature specific heat varies as T/T_K. However the method is not an exact one. The susceptibility is half the correct one obtained by Wilson[21] andNozières.[22] The advantage of this approximation is that the problem becomes very simple and it can be easily generalized to the case of a lattice.

Thus in the static approximation we have to solve now the simple Hamiltonian

$$H = H_0 + V \quad ,$$

where H_0 is given by Eq. (4) and

$$V = \tfrac{1}{2} J \sum_i x_i(d_{i\uparrow}^\dagger c_{i\uparrow} + c_{i\downarrow}^\dagger d_{i\downarrow}) + \tfrac{1}{2} J \sum_i y_i(d_{i\downarrow}^\dagger c_{i\downarrow} + c_{i\uparrow}^\dagger d_{i\uparrow}) + \tfrac{1}{2} J \sum_{i,\sigma} \langle d_{i-\sigma}^\dagger d_{i-\sigma}\rangle c_{i\sigma}^\dagger c_{i\sigma} + \tfrac{1}{2} J \sum_{i,\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma}\rangle d_{i-\sigma}^\dagger d_{i-\sigma} \quad . \quad (12)$$

The partition function Z can be written

$$Z = Z_0 \int dx_i\, dy_i \exp\left[\tfrac{1}{4}\beta J(x_i^2 + y_i^2) + \tfrac{1}{2}\beta J \sum_{i,\sigma} \langle d_{i-\sigma}^\dagger d_{i-\sigma}\rangle \langle c_{i\sigma}^\dagger c_{i\sigma}\rangle\right] \exp \mathrm{Tr} \ln(1 - VG_0)$$

$$= Z_0 \int \exp[-\beta F(x_i, y_i, \langle d_{i\sigma}^\dagger d_{i\sigma}\rangle, \langle c_{i\sigma}^\dagger c_{i\sigma}\rangle)]\, dx_i\, dy_i \quad . \quad (13)$$

Z_0 is the partition function corresponding to H_0 and G_0 is the Green's function for the Hamiltonian H_0. The solution of H gives the energy F as a function of the parameters x_i and y_i. Finally the integration on x_i and y_i is replaced by a saddle-point approximation: The parameters are determined by a minimization of F.

III. PHASE DIAGRAM

In Sec. II we have introduced two kinds of parameters. x_i and y_i describe the scattering of the conduction electrons by the f electrons and thus they are nonzero if there is Kondo coupling. $\langle d_{i\sigma}^\dagger d_{i\sigma}\rangle$ and $\langle c_{i\sigma}^\dagger c_{i\sigma}\rangle$ describe the magnetism of f and s electrons if they are different for up and down spin electrons. In principle both Kondo effect and magnetism can be present in the ground state. However we study here only the cases where the solution is either a pure Kondo solution, or a pure magnetic solution.

A. Kondo state

1. Ground-state energy

In the pure Kondo state, there is no magnetic moment and $\langle d_{i\sigma}^\dagger d_{i\sigma}\rangle = \frac{1}{2}$, $\langle c_{i\sigma}^\dagger c_{i\sigma}\rangle = \frac{1}{2} n$, n being the number of conduction electrons per atom. These relations imply that $x_i = y_i$. Moreover we assume that the state is uniform, i.e., $x_i = y_i = x$ independent on the site i.

The Green's functions corresponding to H, given by Eq. (12) can easily be calculated. The f-electron Green's function is

$$G_d^\sigma(\omega) = \sum_k \left[\omega - E_0 - \tfrac{1}{4} Jn - \frac{J^2 x^2}{4(\omega - \epsilon_k - \frac{1}{4} J)}\right]^{-1} \quad (14)$$

and the conduction-electron Green's function is

$$G_c^\sigma = \sum_k \left[\omega - \epsilon_k - \tfrac{1}{4} J - \frac{J^2 x^2}{4(\omega - E_0 - \frac{1}{4} Jn)}\right]^{-1} \quad . \quad (15)$$

If we assume that the conduction band has a constant density of states, i.e.,

$$\rho_0(\epsilon) = \begin{cases} \dfrac{1}{2D}, & \text{when } -D < \epsilon < D \\ 0, & \text{otherwise} \end{cases} ,$$

we obtain for the density of states of the $4f$ and conduction electrons

$$\rho_d(\omega)=\frac{1}{8D}\frac{J^2x^2}{(\omega-E_0-\frac{1}{4}Jn)^2}\ ,$$
$$\rho_c(\omega)=\frac{1}{2D}\ , \tag{16}$$

when $\omega_1<\omega<\omega_2$ and $\omega_3<\omega<\omega_4$, and $\rho_d=\rho_c=0$ otherwise. ω_1, ω_2, ω_3, and ω_4 are given by

$$\omega_1=\tfrac{1}{2}(-D+E_0+\tfrac{1}{4}J(1+n)-\{[D+E_0-\tfrac{1}{2}J(1-n)]^2+J^2x^2\}^{1/2})\ ,$$
$$\omega_2=\tfrac{1}{2}(D+E_0+\tfrac{1}{4}J(1+n)-\{[D-E_0+\tfrac{1}{4}J(1-n)]^2+J^2x^2\}^{1/2})\ ,$$
$$\omega_3=\tfrac{1}{2}(-D+E_0+\tfrac{1}{4}J(1+n)+\{[D+E_0-\tfrac{1}{4}J(1-n)]^2+J^2x^2\}^{1/2})\ ,$$
$$\omega_4=\tfrac{1}{2}(D+E_0+\tfrac{1}{4}J(1+n)+\{[D-E_0+\tfrac{1}{4}J(1-n)]^2+J^2x^2\}^{1/2})\ .$$

Figure 1 shows the schematic behavior of ρ_d and ρ_c. As soon as $x\neq 0$, there is a gap in the density of states, which is of the order of $J^2x^2/2D$ if the Fermi level is near the middle of the band, i.e., $n\simeq 1$. The width of the peaks, on each side of the gap, is also of this order of magnitude.

The position of the f level, E_0, and the Fermi level E_F must satisfy the following relations, in the case $n<1$ (we restrict to this case, the case $n>1$ can be obtained easily because of the electron-hole symmetry):

$$\langle d^\dagger_{i\sigma}d_{i\sigma}\rangle=\tfrac{1}{2}=\frac{J^2x^2}{8D}\left(\frac{1}{\omega_1-E_0-\frac{1}{4}Jn}-\frac{1}{E_F-E_0-\frac{1}{4}Jn}\right)\ ,$$
$$\langle c^\dagger_{i\sigma}c_{i\sigma}\rangle=\tfrac{1}{2}n=\frac{1}{2D}(E_F-\omega_1)\ , \tag{17}$$

where E_F is in the lower band. For $n=1$, E_F is in the gap. These equations can be solved and we obtain the relation between E_0 and n, and the expression of E_F,

$$E_0=-\tfrac{1}{2}(1-n)D-\frac{1-n}{2n}(n^2D^2+nJ^2x^2)^{1/2}+\tfrac{1}{4}J(1-n)\ ,$$
$$E_F=\tfrac{1}{2}nD-\tfrac{1}{2}(n^2D^2+nJ^2x^2)^{1/2}+E_0+\tfrac{1}{4}Jn\ .$$

x is then determined by minimizing the energy difference $\Delta E(x)$ between the Kondo state and the state without s-f mixing, the f electrons being localized at the energy E_0,

$$\Delta E=-\tfrac{1}{2}(n^2D^2+nJ^2x^2)^{1/2}-\tfrac{1}{2}Jx^2+\frac{J^2x^2}{4D}\ln\frac{(n^2D^2+nJ^2x^2)^{1/2}-nD}{(n^2D^2+nJ^2x^2)^{1/2}+nD}+\tfrac{1}{2}nD\ . \tag{18}$$

The minimum is found to be

$$\frac{J^2x_0^2}{D^2}=4n\frac{e^{2D/J}}{(1-e^{2D/J})^2}\ , \tag{19}$$

which gives for $\Delta E(x)$,

$$\Delta E_K=-nD\frac{e^{2D/J}}{1-e^{2D/J}}\ . \tag{20}$$

We first can remark that we obtain a minimum at x_0 only if $J<0$; if $J>0$ the expression (20) is positive and the minimum is obtained for $x=0$; thus the model gives a Kondo effect only for $J<0$ as it is expected.

When $J<0$ the Kondo ground-state energy is found to have the usual variation $De^{1/\rho J}$ (where ρ is the density of states at the Fermi level), as for a single impurity; the width of the resonance is also of this order.

In order to compare more precisely with the single impurity case, we have calculated the ground-state energy of a single Kondo impurity as a function of the number of conduction electrons, by the same method.[23] For $|J|/D=0.5$ the results are shown in Fig. 2. The following conclusions can be derived: (i) For $n=1$ the ground-state energy ΔE_K is lower for the Kondo lattice than for a single impurity. For $J/D=-0.5$, $\Delta E_K/D$ is -0.45×10^{-2} for a single impurity and -1.85×10^{-2} for the lattice. In fact when the number of impurities increases, the singlet wave

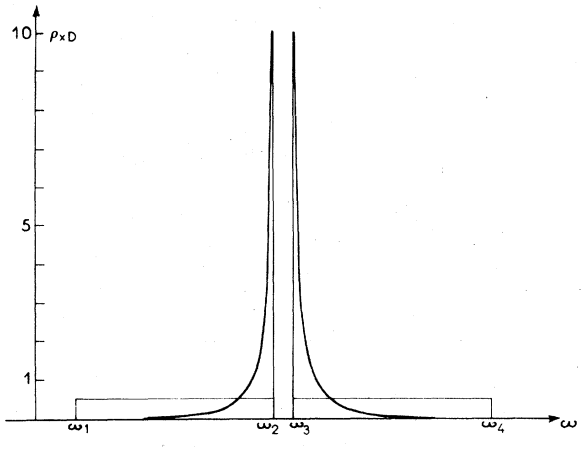

FIG. 1. Schematic density of states in the Kondo state, for the conduction band and for the f electrons.

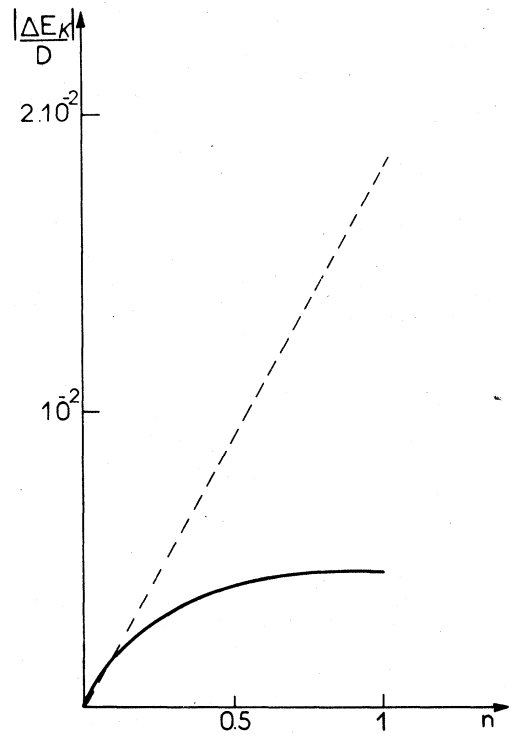

FIG. 2. Variation of the ground-state energy ΔE_K with the number of conduction electrons, for the lattice (dashed line) and for the single impurity (solid line) when $J/D = -0.5$.

functions associated with each impurity are mixed and this mixing is responsible for the decrease in energy. It would be interesting to study the ground-state energy of a concentrated Kondo alloy. Hoshino and Kurata[24] discussed this model recently in the coherent potential approximation, but did not calculate the ground-state energy. We will discuss this problem in a forthcoming publication. (ii) When the number of conduction electrons decreases, the Kondo energy decreases more rapidly in the lattice: when there are less conduction electrons per site, it is more difficult to screen the impurity spins. For the single impurity, this is not very important as there is only one impurity to screen; in fact ΔE_K is almost constant for $0.7 < n < 1$.

The gap is of the order of ΔE_K and exists for all values of J/D, which is not the case in the calculation of Jullien *et al.*[13] They found that the gap disappears when $|J|/D < 0.33$. However we will see in Sec. III B that for low values of $|J|/D$ the ground state is magnetic and the mean-field method used by Jullien *et al.* is not appropriate to the case of a magnetic ground state. By the renormalization-group technique they also found a disappearance of the gap in a one-dimensional lattice,[13] however, this method cannot be generalized to a three-dimensional lattice. Thus other methods should be used in order to find if a metallic Kondo state can be stable in three dimensions for $n = 1$.

As we mentioned in the Introduction, several authors also obtained the same qualitative density of states,[14–17] with a much larger gap of the order of $|V_{kf}|^2/D$, instead of ΔE_K. This is certainly valid for the mixed-valence compounds: In these compounds the Schrieffer-Wolff transformation cannot be applied and our model does not work. We will return to this point in the conclusion.

2. *Kondo temperature of the lattice*

For a single Kondo impurity the Kondo temperature is not a well-defined temperature. It can be calculated from high-temperature expansions: T_K^∞ is then the temperature at which the perturbation expansion diverges; it can also be estimated from low-temperature properties: T_K^0 is the inverse static susceptibility. For a single impurity T_K^∞ and T_K^0 are proportional to each other [22] and also proportional to the ground-state energy ΔE_K.

In the case of two Kondo impurities, this is no longer true. Tsay and Klein[25,26] found from high-temperature expansion that the Kondo temperature varies as $T_K^\infty(1 - W^2/T_K^\infty)^{1/2}$, where W is an effective molecular field on the impurity site[27]; thus the "high-temperature value of T_K" is reduced by the impurity-impurity interaction. Matho and Beal-Monod[28,29] obtained the same qualitative result. However Ishii[30] calculated the ground-state energy of a pair of impurities and did not find the same behavior for the energy.

In the case of the lattice, we have found a ground-state energy proportional to $De^{1/\rho J}$. The high-temperature expansion of Tsay and Klein[26] must be valid in a lattice and would give a decrease of T_K^∞, compared with the single impurity case. We have also calculated the static susceptibility of the impurities at $T = 0$. The result is for $n >> e^{2D/J}$

$$\chi \simeq \frac{g\mu_B + g'\mu_B(J/4D)}{nDe^{2D/J} - J^2/16D} \quad , \tag{21}$$

where g and g' are, respectively, the Landé factor of the f and s electrons. This expression shows that there is no proportionality between ΔE_K and χ^{-1}, contrary to the single impurity case.

Equation (21) shows that χ diverges below a critical value of $|J|/D$; thus if we define T_K^0 by the inverse susceptibility χ^{-1}, T_K^0 vanishes at the critical value. The same behavior is obtained from the high-temperature result: The Kondo temperature vanishes for large value of W/T_K^∞, i.e., for low value of ρJ. This divergence of χ indicates that the ground state is magnetic below a critical value of $|J|/D$. In Sec. III B we discuss the magnetic ground state.

B. Magnetic state

We restrict to ferromagnetic and antiferromagnetic structures, but in principle the RKKY interaction can lead to more complicated structures, as it is found in $CeAl_2$.

1. Ferromagnetic state

In this case we have $x_i = y_i = 0$. As there is no scattering between s and f electrons, the f moment must have its maximum value. Thus we put in Eq. (12),

$$\langle d_{i\uparrow}^{\dagger} d_{i\uparrow}\rangle = 1, \quad \langle d_{i\downarrow}^{\dagger} d_{i\downarrow}\rangle = 0 \ ,$$

$$\langle c_{i\uparrow}^{\dagger} c_{i\uparrow}\rangle = \tfrac{1}{2}(n-\mu), \quad \langle c_{i\downarrow}^{\dagger} c_{i\downarrow}\rangle = \tfrac{1}{2}(n+\mu) \ .$$

$\mu = \langle c_{i\downarrow}^{\dagger} c_{i\downarrow}\rangle - \langle c_{i\uparrow}^{\dagger} c_{i\uparrow}\rangle$ is the magnetic moment of the conduction electrons and the total moment is then equal to $1-\mu$. The self-consistent equations can be solved easily and we obtain

(i) when $n > -J/4D$,

$$\mu = -\frac{J}{4D}, \quad \Delta E_F = -\frac{J^2}{32D} \ , \tag{22}$$

(ii) when $n < -J/4D$,

$$\mu = n, \quad \Delta E_F = n\left(\tfrac{1}{4}J + \tfrac{1}{2}nD\right) \ . \tag{23}$$

μ is the RKKY polarization which is very small for the usual values of J/D; when $J < 0$, this polarization is opposite to the f electron spin.

2. Antiferromagnetic state

In this case the lattice is divided in two sublattices and we have $\langle d_{i\sigma}^{\dagger} d_{i\sigma}\rangle = 0$ or 1 alternatively: $\langle d_{i\sigma}^{\dagger} d_{i\sigma}\rangle = \frac{1}{2}(1+\sigma e^{ipR_i})$ where p is half a reciprocal-lattice vector. For the conduction electrons we have

$$\langle c_{i\sigma}^{\dagger} c_{i\sigma}\rangle = \tfrac{1}{2}(n - \sigma\mu e^{ipR_i}) \ .$$

As in the ferromagnetic case, the self-consistent equations can be solved[31] and we obtain

$$\mu = -\frac{J}{4D}\ln\left(\frac{[\frac{1}{16}J^2 + (1-n)^2D^2]^{1/2} - (1-n)D}{[\frac{1}{16}J^2 + D^2]^{1/2} - D}\right) \ , \tag{24}$$

$$\Delta E_{AF} = \tfrac{1}{8}J\mu + \tfrac{1}{2}(1-n)[\tfrac{1}{16}J^2 + (1-n)^2D^2]^{1/2} - \tfrac{1}{2}(\tfrac{1}{16}J^2 + D^2)^{1/2} + \tfrac{1}{2}Dn(2-n) \ . \tag{25}$$

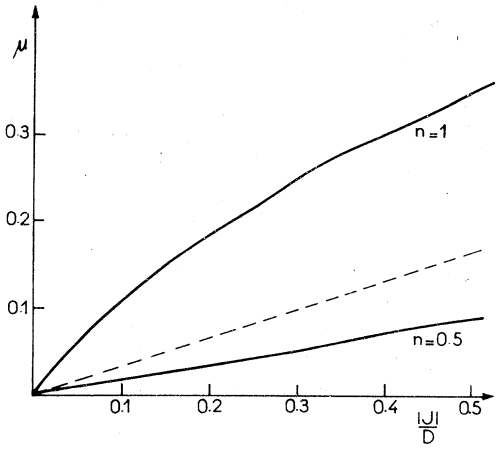

FIG. 3. Magnetic moment of the conduction electrons in the ferromagnetic phase (dashed line) and antiferromagnetic phase (solid lines).

We can remark that the value obtained for the s electrons polarization, given by Eq. (24), can be much larger than in the ferromagnetic case, especially if $n \simeq 1$. Figure 3 shows the variation of μ in the two cases $n = 1$ and $n = 0.5$.

C. Phase diagram

The relative stability of the three phases, Kondo, ferromagnetic, and antiferromagnetic, can be obtained by comparing the energies given by the expressions (20), (22), (23), and (25). The results are shown on Fig. 4. (a) For low values of $|J|/D$ the ground state is magnetic; the Kondo state is obtained only for $|J|/D$ larger than a critical value which depends on the band filling. This is in agreement with the earlier studies of the Kondo lattice of Doniach.[10] (b) Antiferromagnetism is obtained only when the Fermi level is near the middle of the band; when the number of electrons decreases the ferromagnetic structure becomes stable. This is a consequence of the oscillating behavior of the RKKY interactions; when n decreases, k_F decreases also, and the interaction which is proportional to $(\cos 2k_F r)/r^3$ becomes positive between the nearest neighbors.

We have only considered pure Kondo and pure magnetic states; however it would be interesting to study the mixed states, i.e., states where x_i, $y_i \neq 0$

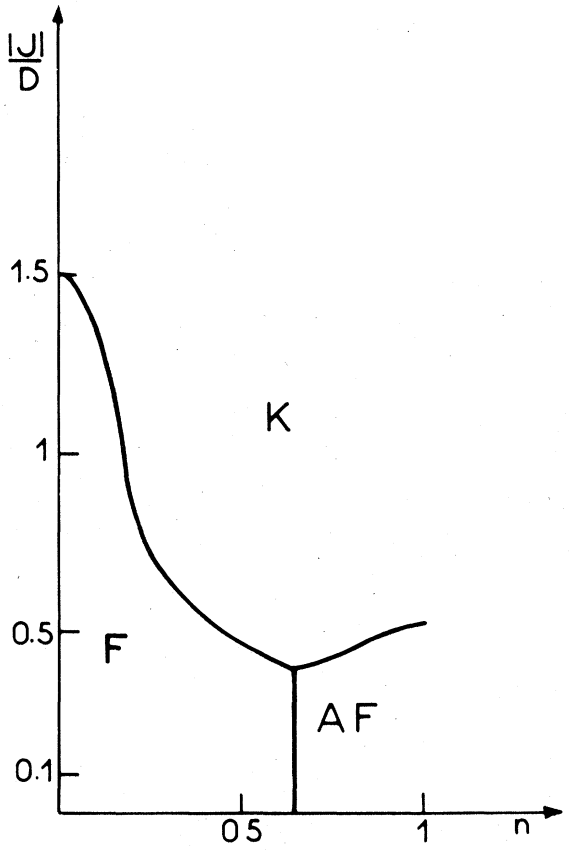

FIG. 4. Phase diagram. The stability region of the Kondo, ferromagnetic, and antiferromagnetic states are indicated by the letters K, F, and AF.

with magnetic moments. As shown by the expression (21), the susceptibility diverges at a critical value of $|J|/D$ which is higher than the value calculated by comparing ΔE_F and ΔE_K. Thus this indicates that the mixed state is the stable state at least between these two critical values.

IV. CONCLUSION

We have obtained the phase diagram of the Kondo-lattice model at zero temperature; the formalism is simple enough to generalize it to the calculation of finite-temperature properties. At zero temperature we obtain magnetic and nonmagnetic states, metallic or insulating depending on the band filling and the parameter $|J|/D$.

However for large values of $|J|/D$ the question arises of the validity of the model. The Schrieffer-Wolff transformation[19] is valid only for small $|J|/D$; J is given by $2V^2/(E_0-E_F)$, but the transformation works only if $|E_0-E_F|$ is larger than the width Δ of the virtual bound state in the Anderson model, $\Delta=\pi\rho(E_F)|V_{kf}|^2$. Thus the condition $|E_0-E_F|<\Delta$ can be written $|J|<1/\pi\rho(E_F)=4D/\pi$, and the phase diagram (Fig. 4) must be restricted to $|J|/D\lesssim 1$; in this case the Kondo state can be obtained only if the number of conduction electrons is greater than a critical value $n_c\simeq 0.2$. For values of $|J|/D$ larger than 1, the model has no physical meaning and we must return to the Anderson model.

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[23]In the case of a single impurity, the Green's function is given by $1/\omega - E_0 - \frac{1}{4}Jn - \frac{1}{4}(J^2x^2)G_0$, where G_0 is the unperturbed Green's function of the conduction electrons:

$$G_0 = \frac{1}{2D} \ln \frac{\omega - D}{\omega + D} .$$

Usually one approximates G_0 by $-i\pi/2D$ for $-D < \omega < +D$; however here we have to keep the exact expression because the impurity level can come near the band edge, when n varies. Thus we have made the calculation with the exact G_0.

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