Analysis realized by means of unitary transformations of the Kondo Hamiltonian of the different phases in the Kondo lattices

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I analyze the possibilities of the Kondo lattice scenario for the different quantum phases appearing in strongly correlated systems. I use in this analysis a formulation of the Kondo Hamiltonian in terms of a renormalized set of canonical operators and the construction of strongly correlated modes involving soft electrons (or holes) and a kind of spin wave. These strongly correlated modes approximately diagonalize the resulting transformed Hamiltonian. The quantum phases arise, in this model, only varying the Kondo J coupling and the density of states at E_F of the noninteracting system (D_F). For small values of D_F and sufficient large values of J, the resulting systems are weak antiferromagnetic insulators. For increasing D_F values and decreasing J couplings, the pattern corresponds to conducting materials which are candidates, in certain conditions, to be heavy-fermion metals. For determined conditions of D_F and J values, there is an interval of the J parameter ($J_c \leqslant J \leqslant J_{\text{top}}$), in which an intriguing ground state appears. The properties of this ground state are close to a gapless and low-temperature zero-resistance system whose energy condensation does not require the existence of electronic pair coupling. [S0163-1829(98)01441-6]

I. INTRODUCTION

The Kondo lattice model (KLM) is generally regarded as a canonical model for strongly correlated systems when one can consider that the high on-site Coulomb repulsion can inhibit the charge fluctuations in the correlated orbitals.[1] An explanation of the phenomenology of these systems[2–5] based on this model, on the Anderson lattice model in the Kondo regime or in any other model,[5] still remains incomplete and controversial.[2–8] There are paradigmatic debates which have implied large experimental and theoretical efforts and remain without consensus.

Some examples of these debated questions are: (i) The nature of the low-energy resonances detected by direct and inverse photoemission;[7,8] in this point, some authors[7] are looking for physical models to find coherence between the features of these resonances and the experimental results, since, in their opinion, the explanation of other authors,[8] based on the impurity models, is inconsistent. (ii) The discussion about whether the existence of a huge specific heat in the heavy fermion state is due to charged particles[9,10] or neutral particles.[11] (iii) The mechanism of the energy condensation in the superconductivity of some heavy-fermion compounds, as UBe_{13}, which remains completely unknown.[2,12] (iv) The existence of the Kondo insulators.[13–15]

On the other hand, some agreements seem to be more or less generalized,[3,4,16] and these are: (i) the existence of the so-called coherence temperature T^*, below which the system behaves as a coherent spin liquid and above which the f-electron atoms act as independent magnetic impurities. (ii) The presence of a certain tendency to antiferromagnetism in which the value of the local magnetic moment is quenched by the fluctuations in the spin liquid. (iii) The existence of large entropy variations, huge specific heat, and magnetic susceptibilities in some Kl materials. (iv) The concomitance of superconductivity and large specific heat in some Ce and U compounds.

In this work, I start from a KLM analysis whose detailed mathematical formalism and calculations are given elsewhere[17] and I use this formalism for analyzing the physical results that are, in author's opinion, essential for the understanding of the phenomenology of the Kondo lattice systems. The main point that I wish to emphasize in this work is the evolution of the electronic pattern offered by the spectrum of the strongly correlated modes for different values of J (Kondo coupling parameter) and D_F (density of states of noninteracting system at E_F). This analysis allows us, on the one hand, to draw three quantum phases (insulator, conductor, and a different phase which may correspond to a kind of superconducting state) depending on the values of JD_F, and on the other hand, to incide in the controversial debates cited above, giving coherent physical interpretations in unified model.

II. THEORETICAL MODEL

We consider a KLM consisting of a conduction band coupled to a lattice of $s=1/2$ local moments by an exchange interaction, namely,

$$H = H_0 + H_K = \sum_{\mathbf{k},\alpha} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + J \sum_i \mathbf{S}_{ei} \cdot \mathbf{S}_{fi}, \qquad (1)$$

where $\mathbf{S}_{ei} = 1/2 \Sigma_{\alpha,\beta} c^{\dagger}_{i\alpha} \boldsymbol{\sigma}_{\alpha\beta} c_{i\beta}$ and $\mathbf{S}_{fi}$ are the spin of the conduction electrons and the ($s=1/2$) local spin at site i, respectively. The essential idea of this formalism is the use of unitary transformations that map the initial operators $c^{\dagger}_{\mathbf{k}\alpha}$, $c_{\mathbf{k}\alpha}$ and $\mathbf{S}_{f\mathbf{k}}$ (Fourier transformations of $c^{\dagger}_{i\alpha}$, $c_{i\alpha}$, and $\mathbf{S}_{fi}$) into a physically meaningful set $\hat{c}_{\mathbf{k}\alpha} = e^{-T} c_{\mathbf{k}\alpha} e^{T}$, $\hat{c}^{\dagger}_{\mathbf{k}\alpha} = e^{-T} c^{\dagger}_{\mathbf{k}\alpha} e^{T}$, $\hat{S}_{f\mathbf{k}} = e^{-T} S_{f\mathbf{k}} e^{T}$. The new operators $\hat{e}_{\mathbf{p}\alpha} = \hat{c}_{\mathbf{p}\alpha}$ and $\hat{h}_{\mathbf{q}\alpha} = \hat{c}^{\dagger}_{-\mathbf{q}-\alpha}$ correspond to electrons and holes that annihilate the *actual* interacting ground state $|\Phi\rangle$, and $\hat{e}^{\dagger}_{\mathbf{p}\alpha}|\Phi\rangle$, $\hat{h}^{\dagger}_{\mathbf{q}\alpha}|\Phi\rangle$ represent the best possible approximations to the ac-

tual charged modes of the system. The generators $\hat{T}$ are taken as the simplest operators involving fermions that preserve all the symmetries of H. The simplest operator involving fermions that satisfies this condition is

$$\hat{T}=\frac{J}{N^{1/2}}\sum_{\mathbf{k}\mathbf{k}'}\hat{T}(\mathbf{k},\mathbf{k}')[(\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}'\uparrow}-\hat{c}^{\dagger}_{\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}'\downarrow})\hat{S}_{0,\mathbf{k}'-\mathbf{k}}+\hat{c}^{\dagger}_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}'\downarrow}\hat{S}_{-1,\mathbf{k}'-\mathbf{k}}+\hat{c}^{\dagger}_{\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}'\uparrow}\hat{S}_{1,\mathbf{k}'-\mathbf{k}}], \tag{2}$$

where the operational part enclosed in parenthesis is equal to that of the Kondo Hamiltonian and $\hat{T}^{\star}(\mathbf{k}',\mathbf{k})=-\hat{T}(\mathbf{k},\mathbf{k}')$ from the unitary condition of $\hat{T}$ [for a larger explanation of the determination and meaning of $\hat{T}(\mathbf{k},\mathbf{k}')$ see Ref. 17]. For small values of J the new operators are expected to be slight deformations of the initial ones, and we can make the approximations:

$$c^{\dagger}_{\mathbf{k}\alpha}=\hat{c}^{\dagger}_{\mathbf{k}\alpha}+[\hat{T},\hat{c}^{\dagger}_{\mathbf{k}\alpha}], \tag{3}$$

$$S_{l,\mathbf{k}}=\hat{S}_{l,\mathbf{k}}+[\hat{T},\hat{S}_{l,\mathbf{k}}] \tag{4}$$

(the index l of $S_{l,\mathbf{k}}$ can take the values 0, 1, -1, corresponding to the operators $S^{z}_{\mathbf{k}}$, $S^{+}_{\mathbf{k}}$, and $S^{-}_{\mathbf{k}}$, respectively).

Substituting expressions (2)–(4) in the initial Kondo Hamiltonian, we obtain the expression of H in terms of the transformed operators

$$H=\hat{C}+\hat{H}_{\text{kinetic}}+\hat{H}_{\text{Kondo}}+\hat{H}_{\text{RKKY}} \tag{5}$$

where $\hat{C}$ is a constant, and

$$\hat{H}_{\text{kinetic}}=\sum_{\mathbf{p},\alpha}\hat{E}(\varepsilon_{\mathbf{p}})\hat{e}^{\dagger}_{\mathbf{p}\alpha}\hat{e}_{\mathbf{p}\alpha}+\sum_{\mathbf{q},\alpha}\hat{E}(-\varepsilon_{\mathbf{q}})\hat{h}^{\dagger}_{\mathbf{q}\alpha}\hat{h}_{\mathbf{q}\alpha}, \tag{6}$$

where $\hat{E}(\varepsilon)$ is the renormalized energy dispersion whose expression is given in Ref. 17; the $\hat{H}_{\text{Kondo}}$-interacting Hamiltonian takes the following form:

$$\hat{H}_{\text{Kondo}}=\sum_{\mathbf{p}\mathbf{p}'}\frac{J(\hat{\varepsilon}_{\mathbf{p}},\hat{\varepsilon}'_{\mathbf{p}})}{N^{1/2}}[(\hat{e}^{\dagger}_{\mathbf{p}\uparrow}\hat{e}_{\mathbf{p}'\uparrow}-\hat{e}^{\dagger}_{\mathbf{p}\downarrow}\hat{e}_{\mathbf{p}'\downarrow})\hat{S}_{0,\mathbf{p}'-\mathbf{p}}+\hat{e}^{\dagger}_{\mathbf{p}\uparrow}\hat{e}_{\mathbf{p}'\downarrow}\hat{S}_{-1,\mathbf{p}'-\mathbf{p}}+\hat{e}^{\dagger}_{\mathbf{p}\downarrow}\hat{e}_{\mathbf{p}'\uparrow}\hat{S}_{1,\mathbf{p}'-\mathbf{p}}]$$
$$+\sum_{\mathbf{p}\mathbf{p}'}\frac{J(\hat{\varepsilon}_{\mathbf{p}},\hat{\varepsilon}'_{\mathbf{p}})}{N^{1/2}}[(\hat{h}^{\dagger}_{\mathbf{q}\uparrow}\hat{h}_{\mathbf{q}'\uparrow}-\hat{h}^{\dagger}_{\mathbf{q}\downarrow}\hat{h}_{\mathbf{q}'\downarrow})\hat{S}_{0,\mathbf{q}'-\mathbf{q}}-\hat{h}^{\dagger}_{\mathbf{q}\uparrow}\hat{h}_{\mathbf{q}'\downarrow}\hat{S}_{-1,\mathbf{q}'-\mathbf{q}}-\hat{h}^{\dagger}_{\mathbf{q}\downarrow}\hat{h}_{\mathbf{q}'\uparrow}\hat{S}_{1,\mathbf{q}'-\mathbf{q}}], \tag{7}$$

where, $\hat{\varepsilon}_{\mathbf{p}}=\hat{E}(\varepsilon_{\mathbf{p}})$, and the renormalized Kondo coupling is

$$J(\varepsilon_1,\varepsilon_2)=J\hat{\eta}^2/[(\varepsilon_1-\varepsilon_2)^2+\hat{\eta}^2], \tag{8}$$

and

$$\hat{H}_{\text{RKKY}}=\hat{H}^{(1)}_{\text{RKKY}}+\hat{H}^{(2)}_{\text{RKKY}}=\frac{1}{2}\sum_{i\neq j}J^{(1)}_{\text{RKKY}}(\mathbf{R}_i-\mathbf{R}_j)\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j+\frac{1}{2}\sum_{i\neq j}J^{(2)}_{\text{RKKY}}(\mathbf{R}_i-\mathbf{R}_j)\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j, \tag{9}$$

where the term $\hat{H}^{(1)}_{\text{RKKY}}$ ($\hat{H}^{(2)}_{\text{RKKY}}$) comes from the transformation of $H_0(H_K)$, and

$$J^{(1)}_{\text{RKKY}}(\mathbf{R})=\frac{J^2}{\Gamma}\int\frac{\varepsilon_{\mathbf{p}}\cos[(\mathbf{q}-\mathbf{p})\mathbf{R}]}{(\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{q}}+\hat{\eta})^2}d\mathbf{p}\,d\mathbf{q},$$

$$J^{(2)}_{\text{RKKY}}(\mathbf{R})=-\frac{J^2}{\Gamma}\int\frac{2\cos[(\mathbf{q}-\mathbf{p})\mathbf{R}]}{\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{q}}+\hat{\eta}}d\mathbf{p}\,d\mathbf{q}, \tag{10}$$

where Γ is the volume of the Brillouin zone. Thus, the physical picture of the system implied by this formalism is a vacuum state consisting of a background of Ruderman-Kittel-Kasuya-Yosida- (RKKY) induced spin correlations, where two kinds of elementary modes can be excited: soft neutral modes associated with the deformations of the spin liquid, and charged modes corresponding to the excitation of electrons and holes on the system. Note that while the resulting Kondo term is proportional to J, the corresponding RKKY Hamiltonian is proportional to J^2. For instance, in the one-dimensional case, we have $J_{\text{RKKY}}(R=na)=J^{(1)}_{\text{RKKY}}(R=na)+J^{(2)}_{\text{RKKY}}(R=na)=0.26J^2$, $-0.20J^2$, $0.14J^2$, $-0.09J^2$, $0.07J^2$, . . . (in bandwidth units) for $n=\pm1,\pm2,\pm3,\pm4,\pm5,\ldots$, respectively, which corresponds to a weak antiferromagnetic ordering. Therefore, taking into account Eqs. (8)–(10) the RKKY Hamiltonian can be considered a negligible contribution in the calculation of the charged spectrum within our KLM analysis.

From the optimal operators $\hat{c}_{\mathbf{k}\alpha}$, $\hat{S}_{l,\mathbf{k}}$ one can now construct the strongly correlated (SC) modes. The general structure of an electron strongly correlated with a spin wave, having $s=s^z=1/2$ and wave vector $\mathbf{k}$, is given by[17]

$$|\text{SCE}_{\mathbf{k},1/2}\rangle=N^{-1/2}\sum_{\mathbf{p}}B(\mathbf{p})(\hat{e}^{\dagger}_{\mathbf{p}\uparrow}\hat{S}_{0,\mathbf{k}-\mathbf{p}}+\hat{e}^{\dagger}_{\mathbf{p}\downarrow}\hat{S}_{1,\mathbf{k}-\mathbf{p}})|\Phi\rangle. \tag{11}$$

The physical image for these SCE states is a many-body electron (hole) excitation produced by the $\hat{c}^{\dagger}_{\mathbf{p}\sigma}$ operator that is coupled with a cloud of $S=1$ spin waves produced by applying the $\hat{S}$ operators to $|\Phi\rangle$. The variational function $B(\mathbf{p})$ is an essential feature of the SCE states because it determines which electrons (their energy locations) are coupled with the spin fluctuations of the spin field. The SCE

energy is a functional of $B(\mathbf{p})$ which should be minimized. The condition for the minimization of $E_{\mathrm{SC},1/2}[B]$ has a solution *only* for antiferromagnetic couplings ($J>0$). This solution, with the approximation $\hat{E}(\varepsilon)\sim\pm(\hat{E}(0)+\varepsilon)$ [the sign $+(-)$ corresponds to states above (below) the Fermi level] leads to $B(\mathbf{p})=Z/[\varepsilon_{\mathbf{p}}+\Omega_{1/2}]$, $E_{\mathrm{SC},1/2}=\pm(\hat{E}(0)-\Omega_{1/2})$, Z being an arbitrary constant used to normalize the SCE states, and $\Omega_{1/2}=e^{-2/JD_F}/2$ [here, D_F is the density of states (DOS) at E_F in the noninteracting system of Eq. (1)]. For ferromagnetic couplings collective states are formed and they should have the structure $|\mathrm{SCE}_{\mathbf{k},3/2}\rangle=N^{-1/2}\Sigma_{\mathbf{p}}D(\mathbf{p})\hat{e}^{\dagger}_{\mathbf{p}\uparrow}\hat{S}_{1,\mathbf{k}-\mathbf{p}}|\Phi\rangle$, which is the general form of a state composed of an electron and a spin wave having wave vector $\mathbf{k}$ and $s=s^z=3/2$. In this case, the condition for minimizing $E_{\mathrm{SC},3/2}[D]$ has a solution only for $J<0$ and it leads to $D(\mathbf{p})=Z/[\varepsilon_{\mathbf{p}}+\Omega_{3/2}]$, $E_{\mathrm{SC},3/2}=\pm(\hat{E}(0)-\Omega_{3/2})$ where $\Omega_{3/2}=e^{4/JD_F}/2$. I should note that if one considers the KLM as a special case of the Hubbard or Anderson lattice Hamiltonians, the ferromagnetic Kondo coupling corresponds to negative U energies, since the step from one paradigm to the other is basically realized with the change $J\propto t^2/U$. For couplings of the same strength, the formation of these states is much more favored in the antiferromagnetic case ($\Omega_{1/2}\gg\Omega_{3/2}$). If Ω stands for either $\Omega_{1/2}$ or $\Omega_{3/2}$, from the expressions of $B(\mathbf{p})$ and $D(\mathbf{p})$ it can be readily seen that the probability of finding in a SCE mode an electron with wave vector $\mathbf{p}$ such that $\varepsilon\leqslant\varepsilon_{\mathbf{p}}\leqslant\varepsilon+d\varepsilon$ is $P(\varepsilon)d\varepsilon$. For obtaining $P(\varepsilon)$, we normalize the B function, and thus $P(\varepsilon)=B^2(\varepsilon)=\Omega/(\varepsilon+\Omega)^2$. This means, for instance, that half of the electrons which constitute these modes have their energies in the layer $0\leqslant\varepsilon_{\mathbf{p}}\leqslant\Omega$, which implies that only a narrow part of the conduction band participates in the formation of the SCE states, since the conduction bandwidth W is much larger than Ω.

Another possible point to analyze is the effect that the RKKY Hamiltonian produces in the SCE states. The RKKY correction in these states ($\langle\mathrm{SCE}|\hat{H}_{\mathrm{RKKY}}|\mathrm{SCE}\rangle$) depends on the product of two effective coupling parameters, $B(\mathbf{p})$ which are the couplings between charged particles and spin-fluctuation waves and the J_{RKKY}'s of Eq. (10). A simple inspection of this correction allows us to neglect it in front of $\langle\mathrm{SCE}|\hat{H}_{\mathrm{kinetic}}+\hat{H}_{\mathrm{Kondo}}|\mathrm{SCE}\rangle$ which give the spectrum of these states. This question is different in the ground state, since, in $\langle\Phi|\hat{H}_{\mathrm{RKKY}}|\Phi\rangle$ the coupling parameters $B(\mathbf{p})$ do not appear. In this case, this correction, $\propto J^2$, takes only significant values in the localized spin field and yields no important effect in the charged modes' wave function.

III. COMMENTS ABOUT THE THEORETICAL MODEL

The unitary transformation of Eq. (2) is completely defined when the functions $\hat{T}(\mathbf{k},\mathbf{k}')$ are determined. The general form of these functions is[17] $\hat{T}(\mathbf{k},\mathbf{k}')=1/(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}+\eta)$, where the low-energy regulator (η) avoids divergences in the transformation $\hat{T}$ and to ensure its unitarity. As said in Ref. 17, the spectrum of the eigenstates ($\hat{c}^{\dagger}_{\mathbf{k}\alpha}|\Phi\rangle$) of the transformed noninteracting Hamiltonian (6) presents a gap between electron and hole states: $2\hat{E}(0)\approx\eta+3J^2/16-2\hat{\eta}/\pi$, where $\hat{\eta}$ is obtained from the Eq. (17) $\hat{\eta}=(3\pi J^2/64)\ln(1/2\hat{\eta})$. The second term of $\hat{E}(0)$, which is the largest in this expression, arises from the transformation of the extended band term of Hamiltonian (1) by means of Eq. (3). In addition, in a concomitant way, this transformation directly yields the RKKY interaction, i.e.,

$$e^{\hat{T}}(\hat{H}_{\mathrm{kinetic}}+\hat{H}^{(1)}_{\mathrm{RKKY}})e^{-\hat{T}}+e^{\hat{T}}(\hat{H}_{\mathrm{Kondo}}+\hat{H}^{(2)}_{\mathrm{RKKY}})e^{-\hat{T}}\approx H_0+H_K.$$

Therefore, in a certain sense, we can admit that the existence of a gap in the kinetic Hamiltonian (6) has a RKKY character, since this gap is opened in the charged particle spectrum of the ground state when (and because) $\hat{H}^{(1)}_{\mathrm{RKKY}}$ arises in the localized spin field due to the unitary transformation. In addition, as commented in Sec. II, the correction $\langle\Phi|\hat{H}_{\mathrm{RKKY}}|\phi\rangle$ and the gap in the charged modes of the vacuum state are $\propto J^2$. One could say that $\hat{E}(0)$ corresponds to the energy condensation of the new ground state of the charged modes that is utilized in antiferromagnetic correlations within the noncharged spin field.

Obviously, if we consider a different order of truncation of the unitary transformation, this gap $\hat{E}(0)$ will quantitatively be different and correlatively the interaction terms of the spin-spin exchange within the spin field will also be different (then terms of the type $J^3\hat{S}_i\hat{S}_j\hat{S}_l$, $J^4\hat{S}_i\hat{S}_j\hat{S}_l\hat{S}_m$, etc. will appear). If J values are small enough, these new spin-spin interactions and new terms of the spectrum gap in Eq. (6) (which always appears), are negligible in front of those arising from the first order since their corresponding exponents of J^n are larger.

The transformation process of the Hamiltonian made here and in previous works (Ref. 17) infers the existence of a transformed vacuum state [the state $|\Phi\rangle$ of Eq. (11)]. This vacuum state is such that: $\hat{e}_{\mathbf{p}\alpha}|\Phi\rangle=0$, $\hat{h}_{\mathbf{q}\alpha}|\Phi\rangle=0$, and $\hat{e}^{\dagger}_{\mathbf{p}\alpha}|\Phi\rangle$ and $\hat{h}^{\dagger}_{\mathbf{q}\alpha}|\Phi\rangle$ are eigenstates of the kinetic Hamiltonian (6). These eigenstates present the cited gap $[2\hat{E}(0)]$ in their charged spectrum. An easy inspection of the Hamiltonian (5) allows us to know that the vacuum state $|\Phi\rangle$ is the ground state of Eq. (5). We have proved in Ref. 17 that the SCE modes (11) are the excited states of this transformed Hamiltonian. Therefore, the spectrum of SCE states depends on the $\hat{H}_{\mathrm{kinetic}}$ and $\hat{H}_{\mathrm{Kondo}}$. As a consequence this spectrum contains the analytic term proportional to J^2 coming from the kinetic term and another exponential term arising from the transformed Kondo Hamiltonian. In this scenario the energy location of the SCE states governs the conducting and magnetic properties of the Kondo lattice materials. Therefore, these properties depend directly on two competing effects: those arising from the RKKY character ($\propto J^2$) and those that are consequence of the transformed Kondo interaction (exponential term). This point, which is variationally determined in this paper, has been suggested previously in the literature.[3,4,11,15,18–22] In Secs. IV, V, and VI, I discuss the conducting and magnetic properties of the KL systems as a function of the location of the SCE states, and discuss how the effects of the two components (J^2 and the exponential one) can yield different phases.

Let me compare our model with other previous Kondo analysis. Fazekas and Muller-Hartmann determine, also variationally, the Kondo lattice ground state considering several trial wave functions. Their results for the energy per particle ($\varepsilon_{\mathbf{p}}$) of ground state in all analyzed cases contain several terms. For the case in that the magnetic ordering coexists with Kondo regime, $\varepsilon_{\mathbf{p}}$ contains a term $\propto J^2$ and other logarithmic one. For the case of coherent superposition of Kondo singlets, $\varepsilon_{\mathbf{p}}$ is the summation of an exponential term and another constant. Therefore, there is a certain structural similarity with the results of the spectrum of SCE states. However, the main difference in both analysis is that the ansatz utilized by the above cited authors is constituted by fermion operators corresponding to extended and localized electrons, while the SCE states of Eq. (11) is a coupling of $S=1$ magnetic bosons with fermionic charged states. This may be the reason for obtaining the quantitative differences between the spectrum of SCE states and $\varepsilon_{\mathbf{p}}$ deduced by Fazekas and Muller-Hartmann.

One of the main results of the Gutzwiller procedures (see, for instance, the second paper of Ref. 9) is the achieving of two hybridized bands formed by *f* levels and extended conduction states which are split by a hybridization gap of exponential form identified with the Kondo effect gap. In the insulating phase, the DOS arising from these bands has two peaks at both sides of E_F. In this phase the results for low-energy scales ($\sim T_K$) can be easily interpreted because the Kondo gap split states whose predominant component in the hybridization can correspond to the localized one. However, in the metallic phase, the physical interpretation is somewhat more difficult. This is so because in this case E_F can cut the lower (or upper) hybridization band in an energy zone where the band states share localized and extended components. This is indicative that the hybridization propitiates the formation of a quasiband *f,* and therefore, the possibility of migrations of *f* (quasilocalized) electrons between different *f* lattice sites. However, the Gutzwiller models[9] for obtaining the hybridized bands, normally, do not consider, in the used Hamiltonian, terms of the type $f_i^{\dagger} f_j$ (i.e., the obtained results imply a *f* hopping in the lattice which is overlooked in the Hamiltonian that is used for obtaining these results). In our model, we do not consider two ''flavors'' of charged particles (*d* extended and *f* localized), since in KL models, the *f* level is deep enough, and therefore, the overlooking in Eq. (1) of the *f* charge freedom degrees is justified. As a consequence, for metallic phases where the *f*-charged quasiparticles lie close to E_F, as it is in the case of $CeSi_2$, the results of our model are indicative and modest. For this latter case, as I say in Sec. V, other supplementary ingredients should be added in order to explain all close E_F features of its electronic structure.

In my opinion, the structure of the ansatz (11) can present disadvantages, due to the complexity, with respect to that of the Guztwiller-like trial wave functions but it also has some advantage. First, Eq. (11) along with the unitary transformation defined by Eqs. (2)–(4) are able to directly yield the RKKY Hamiltonian (9), while in other works[3,4,18,9] it is suggested or introduced by hand. In second place, there is a coherence between the pattern obtained from the SCE states with some experimental facts of the heavy-fermion phenomenology of the Kondo lattices. This phenomenology, as previously suggested,[3,4] is associated to the existence of spin fluctuations waves that, on one hand, can be coupled with charged particles and, on the other hand, quench the weak antiferromagnetism yielded by the RKKY interactions. On the other hand, I wish to remember that similar types of ansatz (11) have been used in analysis of the one-dimensional Kondo lattice.[1,6] An interesting result in some of these analyses[1] is a rigorous proof of that the ground state of a system composed of one extended electron plus the localized one-dimensional spin field is a ferromagnetic state for an antiferromagnetic Kondo coupling. In low conduction electron density (i.e., away from half filling) and for large Kondo coupling parameters the ferromagnetic state is maintained. This is not surprising if one considers all terms which compete in this reduced version of the Kondo lattice. In our model, Eq. (10) is the general induced RKKY term coming from the transformation [Eqs. (3) and (4)] of the initial Hamiltonian (1). This initial Hamiltonian corresponds to a system composed of *N*-extended band electrons interacting with a spin field of arbitrary dimension. Within our model, the results of Eq. (10) are strongly dependent on the extended band structure $\varepsilon_{\mathbf{k}\alpha}$ and also on the crystal geometry included its dimension. Therefore it is not rare that from Eq. (10), we obtain an antiferromagnetic RKKY interaction (as explained in Sec. II) within the spin field when this interacts via a Kondo lattice with *N*-extended electrons in the one-dimensional paramagnetic band. This RKKY interaction (10) competes with the spin fluctuations which are coupled with the charged particles in the SCE modes and whose properties are in coherence with the idea of the spin liquid. In any case, this latter result cannot be considered contradictory with those results of Ref. 1: they are different because the systems in both cases are different. In fact, the authors of Ref. 1 recognize that in similar regimes to those studied in this paper (i.e., half filling or more occupation ratio) for the one-dimensional Kondo lattice, a spin liquid with a tendency to quenched magnetic ordering and even a paramagnetic state are the most probably states.

In short, our model does not present severe contradictions with previous theoretical results and I think that we can explain several features of the conducting phases of the Kondo lattices versus their band parameters, confronting the J^2 effects versus the exponential ones.

IV. INSULATING PHASE

The pattern obtained from the Hamiltonian $\hat{H}_{\text{kinetic}}$ for the renormalized noninteracting system is a Kondo lattice insulator with a gap whose value is

$$\Delta_c = 2\hat{E}(0) = 0.096J^2. \tag{12}$$

Taking into account that this gap is given in bandwidth units and that our model is valid up to $J=J_{\text{top}}\approx 0.3$ (for values of $J \geqslant 0.3$ the expression $c=e^{\hat{T}}\hat{c}e^{-\hat{T}}=\hat{c}+[\hat{T},\hat{c}]$ is dubious), I estimate that the maximum value for this gap will be around 100 meV.

The existence of this gap has been justified and explained in Sec. III. Mathematically, the dependence of Δ_c on J^2 is a consequence of the approximation considered in the transformation of fermion $c_{\mathbf{k}\alpha}$ operators, since this approximation

[Eqs. (2)–(4)] implies that the transformation is linear with J and the kinetic Hamiltonian is quadratic with J. As explained in Ref. 17, the value of Δ_c is obtained in $\hat{E}(\varepsilon_{\mathbf{k}\alpha})$ when including in this spectrum the Kondo interaction effects corresponding to states of very different energies, since the renormalized Kondo interaction ($\hat{H}_{\text{Kondo}}$) is only effective, as explained above and in Ref. 17, between states of similar energies [see Eq. (8)].

Using the ansatz (11) the diagonalization of the total Hamiltonian (5) is possible. whose eigenstates are the SCE states. Obviously, in the calculation of these eigenstates, the whole of the renormalized Kondo interaction (without the RKKY term) is considered. The center of the energy bands of the SCE states (X) is

$$X = 0.048J^2 - \frac{1}{2}\exp\left(-\frac{2s+1}{|J|D_F}\right), \tag{13}$$

where the exponential form is a direct consequence of the Kondo lattice effects ($\hat{H}_{\text{Kondo}}$) whose transformed parameter is given in Eq. (8). This exponential form of the variation gap also appears in the one-dimensional Kondo lattice (see, for instance, Ref. 1).

Obviously, for $s=3/2$ and $s=1/2$, we obtain the location of the centers of the $\text{SCE}_{3/2}$ and $\text{SCE}_{1/2}$ bands, respectively. It must be remembered that for a determined material the SCE bands will be $s=3/2$ or $s=1/2$ according to the J sign is ferro or antiferromagnetic. For moderate density of states (D_F) in the initial Hamiltonian [Eq. (1)], and for values of J large enough, the Kondo coupling can produce a true gap in the whole Fermi surface. In these cases, $X>0$, the SCE will not be occupied at low temperatures (Kondo temperature range) and the charged spectrum will remain essentially the same as in the renormalized noninteracting case ($\hat{H}_{\text{kinetic}}$) of Eqs. (5) and (6), (although the gap is slightly reduced with respect to that of the noninteracting system by the existence of the SCE band states). *Therefore, the pattern drawn in this regime corresponds to clear insulator Kondo systems as those experimentally studied from some years ago.*[13–15] In these materials two different gaps[13] can be considered: a conducting-particle gap (Δ_c) and a spin gap (Δ_s). The former is given by the splitting between states above and below E_F, which are eigenstates of the Hamiltonian $\hat{C}+\hat{H}_{\text{kinetic}}$, and that in our model is given by Eq. (12). It seems plausible that in our analysis, Δ_s is identified by the splitting between the SCE states below and above E_F^0. This identification is reasonable because of the participation of the spin waves originated by the Kondo coupling in the formation of these SCE states. Therefore, we have

$$\Delta_s = \Delta_c - \exp\left(-\frac{2s+1}{|J|D_F}\right). \tag{14}$$

Considering experimental results of Severing *et al.* (see Refs. 13 and 14), $\Delta_s \simeq 180\ \text{cm}^{-1}$ and $\Delta_c \simeq 300\ \text{cm}^{-1}$. Including these data in Eqs. (12) and (14), we obtain that the resulting system should have $J=0.138$, $D_F=2$ and a bandwidth of the noninteracting system $W=0.95$ eV. These theoretical results are within the interval of validity of our model and are perfectly plausible and assimilated to realistic electronic structures.

The location of the SCE states with respect to E_F depends exponentially on J and D_F [the density of states in the noninteracting system (nonhatted kinetic Hamiltonian)]. Therefore the evolution of this location with the temperature depends fundamentally on the variation versus the energy of the DOS. This DOS arises from delocalized band states, and therefore is quasiconstant versus the energy, with the exception of singular points, van Hove singularities, etc. As a consequence, the insulating gap can be quasi-independent of the temperature, this point being in agreement with experimental analysis of Bucher *et al.*[13] This possible constant value of the insulating gap with temperature has been used for qualitatively explaining the behavior of the optical conductivity with T in $Ce_3Bi_4Pt_3$ (see Fig. 2 of Ref. 13). According to our results, the optical conductivity versus frequency, should increase up to frequencies larger than that corresponding to gap (ideally, it could be zero up to its corresponding frequency), and for larger values, the conductivity can have modest variations or be constant. This evolution versus ω is, of course, for low temperatures. For temperatures equivalent to the energy of the gap, the SCE states can be thermally occupied even for $\omega=0$ and thus the behavior is similar to any metal (i.e., constant or slight variations versus ω, above all for low frequencies).

On the other hand, the RKKY term in our model is proportional to αJ^2, α being a parameter which depends on the dimension and symmetry of the crystal and in all cases, we estimate that it is less than 1. This RKKY term provides a weak antiferromagnetism whose local moments can be quenched because the hatted charged states already have a light coupling to spin fluctuations (see Ref. 17). Therefore, according to our results for this J regime, the evolution of μ_{eff} (average local magnetic moment in the spin field) is coherent with Fig. 3 of Ref. 13, since it should increase during the temperature interval which is dominated by the weak antiferromagnetism due to the spin correlations. From a theoretical point of view and within our model, this behavior can be justified because for these temperatures the cloud of spin fluctuations modifies the tendency toward a spin antiferromagnetic ordering[1,23] and thus the macroscopic magnetization tends to be different to zero and increases. For increasing temperatures, the spin correlations are broken and gradually the SCE states are thermally occupied, and increasing with each additional T, the coherence T^* is reached and as a consequence, the structure of the spin field is lost and the incoherent impurity Kondo effect is open. Then the paramagnetic phase dominates and μ_{eff} tends to have a constant value coincident with that arising from the Hund's rule corresponding to an independent f electron atom.

In short, in the Kondo insulators there are three characteristic temperatures whose values will depend on the J value. For each of these T's, the system can display three different behaviors which are gradually attained. For the lowest temperature ($KT_N \simeq J^2$) the weak magnetic ordering is broken; increasing the temperature the SCE states are occupied and the spin liquid is constituted. In this T interval the charged particles are associated with fluctuations in the spin field via the coupling of conduction electrons with the spin waves.

This temperature can be defined by $KT_M \simeq X$ (X has been defined above). The largest temperature is obviously the coherence temperature T^*, above which there are neither SCE states nor Kondo lattices (i.e., there are not SCE states because there is not a Kondo lattice, but incoherent Kondo impurities). Experimental results[13,24] are clearly in agreement, at least qualitatively, with the above behaviors deduced via the structure of the SCE states.

V. CONDUCTING PHASE

For increasing values of D_F and decreasing J, the gap of $\hat{H}_{\text{kinetic}}$, and the resulting total gap decreases. If one considers an effective bandwidth for the flat band of holes and particles of the SCE states, this gap can disappear and could be converted into a pseudogap. Then the metallic phase can arise. In our calculation the SCE bandwidths are null, but this is a nonphysical result due to the variational procedure for obtaining it. However, if the procedure were perturbative some imaginary part in the self-energy would produce a natural width whose effective DOS arising from the corresponding spectral function would be narrow Lorentzian curves. Therefore the assignation of a certain width to the SCE bands is, in my opinion, a physical added result which is clearly justified. In the case of moderated J values and larger D_F than those of the insulating phase, the Kondo interaction cannot open a sufficiently large gap. Thus, for $X > 0$, but Ω of the order of $\hat{E}(0)$, the low-energy electrons are energetically allowed to participate at low temperatures in the formation of the SCE. In this case, as said above, if one considers that the narrow SCE bands are located in the gap of $\hat{H}_{\text{kinetic}}$, the picture of the system tends to resemble that of a conductor. Then, the system will present at low temperatures a very strong renormalization of the electron (and hole) masses around the Fermi level, since the SCE band is very flat. The mass renormalization due to the thermal occupation of such SCE bands should be added to that arising from the dispersion rule $\hat{E}(\varepsilon_{\mathbf{p}})$. The addition of these two renormalization effects would actually explain the important enhancement at the Fermi surface of the masses of the *charged* excitations measured by photoemission and de Haas–van Alphen experiments.[11] However, as I have already mentioned in Sec. II, this electronic mass renormalization occurs in a very narrow part of the charged particle band and therefore it can be neither the main source of the enormous specific heat nor of the huge low-temperature entropy measured in these systems.[4,11] The strong entropy increasing can be reached with the breakdown of the spin correlations and weak antiferromagnetism ordering due to the long-range RKKY interaction term that in our model appears to renormalize the Kondo Hamiltonian. The two combined effects (the occupation of the SCE states and the subsequent mass renormalization, and the action of the RKKY Hamiltonian) can be the cause for the large entropy increase ($\approx N \ln 2$) and the huge specific heat which appear in the heavy-fermion (HF) state.[4,11,17,25] This interpretation which has been suggested in the literature,[3,4,11] is directly obtained in our model from the calculation of the effective Hamiltonian. On the other hand, the SCE modes consist of charged particles located in extended states that are coupled to spin waves, and therefore they can be detected by photoemission spectroscopy (PES) at low temperatures. The flat character of the SCE band would yield a very large peak in the DOS detected by PES. However the relatively small number of charged particles involved in the formation of these SCE modes also implies a softening of the spectroscopical response derived from these strongly correlated states.

In Sec. II, I remarked that this work considers a Kondo lattice Hamiltonian, whose noninteracting system does not contain terms of localized charged particles (f states), but takes into account the spin variables of these states in the interacting term. Therefore, the present KLM analysis, whose main result is the SCE spectrum, cannot explain the near E_F photoemission features of some heavy-fermion metals[7,8] above all when *some of these features* arise from the charged particles localized in the f states. However, although I recognize that the model used in this paper is unable to draw the complete pattern of the electronic structure of KL in the metallic phase, the present analysis foresees a conducting phase for X values close to zero since then the SCE states are located in the middle of the Δ_c gap. The complete electronic structure of the materials in this phase can be determined by means of other models that consider the f-charged spectrum. In previous papers,[25] we have determined several electronic structures of realistic Ce systems and obtained middle-energy resonances near E_F which are occupied by charged quasiparticles with f character lying at energies very close to those of the SCE states. In these calculations,[25] we use different self-energy approximations which are added to the local-density approximation Hamiltonian. Such self-energies do not take into account the interactions included in the KLM analysis of the present work, hence, the middle-energy resonances corresponding to the f charges should be added to the spectrum of the SCE states in order to have a complete pattern of the direct and inverse PES spectrum.

The Kondo nature of *other features* corresponding to the low-energy photoemission spectra located just above E_F in Ce systems is experimentally clear.[8] For instance, in $CeSi_2$, these peaks are softened[8] when decreasing the composition of Si up to $CeSi_{1.6}$, suggesting the extended nature of the charged particles that participate in the Kondo peaks.

Concerning the low-energy resonances of the Ce systems in general and of the $CeSi_2$ in particular, there is a strong controversy fundamentally between two experimental groups.[7,8] The polemic is centered in the validity (or not) of several solutions of the impurity Anderson Hamiltonian. In Ref. 8, authors claim for an interpretation of the low energy spectrum in terms of the impurity version of the Kondo Hamiltonian attributing the possible quantitative failures to lack of resolution, relaxation due to final effects in the photoemission process, and other incontrolled crystal interactions. The result is that the experimental bandwidths are much larger than those predicted for the impurity models, and on the other hand the latter theoretical results are two orders of magnitude larger than the widths deduced from specific-heat measurements. In Ref. 7, other authors give support to a not yet clear solution in which the coherence effects should have a preeminent role. They refute the impurity interpretation given in Ref. 8 in the sense that the foreseen correlation of the Anderson impurity model between the intensity and location of the Kondo peaks with the Kondo

temperature is not confirmed by the experimental results, since, different materials with a similar low-energy pattern have very different Kondo temperatures.[7] Our model gives a coherent lattice solution which can conciliate the PES results with those of specific heat once one conveniently includes the *f*-charged spectrum within the global scheme. In this sense, the model described in this paper reasonably solves some of the contradictions between spectroscopical and thermal measurements pointed out in Ref. 7. However, the Kondo (lattice) nature of some of the low-energy peaks is for us undubious, and in this point we coincide more with the interpretation given in Ref. 8 than with that given in Ref. 7.

In this conducting phase, two characteristic temperatures have a preeminent role: on the one hand, the temperature (defined by $KT_K \simeq X - E_F$) for which the SCE states can be occupied and can therefore be detected via photoemission, and on the other hand, the HF state temperature (T_H), above which the HF state disappears. In the cases where both temperatures are very different and are not correlated, the HF state cannot be explained only by the occupation of the very flat SCE band. Then, the appearance of the HF state (characterized by the giant enhancement of the electronic specific heat and the magnetic susceptibility) can be also justified for this regime ($X>0$) by the breakdown, above a certain temperature T_H, of the magnetic correlations and weak antiferromagnetic ordering produced by the induced RKKY Hamiltonian. The collective character of the SCE wave functions leads to a variation of their occupation probability versus temperature that obviously differs from the temperature evolution of the Kondo peak arising from the impurity Anderson model (IAM). This issue is the second part of the strong controversy in the interpretation of the PES data.[7,8] The second conflictive point of the debate is whether the location and intensity of the Kondo peak behaves with the temperature as the IAM foresees[8] or not.[7] Some experimental results[7] (in certain coherence with our analysis) give support to the inexistence of such a correlation in some HF materials, invalidating the universality of the IAM explanation for the Kondo spectroscopy detected by PES.

VI. NEW PHASE

The most interesting and intriguing conclusion drawn from our analysis occurs when the energy of the SCE modes is such that $E_{SC,S} = 0.048J^2 - \frac{1}{2}\exp[-(2S+1)/|J|D_F] < -0.048J^2$. In this case, a new ground state (GS) appears, since the charged particles of the top of the conduction band spontaneously fall into the SCE modes due to the Kondo-lattice interaction. Therefore an instability that leads to a new quantum phase in the sense of Sondhi *et al.*'s[26] is produced. Strictly, the main parameters which govern this transition are the J coupling of the Kondo Hamiltonian and D_F. The new phase corresponds to a conducting material that can become a nonelectric resistance phase for certain conditions. The new phase occurs in the Kondo antiferromagnetic coupling when

$$2\ln J \leqslant 1.65 - \frac{2}{JD_F}. \tag{15}$$

For $D_F = 1$ the transition is impossible. This is so because for such a small value of D_F, the Kondo coupling always opens the insulating gap for any value of J. Considering $D_F = 2$, the phase transition occurs in the J interval $J_c = 0.21 \leqslant J \leqslant 0.30$ (always in bandwidth units), and for increasing values of D_F J_c decreases (for instance for $D_F = 3$, the corresponding $J_c = 0.11$). In the ferromagnetic case, the phase transition occurs when

$$2\ln|J| \leqslant 1.65 - \frac{4}{|J|D_F}. \tag{16}$$

For $D_F = 2$ the transition is impossible (the same argument that in the antiferromagnetic case can be used), and for $D_F = 3$ the transition occurs for $J_c \leqslant -0.36$. Obviously, for these values of J, the approximation of considering the relation $c^\dagger_{\mathbf{k}\alpha} = \tilde{c}^\dagger_{\mathbf{k}\alpha} + [\tilde{T}, \tilde{c}^\dagger_{\mathbf{k}\alpha}]$ is dubious, and therefore, one can conclude that the phase transition exists with higher probability in the antiferromagnetic Kondo coupling, above all for low values of the density of states at the Fermi level.

The approximations considered in this model, whose details are extensively given in Ref. 17, are fundamentally the consideration of the first order in the unitary transformations [Eqs. (2)–(4)] and those approximations performed for obtaining the determination of the SCE spectrum considering the trial wave functions [Eq. (10)]. I wish to emphasize that the new phase whose appearance conditions are Eqs. (15) and (16) is reached for values of J and D_F within the intervals in which the above cited approximations are valid. In addition, these values are compatible with electronic structures of realistic materials.

Physically, the existence of this new state is linked to two competitive causes: the change of the vacuum state ($|\Phi\rangle = e^{-\hat{T}}|\Phi_0\rangle$) before including the transformed Kondo term $\hat{H}_{\text{Kondo}}$ and the existence of the SCE modes as states of the total Hamiltonian (5). These two causes produce two gaps defined by Eqs. (12) and (14), and for determined values of J and D_F different phases arise. Specifically, for those values that imply $\Delta_s < 0$, the spin-fluctuation waves are spontaneously coupled to the charged modes so that the SCE states are occupied in the ground state and the new phase appears. The existence of different phases depending of the band parameters is a clear fact theoretically established[1] in Kondo lattices in one dimension. In realistic crystals, there are materials which present many-body states whose properties at low temperatures are not yet well explained. However, the existence of these states associated to the coupling between spin-fluctuation waves and charged fermions in KL systems, in the form explained in this paper, seems compatible with the ideas suggested since some years ago.[2–4] The analysis performed in this paper is an attempt to systemize the transition between the different phases modifying the band parameters J and D_F, and in this context, the state is a natural consequence (quantum transition) of the evolution of Δ_s with these band parameters.

A. Is the phase a heavy-fermion state?

In this phase the specific heat of the system suffers a large increase. An evaluation of this specific heat can be obtained by modeling the SCE DOS by a narrow curve as

$$N_{\mathrm{SCE}}(\omega)\approx\frac{2}{\pi}\frac{\Gamma}{(\omega-X)^2+\Gamma^2}. \tag{17}$$

Then, the Fermi level in the GS (E_F^*) can be calculated and takes the value

$$E_F^*=X-\Gamma\,\mathrm{ctg}\left[\frac{2\pi M}{N}\right], \tag{18}$$

M being half of the number of occupied SCE states and N the number of unit cells of the crystal. The evaluation of M is easy. For instance, considering a rectangular DOS of the noninteracting system whose energy band dispersion is given by $\hat{E}(\varepsilon_{\mathbf{k}})$, $M=N/W^*\left|E_F^*\right|-\hat{E}(0)\left|\right.$. In this situation, the total internal energy of the system is

$$\begin{aligned}U(T)=U_0+\frac{\pi}{3}K_\beta^2T^2\left[\frac{1}{\Gamma}\sin^2A+\frac{2\mu_s}{\Gamma^2}\sin^3A\cos A\right]\\+\frac{7\pi^3}{15\Gamma^3}(K_\beta T)^4\left[\frac{1}{2}\cos 2A\,\sin^4A+\sin^4A\,\cos^2A\right.\\\left.+\frac{4\mu_s}{\Gamma}\cos A\,\sin^5A\left(\cos^2A-\frac{1}{2}\right)\right],\end{aligned} \tag{19}$$

where

$$\mu_s=E_F^*-\frac{\pi^3}{3\Gamma}(K_\beta T)^2\sin 2A,$$

$$A=\frac{2\pi M}{N}, \tag{20}$$

$$U_0\simeq\int_{-\infty}^{\mu_s}\hat{E}(x)\hat{N}(x)dx+M[\Omega-\hat{E}(0)].$$

Therefore, if one considers that $M<N$ and that the chemical potential is at this temperatures almost invariable with the temperature, the specific heat is

$$\begin{aligned}C_V=\frac{\pi^2K_\beta^2T}{3}\hat{N}(\mu_s)+\frac{8\pi K_\beta^2T}{3\Gamma}\left[\left(\frac{\pi M}{N}\right)^2+\frac{4\mu_s}{\Gamma}\left(\frac{\pi M}{N}\right)^3\right]\\+K_\beta^4\left(\frac{\pi T}{\Gamma}\right)^3\left[\frac{224}{5}\left(\frac{\pi M}{N}\right)^4+\frac{1792\mu_s}{15\Gamma}\left(\frac{\pi M}{N}\right)^5\right].\end{aligned} \tag{21}$$

In the limit $X=0$, $M\to 0$ and then $C_V=C_V^0$, C_V^0 being the specific heat yielded by $\hat{N}(x)$ (the first term of former equation). When the binding energy ($|X|$) increases, the number of occupied SCE states in the GS increases, and then the specific heat quickly increases due to the narrowness of the SCE bands (Γ). The expression of this C_V is a polynomial of the kind $\gamma^*T+\beta^*T^3+\cdots$. Some materials (for instance UBe_{13}) present at low temperatures specific heat with polynomial expressions (see Fig. 4 of Ref. 2), and Eq. (21) can imply a specific heat thousands of times larger than that of the normal phases of conventional metals, the reason for this enhancement being the coupling of electrons with spin waves as suggested previously in literature.[2–4] *Expressions (18)–(21) show that the huge specific heat and the magnetic-susceptibility characteristic of the HF state could be explained by this phase with the only mechanism of the occupation of the SCE states.* On the other hand, the entropy variation with T is also very large because of the partial occupation in the GS of the narrow SCE band. In addition, the occupation of these SCE states is not the only source of mass and entropy enhancement, since the RKKY term also operates in the phase producing spin correlations and a tendency to a weak antiferromagnetism that can be destroyed at low temperatures which can increase yet more C_V. However, the spin correlations produced by $\hat{H}_{\mathrm{RKKY}}$ can be damped in this phase because of the occupation of the SCE states in the ground state since the SCE states imply spin fluctuations within the spin field which compete with the spin-spin correlations (the damping of the local moments by the spin fluctuations is an old experimental result in materials in the heavy-fermion state[3,4,16]).

If the HF state can occur when the charged particles fall into the collective SCE states, the debated question about the nature of the particles (charged fermions[10,9] or neutral particles[11]) that are responsible for the HF transition, can be answered mixing these disjunctive propositions. This is so because the SCE states are, as it is insisted throughout this paper, constituted by the coupling of renormalized charged particles (fermions) with collective spin excitations (bosons) originated by the exchange Kondo interaction.

B. Is this phase a superconducting heavy-fermion state?

An issue that has caused large expectation is the relation between the magnetic spin fluctuations and the quenched antiferromagnetism with the appearance of a matter state in which the zero-resistance property is one, and not the only, surprising manifestation.[2–4] A fascinating question opened in the analysis of this new GS is whether the energy condensation which produces the instability in the Fermi surface can lead to a situation similar to superconductivity or whether it is a simple manifestation of dressed electrons mixed with spin-density waves. However, in any case, the phase should present large variations in the conducting behaviors, since the charged particles trapped in the flat band of SCE states are responsible for the conductivity properties. These particles present small mobilities due to their large effective masses and consequently their velocities are very low, since $v_F\simeq v_e(C_V^0/C_V)$, $v_F(v_e)$ being the velocity of the SCE (free electron) particles, and $C_V(C_V^0)$ the calculated (free-electron gas) specific heat. In the Hilbert space whose basis is constituted by SCE states, the transformed Kondo Hamiltonian (5) is approximately diagonal, then, the SCE states should only interact with the lattice via absorption and emission of phonons. However, when the velocity of the particles in the SCE states (v_F) is less than the sound velocity in the material (v_s), the charges located at energies next to E_F cannot interact with the lattice and therefore are unable to produce electrical resistance. Using the linearized Euler model[27] of motion of two fluids, $v_F<v_s$ if the specific heat C_V satisfies the following condition:

$$C_V>C_V^0\left(\frac{3M}{Zm}\right)^{1/2}, \tag{22}$$

where $M(m)$ is the mass of the atoms (free electron) of the solid and Z their charge. *With these latter conditions, a zero-*

resistance transition could appear by the only mechanism of the occupation of the SCE states, without requiring the pair coupling of the charged particles close to E_F. The transition temperature should be low because it is given by the widths of the SCE band since the small v_F is only ensured within this band. In addition, if this zero-resistance transition is only caused by the SCE band occupation, the corresponding state is gapless, since the gap is associated with the existence of pair condensation. In coherence with this point, the specific heat in this phase does not vary exponentially, but as a T^3 polynomial, similar to that of some characteristic gapless superconductors as UBe_{13}.

In this phase, external magnetic fields (**H**) can inhibit the spin fluctuations via Zeeman effects, thus making possible the breaking of the coupling between charged and spin waves when **H** is larger than a critical value. Using a thermodynamical reasoning analog to that used for the standard superconductivity, the critical field $H_c(T)$ and transition temperature can be deduced from the differences between the free energies of the normal and new phases. Therefore, one can consider that

$$\frac{2}{3}\mu_0\pi r_0^3 H_c^2(T) = -\frac{1}{\beta}\int_{-\infty}^{\infty}\hat{N}(x)\ln\left[\frac{1+e^{-\beta(x-\mu)}}{1+e^{-\beta(x-\mu_s)}}\right]dx + \frac{1}{\beta}\int_{-\infty}^{\infty}N_{SCE}(x)\ln[1+e^{-\beta(x-\mu_s)}]dx, \tag{23}$$

where r_0 is the interparticle spacing; μ and μ_s are the chemical potentials of the noninteracting system and the new phase, respectively. Following the superconducting analogy, the transition temperature T_c can be obtained in a function of system parameters considering in Eq. (23) H_c equal to zero.

I wish to emphasize that, in this phase the possible appearance of superconductivity is concomitant with the narrowness of the active SCE bands and the subsequent large specific heat which is provided to the system (this concomitance was suggested from experimental point of view by Fisk *et al.*[3]). A candidate to present this kind of (pseudo?) superconductivity could be UBe_{13}, since it is experimentally known[3] that this material presents a heavy-fermion specific heat varying as T^3 and it is clearly a gapless superconductor of very low transition temperature[2–4,9,16] ($\simeq 1$ K).

On the other hand, it is necessary to note some differences between the phase described in this section and the standard superconducting state caused by the electron pairing: (i) The charge carriers are the SCE states that are fermions, in contradiction with the standard paired superconductors where they are electron pairs (false bosons). (ii) In the GS described here, there is not superconducting coherence as with the standard superconductors, since it is caused because the mass center of the charged particles are in the same wave functions, logically, in contradiction with the fact that in this GS all charges are fermion states. (iii) Possibly, the scattering with the crystal impurities should present differences that will have to be determined.

It is clear that for obtaining an incipient description of this possible superconducting state, a quantitative analysis of its conducting and superconducting properties must be carried out. A particular point that should be considered is the influence in the superconducting transition of the possible existence of a middle-energy resonance band corresponding to the charged *f* particles which, as said above, are excluded in this KLM analysis. In addition, the question of whether the superconducting transition operates by means of two Fermi liquids (the SCE occupied states and the charged *f* particles) or whether the charged *f* particles also participate in the superconducting energy condensation should be answered.

VII. SUMMARY AND CONCLUDING REMARKS

The analysis presented in this paper can be summarized as follows: we have two subsystems, charged particles in extended bands and a spin field in a quasiantiferromagnetic ordering. When both subsystems interact via spin exchange coupled particle states can be formed by charged $s=1/2$ particles and neutral $s=1$ ones. These states have $S=1/2$ for the antiferromagnetic initial Kondo parameter (J), and $S=3/2$ for the ferromagnetic case. The spectrum of these states confirms the conducting and magnetic properties of the KL systems. This spectrum contains two terms: one of them $\propto J^2$ and another exponential. The first term arises in these charged modes because the unitary transformation yields the RKKY interaction that acts within the localized spin field. The exponential term arises from the transformed Kondo Hamiltonian. Varying the coupling strength (J) both terms of the spectrum of the SCE states vary differently and thus the quantum phases appear. For large J and the small density of states of the noninteracting system (D_F), the Kondo lattice interaction yields a GS that corresponds to a small-gap Kondo insulator. Decreasing J and increasing D_F the gap also decreases and the conducting phase is then possible. In this phase, thermal excitation of electrons can be produced and then spin-flip effects in the weak antiferromagnetic ordering generate spin waves which are coupled with some (a small number) of these electrons. This fact increases the effective mass of the conduction electrons. In this phase other apparent mass enhancement can be associated to the entropy increase due to the thermal breakdown of the spin correlations induced by the RKKY interaction. For a critical value of J, spontaneous spin waves arise at $T=0$ K, and thus a true phase is produced since the coupled states are occupied in the GS. The effective mass of electrons in an energy interval around E_F is then very large and the mobility of the particles in such an interval is so small that it can hinder the interaction with the lattice. Then the zero-resistance state condition arises in the Kondo lattice system. In other words, the occupation of the SCE states in the GS implies the spontaneous coupling of the electrons with the spin waves generated by their interaction with the spin field. This fact can be a sufficient mechanism for the energy condensation of a special (super?) conducting state, although it does not exclude the concomitance with other mechanisms.

Note added in proof. Equation (19) is obtained from Sommerfeld's method. Obviously, other methods will yield different functions for $U(T)$. The important point of Eq. (19) is that the terms in T, T^3, T^5,… cannot be neglected because they are proportional to Γ^{-1}, Γ^{-3}, Γ^{-5},…, respectively.

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[1] H. Tsunetsugu, M. Sigrist, and K. Ueda, Rev. Mod. Phys. **69**, 809 (1997); M. Sigrist, H. Tsunetsugu, and K. Ueda, Phys. Rev. Lett. **67**, 2211 (1991).

[2] P. W. Anderson, Proc. Natl. Acad. Sci. USA **92**, 6668 (1995).

[3] Z. Fisk, J. L. Sarrao, J. L. Smith, and J. D. Thompson, Proc. Natl. Acad. Sci. USA **92**, 6663 (1995).

[4] Z. Fisk, D. W. Hess, C. J. Pethick, D. Pines, J. L. Smith, J. D. Thompson, and J. O. Willis, Science **239**, 33 (1988).

[5] P. Fulde, J. Keller, and G. Zwicknagl, *Solid State Physics: Advances in Research and Applications* (Academic, New York, 1988), Vol. 41, p. 1; P. Fulde, *Electron Correlations in Molecules and Solids* (Springer, Berlin, 1995).

[6] K. Tsutsui, Y. Ohta, R. Eder, S. Maekawa, E. Dagotto, and J. Riera, Phys. Rev. Lett. **76**, 279 (1996).

[7] J. J. Joyce, A. J. Arko, J. Lawrence, P. C. Canfield, Z. Fisk, R. J. Bartlett, and J. D. Thompson, Phys. Rev. Lett. **68**, 236 (1992); J. J. Joyce and A. J. Arko, *ibid.* **70**, 1181 (1993); J. J. Joyce, A. J. Arko, P. S. Riseborough, P. C. Canfield, J. M. Lawrence, R. I. R. Blyth, R. J. Bartlett, J. D. Thompson, and Z. Fisk, Physica B **186-188**, 31 (1993); A. B. Andrews, J. J. Joyce, A. J. Arko, J. D. Thompson, J. Tang, J. M. Lawrence, and J. C. Hemminger, Phys. Rev. B **51**, 3277 (1995); A. B. Andrews, J. J. Joyce, A. J. Arko, Z. Fisk, and P. S. Riseborough, *ibid.* **53**, 3317 (1996); A. J. Arko, J. J. Joyce, A. B. Andrews, J. L. Smith, J. D. Thompson, E. Moshopoulou, Z. Fisk, A. A. Menovsky, and P. C. Canfield, Physica B **230&232**, 16 (1997).

[8] F. Patthey *et al.*, Phys. Rev. Lett. **70**, 1179 (1993); D. Malterre, M. Grioni, P. Weibel, B. Dardel, and Y. Baer, Europhys. Lett. **20**, 445 (1992); Phys. Rev. B **48**, 10 599 (1993); D. Malterre, M. Grioni, and Y. Baer, Adv. Phys. **45**, 299 (1996); L. Duó, P. Vavassori, L. Braicovich, M. Grioni, D. Malterre, Y. Baer, and G. L. Olcese, Phys. Rev. B **53**, 7030 (1996); M. Grioni, P. Weibel, D. Malterre, Y. Baer, and L. Duó, *ibid.* **55**, 2056 (1997); M. Garnier, K. Breuer, D. Purdie, M. Hengsberger, Y. Baer, and B. Delley, Phys. Rev. Lett. **78**, 4127 (1997).

[9] T. M. Rice and K. Ueda, Phys. Rev. Lett. **55**, 995 (1985); Phys. Rev. B **34**, 6420 (1986).

[10] A. Millis and P. Lee, Phys. Rev. B **35**, 3394 (1987).

[11] Y. Kagan, K. A. Kikoin, and N. V. Prokof'ev, Physica B **182**, 201 (1992); **194**, 1171 (1994).

[12] P. W. Anderson, Science **267**, 1610 (1995).

[13] B. Bucher, Z. Schlesinger, P. C. Canfield, and Z. Fisk, Phys. Rev. Lett. **72**, 522 (1994).

[14] A. Severing *et al.*, Phys. Rev. B **44**, 6832 (1991).

[15] A. E. Sikkema, I. Affleck, and S. R. White, Phys. Rev. Lett. **79**, 929 (1997).

[16] K. Andres, J. E. Graebner, and H. R. Ott, Phys. Rev. Lett. **35**, 1779 (1975); G. R. Stewart, Rev. Mod. Phys. **56**, 755 (1984).

[17] J. M. Prats and F. López-Aguilar, Nucl. Phys. B **483**, 637 (1997).

[18] P. Fazekas and E. Muller-Hartmann, Z Phys. B **85**, 285 (1991).

[19] B. A. Jones, C. M. Varma, and J. W. Wilkins, Phys. Rev. Lett. **61**, 125 (1988).

[20] C. Godart, L. C. Gupta, C. V. Tomy, J. D. Thompson, and R. Vijayaraghavan, Europhys. Lett. **8**, 375 (1989).

[21] C. C. Yu and S. R. White, Physica B **199&200**, 454 (1994).

[22] S. R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996).

[23] H. Tsunetsugu, Y. Hatsugai, K. Ueda, and M. Sigrist, Physica B **186&188**, 882 (1993).

[24] H. v. Lohneysen, T. Pietrus, G. Portisch, H. C. Schlager, A. Schroder, M. Sieck, and T. Trappmann, Phys. Rev. Lett. **72**, 3262 (1994).

[25] F. López-Aguilar, J. Costa-Quintana, and L. Puig-Puig, Phys. Rev. B **48**, 1128 (1993); **48**, 1139 (1993); M. M. Sánchez-López, J. Costa-Quintana, and F. López-Aguilar, Europhys. Lett. **27**, 235 (1994); J. Costa-Quintana, E. González-León, F. López-Aguilar, L. Puig-Puig, and M. M. Sánchez-López, Physica B **206&207**, 186 (1995); J. Costa-Quintana, M. M. Sánchez-López, and F. López-Aguilar, Phys. Rev. B **54**, 10 265 (1996); F. López-Aguilar, J. Costa-Quintana, and M. M. Sánchez-López, *ibid.* **56**, 1335 (1997).

[26] S. L. Sondhi *et al.*, Rev. Mod. Phys. **69**, 315 (1997).

[27] G. Rickayzen, *Theory of Superconductivity* (Wiley, New York, 1965).