Spectrum and phase transitions in Kondo lattices

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In this paper, I analyze the spectra of composite systems of charged modes and localized spin fields. I determined the structure of the ground state and the excited states based on the coupling of charged modes and spin-fluctuation waves traveling into the spin field. This is carried out considering the interplay of the renormalized Kondo Hamiltonian and the induced Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction. The spectrum of these states is deduced in several cases, when the spin field state is magnetically nonordered and when it is antiferromagnetic. I show that in both spin field states the fluctuation waves can confer a narrow band structure character to these excited states, whose **k** dispersion is due to the J_{RKKY} interaction. In addition, for both spin field states, the Kondo effects compete with the RKKY effects and the concatenation of the two actions can produce different phases. I analyze the conditions for the appearance of such phases and outline some of their properties.

I. INTRODUCTION

The conduction-band electrons within the Kondo lattice produce a coherent interaction with the components of the localized spin fields.[1–8] As it is well known, this coherent interaction induces a Heisenberg-like coupling within the spin field that is the so-called Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction.[2,4,6,7] The most simplified version of this induction is given in the model of two impurities (see, for instance, Ref. 1). The joint action of the Kondo and RKKY interactions generates fluctuation waves in the spin field which largely modify the Kondo exchange effects between the conduction electron sea and the spin field lattice. This leads to coupled states of charged modes and fluctuation waves in an analogous way to the case of the polaron, which could allow us by analogy to call them magnetic polarons. The formal expression of these magnetic polarons are linear combinations of composed states of charged modes $e^{\dagger}_{\mathbf{p}}|\mathrm{GS}\rangle$ and spin fluctuation waves $\mathbf{S}_{\mathbf{k}-\mathbf{p}}|\mathrm{GS}\rangle$, where $|\mathrm{GS}\rangle$ is the ground state of the mixed system $[|\mathrm{GS}\rangle=|\Phi\rangle|F\rangle$ and $|\Phi\rangle$ $(|F\rangle)$ is the ground state of the charged particle system (the localized spin field)]. This allows us to introduce an ansatz inspired in trial wave functions that have been used in other previous works.[7,9,10] The spin field state can be magnetically ordered or not. In any case, the magnetic status of this $|F\rangle$ state modifies the phenomenology of the Kondo lattice. In the present paper, I variationally determine the wave function of $|\mathrm{GS}\rangle$ and the excited states, as well as the corresponding spectrum. This is carried out considering the different above-mentioned possibilities for the $|F\rangle$ state. These excited states of the system are many-body excitations which propagate through the lattice with a well defined quasimomentum. Therefore they can be regarded as quasiparticle-state bands whose dispersion energy is $E_{excited}(\mathbf{k})-E_{\mathrm{GS}}$, where $E_{\mathrm{GS}}[E_{excited}(\mathbf{k})]$ is the energy of the ground [**k**-momentum excited] state. The spectrum of these quasiparticles contains competitive terms arising from the RKKY and renormalized Kondo effects, being possible that the energy of the excited states is, in certain conditions, less than that of the state initially considered as the ground state. In this case, insulator-conducting phase transitions occur and new metallic phases appear. The main objetive of this paper is to formalize the determination of the wave functions for the ground state and excited states of the mixed system (charged modes and spin-fluctuation waves) and to obtain the quasimomentum dependence of their spectrum. As a consecutive study, I will analyze the conditions for the appearance of the different phases: Kondo insulators,[11–15] and conducting materials.[4,16–18] The band character of these quasiparticle structures is conferred by the RKKY interaction and the resulting width of these bands can be narrow, strongly enhancing the effective masses of the charges located in them. A property of this mass enhancement is its magnetic origin, since it is produced by the coupling of initially extended states with spin-fluctuation waves. Since some years ago, different authors have suggested such an origin for the heavy-fermion phenomenology.[2–5,19,20] Therefore the occupation of these strongly correlated electron (SCE) states can lead to find explanations for this phenomenology.

II. SUMMARY OF THE MODEL AND TRIAL WAVE FUNCTIONS

A more extensive explanation of the model can be found in Refs. 16 and 18. We consider the $s-f$ (or $s-d$) exchange Hamiltonian[3] which usually is named Kondo lattice model (KLM) and whose expression is[3,6,7]

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

where $\mathbf{S}_{ei}$ and $\mathbf{S}_{fi}$ are the spin of the conduction electrons and the $(s=1/2)$ local i spin, respectively. In our analysis of this model, we consider a unitary transformation of the initial operators $c^{\dagger}_{\mathbf{k}\alpha}$, $c_{\mathbf{k}\alpha}$, and $\mathbf{S}_{f\mathbf{k}}$ into a new 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 transformed operators $\hat{e}_{\mathbf{p}\alpha}=\hat{c}_{\mathbf{p}\alpha}$ and $\hat{h}_{\mathbf{q}\alpha}=\hat{c}^{\dagger}_{-\mathbf{q}-\alpha}$ are such that $\hat{e}_{\mathbf{p}\alpha}|\mathrm{GS}\rangle=\hat{h}_{\mathbf{q}\alpha}|\mathrm{GS}\rangle=0$, where $|\mathrm{GS}\rangle$ is the ground state of the interacting system. The generator of the transformation $\hat{T}$ can be arbitrary whenever $\hat{T}|\mathrm{GS}\rangle\neq 0$ and preserve all symmetries of the initial Hamiltonian. In addition, for small

Kondo coupling parameter J, and any $\hat{O}$ operator, the following equality should be valid:

$$O = e^{-\hat{T}}\hat{O}e^{\hat{T}} \approx \hat{O} + [\hat{T},\hat{O}]. \tag{2}$$

Substituting the original creation and annihilation operators in function of the corresponding transformed operators in the initial Kondo Hamiltonian, we obtain the expression of H in terms of the new degrees of freedom.

$$H = \hat{C} + \hat{H}_{kinetic} + \hat{H}_{Kondo} + \hat{H}_{RKKY}, \tag{3}$$

where the different terms of the Hamiltonian are given in Refs. 16 and 18.

The general structure of the above transformed Hamiltonian's eigenstates with $s = s^z = 1/2$ and wave vector $\mathbf{k}$ is[16,18]

$$|\mathrm{SCE}_{\mathbf{k},1/2}\rangle = AN^{-1/2}\sum_{\mathbf{p}} B(\mathbf{p})(\hat{e}^{\dagger}_{\mathbf{p}\uparrow}\hat{S}_{0,\mathbf{k}-\mathbf{p}} + \hat{e}^{\dagger}_{\mathbf{p}\downarrow}\hat{S}_{1,\mathbf{k}-\mathbf{p}})|\Phi\rangle|F\rangle. \tag{4}$$

A similar expression is obtained for the states constructed with hole operators,

$$|\mathrm{SCE}_{\mathbf{k},1/2}\rangle = AN^{-1/2}\sum_{\mathbf{p}} B(\mathbf{p})(\hat{h}^{\dagger}_{\mathbf{p}\uparrow}\hat{S}_{0,\mathbf{k}-\mathbf{p}} + \hat{h}^{\dagger}_{\mathbf{p}\downarrow}\hat{S}_{1,\mathbf{k}-\mathbf{p}})|\Phi\rangle|F\rangle, \tag{5}$$

where A is a normalization constant. These SCE states are many-body electron (hole) excitations $\hat{e}^{\dagger}_{\mathbf{p}\sigma}|\Phi\rangle$ ($\hat{h}^{\dagger}_{\mathbf{p}\sigma}|\Phi\rangle$) that are coupled to a cloud of spin-fluctuation waves whose wave functions are given by $\hat{S}_{l\mathbf{k}}|F\rangle$. The structure of the $|\Phi\rangle$ state is constituted by the true GS of the charged modes without coupling with the spin-fluctuation waves and $|F\rangle$ is the spin field ground state.

The structure of these $|\mathrm{SCE}_{\mathbf{k},s}\rangle$ states depends on the nature of the spin field. In general, the wave functions of a spin-field state $|F\rangle$ can be written as

$$|F\rangle = \sum_{\alpha_1=\uparrow,\downarrow}\sum_{\alpha_2=\uparrow,\downarrow}\cdots\sum_{\alpha_N=\uparrow,\downarrow} C_{\alpha_1\alpha_2\cdots\alpha_N}\hat{f}^{\dagger}_{\alpha_1}\hat{f}^{\dagger}_{\alpha_2}\cdots\hat{f}^{\dagger}_{\alpha_N}|0\rangle, \tag{6}$$

where the $C_{\alpha_1\alpha_2\cdots\alpha_N}$ coefficients define the magnetic state of $|F\rangle$. The only difference between Eqs. (4) and (5) and the trial wave functions of our previous papers[16,18] is that the results depend here on the magnetic structure of the spin field state $|F\rangle$, while in Refs. 16 and 18 the spectrum was obtained without considering the RKKY action, thus overlooking the structure of the spin field state. The above $|F\rangle$ wave function for a system in a general case can be rewritten as

$$|F\rangle = \prod_j |[\alpha_j,\beta_j]\rangle, \tag{7}$$

where $|[\alpha_j,\beta_j]\rangle = (a_j e^{i\theta_j}\hat{f}^{\dagger}_{j\uparrow} + b_j e^{i\theta'_j}\hat{f}^{\dagger}_{j\downarrow})|0\rangle = (a_j e^{i\theta_j}|\uparrow\rangle_j + b_j e^{i\theta'_j}|\downarrow\rangle_j)$, and in all j sites $a_j^2 + b_j^2 = 1$. The phases θ and θ' are arbitrary. Both the modules and phases of the variational α_j and β_j parameters define the magnetic structure. The actual Kondo materials are either antiferromagnetic, such as UPt_3 and UPd_2Al_2,[20,21] or magnetically nonordered as $CeSi_2$ and UBe_{13}.[20] Therefore I shall consider in this work only these two cases.

For the magnetically nonordered system, I consider a spin field state such that $\langle F|\hat{S}_{jz}|F\rangle = 0$ for all j sites. In this case, the $|F\rangle$ state can be defined by

$$|F\rangle = 2^{-N/2}\prod_j |[1,1]_j\rangle, \tag{8}$$

where $|[1,1]_j\rangle = (e^{i\theta_j}\hat{f}^{\dagger}_{j\uparrow} + e^{i\theta'_j}\hat{f}^{\dagger}_{j\downarrow})|0\rangle = (e^{i\theta_j}|\uparrow\rangle_j + e^{i\theta'_j}|\downarrow\rangle_j)$.

In this case, the $\hat{S}_{l\mathbf{k}}|F\rangle$ states are perturbations of the spin field in a magnetically nonordered state, i.e., these states constitute a spin liquid of excitations within the paramagnetic spin field. The wave functions of such excitations can be formally expressed as

$$\hat{S}^{+}_{\mathbf{k}}|F\rangle = \sum_j^N \frac{e^{i\mathbf{k}\cdot\mathbf{R}_j}}{\sqrt{N2^N}}|[1,1]_1\cdots[1,0]_j\cdots[1,1]_N\rangle, \tag{9}$$

$$\hat{S}^{z}_{\mathbf{k}}|F\rangle = \sum_j^N \frac{e^{i\mathbf{k}\cdot\mathbf{R}_j}}{\sqrt{N2^N}}|[1,1]_1,\cdots,[1,-1]_j,\cdots,[1,1]_N\rangle, \tag{10}$$

$$\hat{S}^{-}_{\mathbf{k}}|F\rangle = \sum_j^N \frac{e^{i\mathbf{k}\cdot\mathbf{R}_j}}{\sqrt{N2^N}}|[1,1]_1\cdots[0,1]_j\cdots[1,1]_N\rangle. \tag{11}$$

From an easy inspection of the above equations one can see that in this case, the trivector $(\hat{S}^{+}_{\mathbf{k}},\hat{S}^{z}_{\mathbf{k}},\hat{S}^{-}_{\mathbf{k}})|F\rangle$ is truly one dimensional because its three components are linearly dependent (for a lattice with $N\to\infty$, $\hat{S}^{+}_{\mathbf{k}}|F\rangle$, and $\hat{S}^{-}_{\mathbf{k}}|F\rangle$ are parallel). Therefore, in the magnetically nonordered case, the spin excitations within the spin liquid have $S=0$ and thus the $|\mathrm{SCE}\rangle$ states can only have $S=1/2$.

For an antiferromagnetically ordered $|F\rangle$ state, the components of the trivector $(\hat{S}^{+}_{\mathbf{k}},\hat{S}^{z}_{\mathbf{k}},\hat{S}^{-}_{\mathbf{k}})|F\rangle$ can be given in one dimension by

$$\hat{S}^{\pm}_{\mathbf{k}}|F\rangle = \sum_j \frac{e^{i\mathbf{k}\cdot\mathbf{R}_j}}{\sqrt{N}}|\uparrow\rangle_1|\downarrow\rangle_2\cdots S^{\pm}_j|m_s\rangle_j\cdots\rangle, \tag{12}$$

$$\hat{S}^{z}_{\mathbf{k}}|F\rangle = \sum_j \frac{e^{i\mathbf{k}\cdot\mathbf{R}_j}}{\sqrt{N}}|\uparrow\rangle_1|\downarrow\rangle_2\cdots S^{z}_j|m_s\rangle_j\cdots\rangle \tag{13}$$

(the extension to any dimension is straightforward). For the sake of simplicity I consider here an antiferromagnetic structure of two sublattices with antiparallel spin direction, the calculations for any other antiferromagnetic structure can be deduced from this simple one. The three states in the antiferromagnetic $|F\rangle$ state above defined are linearly independent and hence the trivector $(\hat{S}^{+}_{\mathbf{k}},\hat{S}^{z}_{\mathbf{k}},\hat{S}^{-}_{\mathbf{k}})|F\rangle$ corresponds to $S=1$ spin waves propagating with momentum $\mathbf{k}$ through the spin field. As a consequence, the $|\mathrm{SCE}\rangle$ states in an antiferromagnetic spin field can have $S=1/2$ and $S=3/2$.

III. STRUCTURES AND ENERGIES OF THE GROUND STATE

The ground state $|\mathrm{GS}\rangle$ is composed, as mentioned above, by a many-body charged mode wave function $|\Phi\rangle$, and a spin field wave function $|F\rangle$. Given the operational structure[16,18] of $\hat{H}_{kinetic}$, $\hat{H}_{Kondo}$, and $\hat{H}_{RKKY}$, it is obvious

that $|\Phi\rangle$ is eigenstate of both $\hat{H}_{kinetic}$ and $\hat{H}_{kinetic}+\hat{H}_{Kondo}$. As a consequence, the structure of $|\Phi\rangle$ is totally determined because $\hat{H}_{kinetic}$ is a noninteracting system of energy $\hat{C}$.

In the case of magnetically nonordered $|F\rangle$ states, we obtain

$$E^0_{RKKY}=\left\langle F\left|\frac{1}{2}\sum_{i\neq j} J_{ij}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j\right|F\right\rangle = \frac{1}{8}\sum_{i\neq j} J_{ij}\cos(\theta_i+\theta'_j-\theta'_i-\theta_j). \tag{14}$$

The above energy only depends on the phases θ_i, θ_j, θ'_i, and θ'_j that define a given nonordered state. As an example, we can consider the one-dimensional lattice; here, the lowest energy for a nonordered $|F\rangle$ state is obtained with a distribution of phases such that $\theta'_j=\theta_j+(-1)^{j(\pi/2)}$. The corresponding minimum energy is then

$$E^0_{RKKY}=\langle F|\hat{H}_{RKKY}|F\rangle=-\frac{1}{8}\sum_{i\neq j}|J_{ij}|. \tag{15}$$

For an antiferromagnetic $|F\rangle$ state, the energy of the ground state of the $|F\rangle$ spin field is

$$E^0_{RKKY}=\langle F|\hat{H}_{RKKY}|F\rangle=-\frac{1}{8}\sum_{i\neq j}J_{ij}+\frac{1}{2}\sum_{i\neq j}^{++}J_{ij}, \tag{16}$$

where $\Sigma^{++}_{i\neq j}$ stands for the (ij) indexes that run over the spin-up sublattice.

IV. CALCULATION OF THE TOTAL SCE ENERGY

The SCE energy is a functional of the variational $B(\mathbf{p})$ parameters of Eqs. (4) and (5) which should be minimized in order to determine the SCE spectra. Therefore we have that

$$E_{\mathrm{SCE}}(\mathbf{k})=\langle \mathrm{SCE}_{\mathbf{k},\sigma}|\hat{C}+\hat{H}_{kinetic}+\hat{H}_{Kondo}+\hat{H}_{RKKY}|\mathrm{SCE}_{\mathbf{k},\sigma}\rangle = \hat{C}+\langle\hat{H}_{kinetic}\rangle+\langle\hat{H}_{Kondo}\rangle+\langle\hat{H}_{RKKY}\rangle. \tag{17}$$

The calculation of $E_{\mathrm{SCE}}(\mathbf{k})$ obviously depends on the structure of the $|F\rangle$ state.

A. Nonordered $|F\rangle$ case

The calculation of the different average values of Eq. (17) is large but can easily be systematized by considering the structure of the $|F\rangle$ states given in Eqs. (8)–(13). Then, we have that $\langle\hat{H}_{RKKY}\rangle$ reads

$$\langle\hat{H}_{RKKY}\rangle=\frac{A^2}{2N}\sum_{i\neq j}\sum_{\mathbf{p}} J_{ij}|B(\mathbf{p})|^2\{\langle\hat{S}^0_{\mathbf{p}-\mathbf{k}}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j\hat{S}^0_{\mathbf{k}-\mathbf{p}}\rangle + \langle\hat{S}^-_{\mathbf{p}-\mathbf{k}}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j\hat{S}^+_{\mathbf{k}-\mathbf{p}}\rangle\}. \tag{18}$$

The $\langle\hat{H}_{Kondo}\rangle$ term is

$$\langle\hat{H}_{Kondo}\rangle=\frac{A^2}{2N^{3/2}}\sum_{\mathbf{p}\mathbf{p}'}B^*(\mathbf{p})B(\mathbf{p}')J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'}) \times\sum_{ijm} e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_i}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{R}_j}e^{i(\mathbf{k}-\mathbf{p}')\cdot\mathbf{R}_m}\{\langle\hat{S}_{iz}\hat{S}_{jz}\hat{S}_{mz}\rangle - \langle\hat{S}^-_i\hat{S}_{jz}\hat{S}^+_m\rangle+\langle\hat{S}^-_i\hat{S}^+_j\hat{S}_{mz}\rangle+\langle\hat{S}_{iz}\hat{S}^-_j\hat{S}^+_m\rangle\}. \tag{19}$$

$\langle\hat{H}_{kinetic}\rangle$ reads

$$\langle\hat{H}_{kinetic}\rangle=\frac{A^2}{2N}\sum_{\mathbf{p}}|B(\mathbf{p})|^2\hat{E}(\varepsilon_{\mathbf{p}}). \tag{20}$$

By putting together the resulting expressions for $\langle\hat{H}_{kinetic}\rangle$, $\langle\hat{H}_{Kondo}\rangle$ and $\langle\hat{H}_{RKKY}\rangle$, we have that

$$E_{\mathrm{SCE}}(\mathbf{k})=E_{\mathrm{GS}}+\frac{A^2}{2N}\sum_{\mathbf{p}}|B(\mathbf{p})|^2\hat{E}(\varepsilon_{\mathbf{p}})-\frac{A^2}{4N^2} \times\sum_{\mathbf{p}\mathbf{p}'}B^*(\mathbf{p})J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})B(\mathbf{p}') -\frac{A^2}{4N^2}\sum_{i\neq j}\left(\frac{3}{4}|J_{ij}|-\frac{1}{4}J_{ij}\right) \times\sum_{\mathbf{p}}|B(\mathbf{p})|^2\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]. \tag{21}$$

The above energy corresponds to the excitation of the system by adding a new particle to the GS. This excitation propagates with a $\mathbf{k}$ momentum and can be interpreted as a quasiparticle of energy $E_{\mathrm{SCE}}(\mathbf{k})-E_{\mathrm{GS}}$.

B. Antiferromagnetic $|F\rangle$ case

The expressions (18) and (19) hold also in this case. However, the average values are different because of the different $|F\rangle$ state. Expressing the $\hat{H}_{RKKY}$ Hamiltonian as in Eq. (18) and considering all different average values calculated with the corresponding $|F\rangle$ state, we obtain the following $\mathbf{k}$ dependence of the SCE energy:

$$E_{\mathrm{SCE}}(\mathbf{k})=E_{\mathrm{GS}}+\frac{A^2}{2N}\sum_{\mathbf{p}}|B(\mathbf{p})|^2\hat{E}(\varepsilon_{\mathbf{p}}) -\frac{A^2}{4N^2}\sum_{\mathbf{p}\mathbf{p}'}B^*(\mathbf{p})J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})B(\mathbf{p}') +\frac{A^2}{2N^2}\sum_{i\neq j}^{--}J_{ij}\sum_{\mathbf{p}}|B(\mathbf{p})|^2\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]. \tag{22}$$

The energies of Eqs. (21) and (22) are not determined because they depend on the $B(\mathbf{p})$-variational parameters. Therefore they lack physical meaning until these parameters are determined by minimizing $E_{\mathrm{SCE}}(\mathbf{k})$. This is performed by using the variational techniques of the following section.

V. VARIATIONAL PRINCIPLE APPLIED TO THE $E_{\mathrm{SCE}}(\mathbf{k})$ SPECTRA

The $B(\mathbf{p})$ functions can be determined in a similar procedure to Eq. (84) of Ref. 16 [i.e., by minimizing the $E_{\mathrm{SCE}}(\mathbf{k})$ energy with respect to these variational functions]. This minimization principle leads to the following expressions:

Nonordered $|F\rangle$ state,

$$[E_{\mathrm{SCE}}(\mathbf{k})-E_{\mathrm{GS}}]B(\mathbf{p}) = \hat{E}(\varepsilon_{\mathbf{p}})B(\mathbf{p})-\frac{1}{2N}\sum_{\mathbf{p}'} J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})B(\mathbf{p}') - \frac{1}{2N}\sum_{i\neq j}\left(\frac{3}{4}|J_{ij}|-\frac{1}{4}J_{ij}\right)\sum_{\mathbf{p}} B(\mathbf{p})\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]. \tag{23}$$

Antiferromagnetic $|F\rangle$ state,

$$[E_{\mathrm{SCE}}(\mathbf{k})-E_{\mathrm{GS}}]B(\mathbf{p}) = \hat{E}(\varepsilon_{\mathbf{p}})B(\mathbf{p})-\frac{1}{2N}\sum_{\mathbf{p}'} J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})B(\mathbf{p}') + \frac{1}{N}\sum_{i\neq j}^{--} J_{ij}\sum_{\mathbf{p}} B(\mathbf{p})\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]. \tag{24}$$

In the cases in which $\langle\hat{H}_{Kondo}\rangle$ is much larger than $\langle\hat{H}_{RKKY}\rangle$, we can operate in a similar way to that of Ref. 16. We can initially drop the term arising from the RKKY interaction in order to obtain $B(\mathbf{p})$ and then, by substituting in $\langle\hat{H}_{RKKY}\rangle$ the calculated values for the variational functions we determine $E_{\mathrm{SCE}}(\mathbf{k})$.

For the magnetically nonordered $|F\rangle$ state, we obtain

$$E_{\mathrm{SCE}}(\mathbf{k}) = E_{\mathrm{GS}}+\hat{E}(0)-\frac{1}{2}\exp\left(-\frac{2}{JD_F}\right) - \frac{1}{4N^2}\sum_{i\neq j}\left(\frac{3}{4}|J_{ij}|-\frac{1}{4}J_{ij}\right) \times\sum_{\mathbf{p}} b(\mathbf{p})\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}] \tag{25}$$

and for the antiferromagnetic $|F\rangle$ state,

$$E_{\mathrm{SCE}}(\mathbf{k}) = E_{\mathrm{GS}}+\hat{E}(0)-\frac{1}{2}\exp\left(-\frac{2}{JD_F}\right) + \frac{1}{2N^2}\sum_{i\neq j}^{--} J_{ij}\sum_{\mathbf{p}} b(\mathbf{p})\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]. \tag{26}$$

$\hat{E}(0)$ is the value $\hat{E}(\varepsilon_{\mathbf{p}})$ for $\varepsilon_{\mathbf{p}}=0$. This value is $0.048J^2$ (Ref. 16) when a simple band structure ($\varepsilon_{\mathbf{p}}=\gamma|\mathbf{k}|-1/2$) in the initial Hamiltonian (1) is considered. Then, the $b(\mathbf{p})$ functions are

$$b(\mathbf{p})=2\frac{\Omega(\Omega+\delta/2)}{(\varepsilon_{\mathbf{p}}+\Omega)^2} \tag{27}$$

with $\Omega=\frac{1}{2}\exp(-2/JD_F)$.

An important point in the heavy-fermion issue is the narrowness of the band structure of the SCE states, since this determines the features of this strongly correlated state. The band structure of Eqs. (25) and (26) can be written in a single expression:

$$\Delta(\mathbf{k})=-\frac{\Omega}{2N}\sum_{\mathbf{p}}\frac{\delta/2+\Omega}{(\varepsilon_{\mathbf{p}}+\Omega)^2}\sum_i J_i\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_i]. \tag{28}$$

In this equation the J_i parameters are the RKKY exchange terms with respect to a given site considered as origin. In order to estimate the band structure and analyze its width, one can consider a one-dimensional system with a distribution of J_n parameters such that they can be expressed as $J_n=J_1\alpha^{-(n-1)}$ (for instance, in the calculation carried out in Ref. 18, I obtain $\alpha\approx 2$). Then, the band structure is

$$\Delta(\mathbf{k})=-\frac{\Omega\alpha}{2N}\sum_{\mathbf{p}}\frac{\delta/2+\Omega}{(\varepsilon_{\mathbf{p}}+\Omega)^2}\frac{\alpha\cos[(p-k)a]-1}{\alpha^2+1-2\alpha\cos[(p-k)a]}. \tag{29}$$

A new simplification can be obtained if we use the exhaustion Nozières phenomenon.[22] We can thus consider only the term in the $\mathbf{p}$ summatory for $\mathbf{p}=0$. Thus we have

$$\Delta(\mathbf{k})\approx-\frac{J_1(\delta_2+\Omega)}{2\Omega}\frac{\alpha^2\cos(ka)-\alpha}{\alpha^2+1-2\alpha\cos(ka)}. \tag{30}$$

This band structure has the minimum at $k=0$, the maximum at $k=\pm\pi/a$ and its bandwidth is

$$\delta_{\mathrm{SCE}}=\frac{J_1(\delta/2+\Omega)}{\Omega}\frac{\alpha^2}{\alpha^2-1}. \tag{31}$$

Therefore the heavy-fermion band-structure condition will require that the RKKY term should be preferably weak (i.e., J_1 small), short ranged, and/or fast decreasing (i.e., α large), and the initial bandwidth of Hamiltonian (1) should be as narrow as possible (i.e., small δ).

A. Alternative method to obtain $E_{\mathrm{SCE}}(\mathbf{k})$

An alternative method within the variational calculation consists in determining the characteristic integral equation as in the superconducting equation cases. We start from Eqs. (24) and (25), which can be rewritten as

$$[E_{\mathrm{SCE}}(\mathbf{k})-E_{\mathrm{GS}}-\hat{E}(\varepsilon_{\mathbf{p}})+\Delta_{\mathbf{k}}(\mathbf{p})]B(\mathbf{p}) = -\frac{1}{2N}\sum_{\mathbf{p}'} J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})B(\mathbf{p}'), \tag{32}$$

where $\Delta_{\mathbf{k}}(\mathbf{p})$ takes the following expressions: for the nonordered $|F\rangle$ state

$$\Delta_{\mathbf{k}}(\mathbf{p})=\frac{1}{2N}\sum_{i\neq j}\left[\frac{3}{4}|J_{ij}|-\frac{1}{4}J_{ij}\right]\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}], \tag{33}$$

for the antiferromagnetic case

$$\Delta_{\mathbf{k}}(\mathbf{p})=-\frac{1}{N}\sum_{i\neq j}^{--} J_{ij}\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]. \tag{34}$$

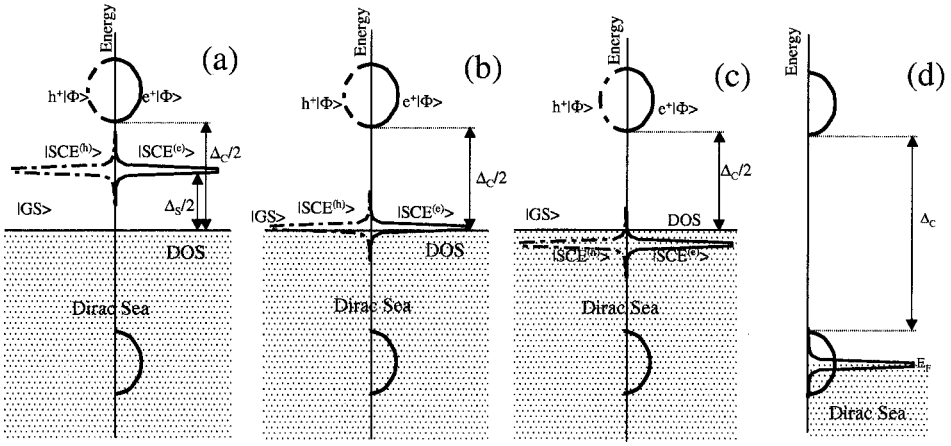

FIG. 1. Schematic drawing of the electronic structure of the different phases described in the text. (a) Insulating A phase. (b) Conducting B phase. (c) Insulating C phase. (d) Conducting D phase. The solid (discontinuous) line correponds to the density-of-states of particles (holes); GS in (a), (b), and (c) stands for the energy level corresponding to the ground state and $\Delta_c(\Delta_s)$ is the charged (spin) gap. The widths of these gaps are exaggerated in order to preserve the clearness of the figure.

From Eq. (32), we arrive to the following integral equation:

$$1=-\frac{1}{2N}\sum_{\mathbf{p}'}\frac{J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})}{E_{\mathrm{SCE}}(\mathbf{k})-E_{\mathrm{GS}}-\hat{E}(\varepsilon_{\mathbf{p}})+\Delta_{\mathbf{k}}(\mathbf{p})}. \quad (35)$$

The minimization of $E_{\mathrm{SCE}}(\mathbf{k})$ from Eqs. (25) and (26) implies that the kinetic energy $\hat{E}(\varepsilon_{\mathbf{p}})$ must be small, which requires that $B(\mathbf{p})$ have all its weight concentrated in a very narrow layer around the Fermi level (this argument is coherent with the exhaustion phenomenon explained by Nozières[22]). Therefore the integration limits of the characteristic integral equation in this layer are such that $J(\varepsilon_{\mathbf{p}},\varepsilon_{\mathbf{p}'})=J$. Then, the above integral equation can be given as

$$1=-\frac{J}{2\Gamma}\int_{\Delta\mathbf{k}}\frac{d\mathbf{p}}{E_{\mathrm{SCE}}(\mathbf{k})-E_{\mathrm{GS}}-\hat{E}(\varepsilon_{\mathbf{p}})+\Delta_{\mathbf{k}}(\mathbf{p})}. \quad (36)$$

The solution is not an easy problem and requires computational procedures, but single cases allow us to make estimations which are not too different from the actual ones. For example, considering one-dimensional lattices and short-range J_{ij} parameters, we arrive to the following solution for the SCE spectra for the nonordered $|F\rangle$ state:

$$E_{\mathrm{SCE}}(\mathbf{k})=E_{\mathrm{GS}}+\hat{E}(0)-(J_1/4)\cos ka+\beta(\mathbf{k})\,\delta \times\exp[4\pi\beta(\mathbf{k})/Ja)],$$

where $\beta(\mathbf{k})=-\gamma+(J_1a/4)\sin(ka)$ and for the antiferromagnetic case: $E_{\mathrm{SCE}}(\mathbf{k})=E_{\mathrm{GS}}+\hat{E}(0)-(J_1/2)\cos 2ka+\beta(\mathbf{k})\,\delta\exp[4\pi\beta(\mathbf{k})/Ja]$, with $\beta(\mathbf{k})=-\gamma+J_1a\sin(2ka)$, where J_1 is the value of J_{ij} for nearest neighbors; γ is the proportionality constant between the initial conduction band structure and the module of the momentum (i.e., $\varepsilon_{\mathbf{p}}=\gamma|\mathbf{k}|$); a is the lattice parameter; J stands for the Kondo coupling parameter of Hamiltonian (1) given in noninteracting system bandwidth units; δ is the part of the conduction band which supplies the charged modes that couple with the spin-fluctuation waves to form the SCE states. Considering the latter approximations, one can arrive at similar values for the SCE spectra from Eqs. (25) and (26). In the case of extremely short range and weak $\hat{H}_{RKKY}$, we again find the expressions of $E_{\mathrm{SCE}}(\mathbf{k})$ of Ref. 16, namely $E_{\mathrm{SCE}}(\mathbf{k})=E_{\mathrm{GS}}+\hat{E}(0)-\frac{1}{2}\exp(-2/JD_F)$.

All calculations of Secs. IV and V have to be also realized considering SCE states constructed with hole operators [i.e., Eq. (5)]. However, the calculation procedure and the results are strictly equal because we have considered a half filling condition in the initial Hamiltonian (1). Therefore I drop them in order to avoid repetitions.

B. Comments on the SCE spectra

In previous papers,[16,18] we have shown how the initial noninteracting system consisting of a partially occupied extended conduction band and a localized spin field is transformed when an appropriate transformation of the degrees of freedom is applied. The resulting noninteracting ground state presents a gap between a completely occupied valence band and another totally unoccupied conduction band. This gap can be called charge gap and its value depends on the band structure of the initial noninteracting system [an example is given in Ref. 16 and the gap value which depends on the initial band structure of the H_0 Hamiltonian in that case is $2\hat{E}(0)=0.096J^2$ (in bandwidth units). Any other band structure will yield the same J^2 dependence but with a different proportionality constant]. The ground state of the system is completed with a spin field state whose energy is given in Eqs. (14) for the general case. Equations (15) and (16) give the GS energies for the magnetically nonordered and antiferromagnetic case, respectively.

In the present work, I have determined the SCE spectra [Eqs. (25) and (26)] considering the competition between the renormalized Kondo effects and the induced RKKY interaction. The Kondo term of these spectra is always negative, i.e., it tends to lower the excitation energy of the charged mode. On the other hand, the RKKY term yields two different effects: (i) a positive term (gap) $\hat{E}(0)$ that is produced due to the transformation of H_0 (which generates $\hat{H}_{kinetic}$ and a part of $\hat{H}_{RKKY}$), and (ii) a $\mathbf{k}$-depending term that provides the band character to the SCE states.

Another physical image of the SCE states and their corresponding SCE spectra is described in terms of charged particle excitations from the valence band to the conduction band. Actually, when one of these excitations is produced, the excited charge interacts with the spin field, producing local spin fluctuations and coupling to them. As a consequence of this coupling, the excitation energy is decreased in

such a way that the corresponding hole suffers the same process. The situation [see Fig. 1] is that while the production of an electron-hole pair without spin field implications costs an energy $\Delta_c = 2\hat{E}(0) = 0.096J^2$, when we consider the Kondo Hamiltonian and the RKKY interaction, this energy is: $\Delta_s(\mathbf{k}) = 0.096J^2 - 2\Omega + 2\Delta(\mathbf{k})$, where $\Delta(\mathbf{k})$ is the band dispersion of Eqs. (28) and (29). Δ_c and Δ_s [the latter value can be considered the average of $\Delta_s(\mathbf{k})$ in the Brillouin zone] are the charge and spin gaps. Therefore the charge gap Δ_c is the necessary energy for obtaining an electron-hole pair without considering the coupling of the charged modes with the spin-fluctuation waves (see Fig. 1). This electron-hole pair energy is reduced when each component of the pair is coupled with the magnetic bosons, thus appearing the spin gap $\Delta_s(\mathbf{k})$. Therefore, as shown in Fig. 1, the Kondo lattice system contains two types of collective excitations: (i) noncoupled charged particle (hole) modes $\hat{e}^{\dagger}_{\mathbf{p}\sigma}|\Phi\rangle$ $(\hat{h}^{\dagger}_{\mathbf{q}\sigma}|\Phi\rangle)$, and (ii) the SCE quasiparticles that consist of charged modes strongly correlated with spin-fluctuation waves induced in the localized spin field. These latter $2N$ states which are quasieigenstates of $\hat{H}_{kinetic} + \hat{H}_{Kondo} + \hat{H}_{RKKY}$ are split by an average gap $[\Delta_s = 0.096J^2 - \exp(-2/JD_F)]$.

A point on which I wish to remark is the relevance of the **k**-dependent SCE spectra in yielding the quantitative explanation of the different phases. In previous papers,[16,18] we determined the SCE spectra without considering the RKKY Hamiltonian and as a consequence, the SCE bands were totally flat, i.e., without any **k** dependence, and therefore these states did not present a band character, being instead truly $2N$-degenerate energy levels. In Ref. 18 I discussed the appearance of different phases varying the values of J and D_F parameters. For increasing J values (keeping the value of D_F fixed) the SCE level crosses the zero energy and produces an essential instability, because all SCE states transit from a total unoccupation to a total occupation due to the $2N$-degenerate SCE levels. Therefore in Ref. 18 the idea of a metallic phase defined as an intermediate occupation of this SCE level is an intuitive and heuristic concept which only acquires physical meaning when a **k** dispersion is obtained due to the action of the RKKY effects. In Ref. 18, the bandwidth was included by hand in order to justify the appearance of this metallic phase. In that paper, the conducting phase was a foresight but its existence was not truly proved. On the contrary, in the present paper I have determined the band character of the SCE states in such a way that we can obtain the occupation ratio, the Fermi level, the mobility of the charge carriers, etc., depending on their energy locations and the $E_{\mathrm{SCE}}(\mathbf{k})$ dispersion. Therefore the metallic phase can be now quantitatively determined thanks to the RKKY interaction, which was overlooked in Ref. 18.

VI. DIFFERENT PHASES OF THE SYSTEM

The center (X) of the narrow SCE bands is located at an energy $X = \Delta_s/2 = 0.048J^2 - \frac{1}{2}\exp(-2/JD_F)$ with respect to the ground state (zero energy). For different values of J and density of states at E_F (D_F) of the initial noninteracting Hamiltonian H_0, we obtain different patterns corresponding to the insulating and conducting phases of Fig. 1. Each of the four phases of this figure appears in a determined J interval $J_c < J < J_{max}$, where J_c is the critical value and J_{max} is the maximum value for which the corresponding phase is maintained. Obviously, the value of J_c depends on D_F. For every $J = J_c$ new quantum phases, in Sondhi *et al.*'s sense,[24] are produced. The name quantum phases is due to the fact that these phases appear by variations of the parameters which govern the quantum Hamiltonian in contrast to the phases yielded by the variation of temperature.

A. Phase *A*

In this phase [see Fig. 1(a)], the occupied and unoccupied states are split as in any insulator. The SCE states consist of spin-fluctuation waves coupled to charged states, therefore the structure of these bands in these insulators can be determined by paramagnetic scattering function measurements.[12] These experimental data can detect the spin gap (Δ_s) and the SCE bandwidths which are usually narrower than that of the spectrum of the noncoupled charged modes.[12] The noncoupled charged modes are split by the Δ_c gap; therefore, in principle, the conductivity $\sigma(\omega)$ is obviously zero for $\omega = 0$, and for $T = 0$ it should present a peak at $\omega \sim \Delta_c/2$. For increasing frequencies (beyond $\Delta_c/2$) $\sigma(\omega)$ should show the normal-metal behavior. The electronic structure of Fig. 1(a) does not change with the thermal action, therefore $\sigma(\omega)$ should increase with T in the interval $0 < \hbar\omega < \Delta_c/2$, and it should be quasiconstant versus T for frequencies larger than $\Delta_c/2$. Δ_c and Δ_s have been experimentally detected[12,11,13,14] and their features are in agreement with the structure given in Fig. 1(a).

B. Phase *B*

When $\Delta_s < 2\delta_{\mathrm{SCE}}$, [see Fig. 1(b)], some SCE states can have less energy than the GS constructed only with the N electrons located in the charged modes without coupling with spin fluctuations. Then, an instability appears because, in the actual ground state of the interacting system, a spontaneous production of particle-hole pairs located in the SCE states is favored. Therefore the two SCE bands can be partially occupied and as a consequence a conducting phase is produced.

In a perfect impurity-lacking Kondo lattice within this phase, the conductivity is governed by the phonon interchange from both intraband and interband (or umklapp) processes, $|\langle \mathrm{SCE}_{\mathbf{k}\alpha}|H_{e\text{-}ph}|\mathrm{SCE}_{\mathbf{k}\alpha}\rangle|^2$ and $|\langle \mathrm{SCE}_{\mathbf{k}\alpha}|H_{e\text{-}ph}|\hat{e}^{\dagger}_{\mathbf{k}\alpha}\Phi\rangle|^2$, respectively. The umklapp scatterings are different from zero but their contribution can be negligible because the energies of the initial and final charged states are split by a gap ($\simeq \Delta_c/2$), and this gap can be much larger than $K_B T^*$ (T^* is the coherence temperature). Therefore the conductivity in this case is $\sigma = 2e^2 n\tau^*/m^*$, where all variables concern the SCE band (the factor 2 is due to the existence of identical SCE bands, one of particles and another of holes). In general, the relaxation time in an ideal system without impurities is caused by the inelastic interaction with the lattice, which is given by:[25] $\tau^{-1} = \Sigma_{\mathbf{q}\nu} G_{\nu}(\mathbf{q},T)\,\delta[\varepsilon_{\mathrm{SCE}}(\mathbf{k}_F + \mathbf{q}) - \varepsilon_{\mathrm{SCE}}(\mathbf{k}_F) - \hbar\omega_{\mathbf{q}\nu}]$, where G_{ν} is a function which includes the electron-phonon coupling strength for any temperature corresponding to the SCE band of charged particles and the ν band of phonons. A

fundamental point to obtain the relaxation time τ is to know the band structures within the argument of the Dirac delta function of the above expression. Taking into account the calculations that lead to the band-structure expressions of Eqs. (28) and (29) for the SCE states, we have a procedure for obtaining the relaxation time and therefore the conductivity. The partial occupation of both the hole- and the particle-SCE band ensures the nonzero conductivity, and therefore the metallic behavior of the material in this phase. The quantitative analysis of these relaxation times requires a large and complex systematic which is out of the scope of this paper, and it deserves a detailed analysis.

An important point is that the particle SCE band in the *B* phase cannot be analyzed without considering simultaneously the hole SCE band, since the existence of the former generates *a fortiori* the latter. In this excitonic gas, for each particle SCE state occupied with an energy E, a momentum $\mathbf{k}$, a charge e^-, and a spin σ, another hole SCE state is occupied with the same energy E, $-\mathbf{k}$, e^+, and $-\sigma$. This picture, although being obvious, can lead, I believe, to drastic and interesting consequences. Namely, from the Lorentz force point of view, the SCE pair in this *B* phase ($|\mathrm{SCE}^{(e)}_{\mathbf{k}\sigma};\mathrm{SCE}^{(h)}_{-\mathbf{k}-\sigma}\rangle$) maintains its structure in the presence of an external electric field. This field increases the $\mathbf{k}$ momentum of each pair component but keeps null the momentum of the gravity center of the pair, and doubles the electric current generated by each mate. On the other hand, the magnetic field can produce a current orthogonal to this field in a similar way to that produced by an electron pair. In addition, when a electron-hole SCE pair is spontaneously occupied in the ground state, an attractive interaction arises because the interacting process $\langle \mathrm{SCE}^{e}_{\mathbf{k}\sigma};\mathrm{SCE}^{h}_{-\mathbf{k}-\sigma}|\hat{H}_{RKKY}|\mathrm{SCE}^{e}_{\mathbf{k}\sigma};\mathrm{SCE}^{h}_{-\mathbf{k}-\sigma}\rangle$ can be negative. Therefore each SCE-excitonic pair forms a composite boson whose features and their influence in the macroscopic physical responses of the excitonic gas should be analyzed.

C. Phase *C*

When J increases further [see Fig. 1(c)], for X values in the interval $-\delta_{\mathrm{SCE}}>X>-\Delta_c/2$, every hole- and particle-SCE state is below the zero energy of the Dirac sea. Therefore all SCE states are occupied and the insulating phase appears again because $\Delta_s(\mathbf{k})$ becomes negative for all $\mathbf{k}$ momenta. This situation remains in the parameter space until the gravity center of the SCE bands tends toward values close to $-\Delta_c/2$. The thermodynamic and conducting properties of this phase differ from those of phase *A*, since now the states that can be occupied by thermal or electromagnetic interactions are the noncoupled states instead of the SCE states (as it is the case in phase *A*). This implies that the magnetic amplitude response of the system $\chi(\omega)$ does not contain any peak for $\hbar\omega=\Delta_s$ as it can occur in phase *A*,

D. Phase *D*

When $X<-\Delta_c/2$, a new insulating-conducting phase transition arises. In this phase, the Dirac sea is transformed and
a new lower energy state appears [see Fig. 1(d)]. The SCE states can be redefined as: $|\mathrm{SCE}_{\mathbf{k},1/2}\rangle=\Sigma_{\mathbf{p}}[B(\mathbf{p})/\sqrt{N}](\hat{e}^{\dagger}_{\mathbf{p}\uparrow}\hat{S}_{0,\mathbf{k}-\mathbf{p}}+\hat{e}^{\dagger}_{\mathbf{p}\downarrow}\hat{S}_{1,\mathbf{k}-\mathbf{p}})|0\rangle$, where $|0\rangle$ is the total vacuum state. The SCE band is partially occupied and the ground state in this case is given by:

$$|\Phi^*\rangle=\prod_{\alpha\mathbf{q}\leqslant\mathbf{q}_F}|\mathbf{q}\alpha\rangle|\mathrm{SCE}_{\mathbf{q}\alpha}\rangle$$

$$=\prod_{\alpha\mathbf{q}\leqslant\mathbf{q}_F}\{\hat{c}^{\dagger}_{\mathbf{q}\alpha}\Sigma_{\mathbf{p}}[B(\mathbf{p})/\sqrt{N}](\hat{e}^{\dagger}_{\mathbf{p}\uparrow}\hat{S}_{0,\mathbf{q}-\mathbf{p}}+\hat{e}^{\dagger}_{\mathbf{p}\downarrow}\hat{S}_{1,\mathbf{q}-\mathbf{p}})\}|0\rangle,$$

where the wave function $|\Phi^*\rangle$ should be totally antisymmetrized because this state is formed by fermion states. The Dirac sea is transformed in such a way that at $T=0$, the SCE states in $|\Phi^*\rangle$ are occupied without production of SCE particle-hole pairs. The occupation of these SCE states is produced by the unoccupation of some noncoupled charged modes at the top of the valence band which have, in this phase, a larger energy. As a consequence, SCE states coexist at E_F with charged modes noncoupled to the spin-fluctuation waves [see Fig. 1(d)]. The conducting properties of this *D* phase become again those of a metallic material. The difference between the *B* and *D* phases [compare Figs. 1(b) and (d)] is that in *B* there are only SCE states at E_F, while in *D*, SCE states and noncoupled charged modes are located at E_F (the latter, however, in less number). The relation between the number of noncharged modes and SCE states at E_F is a feature which has crucial influence in the low-energy properties, and depends on the narrowness of the corresponding bands.

The coexistence, in this *D* phase, of $\hat{c}^{\dagger}_{\mathbf{q}\alpha}|0\rangle$ modes and SCE states at E_F, implies that the phonon relaxation is governed by the intraband processes of the types $|\langle \mathrm{SCE}_{\mathbf{k}\alpha}|H_{e\text{-}ph}|\mathrm{SCE}_{\mathbf{k}\alpha}\rangle|^2$ and $|\langle 0|\hat{c}_{\mathbf{k}\alpha}H_{e\text{-}ph}\hat{c}^{\dagger}_{\mathbf{k}'\alpha}|0\rangle|^2$, and the umklapp processes of the type $|\langle \mathrm{SCE}_{\mathbf{k}\alpha}|H_{e\text{-}ph}\hat{c}^{\dagger}_{\mathbf{q}\alpha}|0\rangle|^2$. Therefore the conductivity cannot be expressed by means of additive formulas for each band [i.e., $\sigma\neq\Sigma_i(e^2n_i\tau_i/m_i^*)$] due to the existence of nonvanishing umklapp processes between SCE states and single charged states such as $\hat{c}^{\dagger}_{\mathbf{k}\alpha}|0\rangle$. However, the strength of the umklapp scattering is necessarily smaller than that of the SCE states (although nonvanishing) because the corresponding mixed matrix elements are different from zero due to the action of the electron-phonon interaction terms assisted by spin fluctuations. Obviously, these spin-fluctuation-assisted electron-phonon terms are smaller than those provided by the direct $\hat{H}_{e\text{-}ph}$. Therefore the conduction behavior of the *D* phase is more standard than that of *B*, since the presence of SCE states and noncoupled charged states at E_F activates the interband inelastic scattering. The influence of these interband phonon interactions implies that τ^{-1} in the *D* phase is close to that of the Kondo lattice with the features of a normal heavy-fermion metal.

Relation of this D phase with the heavy-fermion metallic state. An interesting analysis of this phase is the relation with the heavy-fermion state. Strictly speaking, the heavy-fermion metals are conducting compounds whose charge carrier gas present an anomalously large effective heat (between 100 and 2000 times larger than that of the free-electron gas).[3,5,26] The origin of such heavy-fermion feature, common to some metals, is still strongly debated. However, the spin-

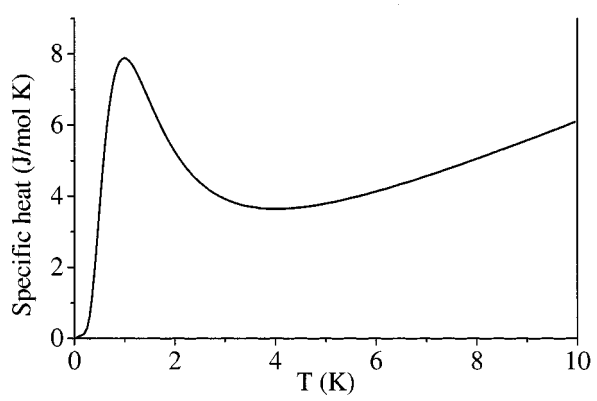

FIG. 2. $C(T)$ for $\delta=8$ meV and $X-E_F=0.2$ meV.

fluctuation influence seems to be the most extensively accepted origin (see for instance, Refs. 3, 4, 26, and 27). In any case, this property is not acquired through a quantum phase transition, as occurs in the different phases described above. It corresponds to a gradual property which can be present in any Kondo lattice according to how the magnetic bosons influence the charges located in states close to E_F. This influence clearly appears in the temperature evolution of the system specific heat. In Fig. 1, one can see that the D phase corresponds to a conductor whose specific heat can be strongly affected by the presence of the SCE states. In order to obtain the possible heavy-fermion feature, the SCE density of states (DOS) can be modelized by a narrow Lorentzian curve: $N_{\mathrm{SCE}}(\omega)\approx(2N/\pi)\,\delta_{\mathrm{SCE}}/[(\omega-X)^2+\delta_{\mathrm{SCE}}^2]$. Then, the SCE states in the D phase are occupied up to a level (E_F^*) that is given by: $E_F^*=X-\delta_{\mathrm{SCE}}\cot[\pi M/N]$, M being the number of occupied SCE states and N the number of crystal unit cells. In the D phase, E_F^* coincides with the true E_F of the system. In these conditions, the enhancement of the specific heat with respect to that of the free-electron gas can be calculated by means of the thermodynamic relation $C(T)=-T(\partial^2F/\partial T^2)$, where F is the free energy defined by $F=-Nk_\beta T\ln Z$, and Z is the partition function considering the vacuum state $|\mathrm{GS}\rangle$ and the $|\mathrm{SCE}_{\mathbf{k}\alpha}\rangle$ states. The resulting specific heat of this D phase, with the assumption of narrow SCE bands, can easily be obtained by means of the above systematic and its expression is

$$\frac{C(T)}{C^0(T)}=\frac{m^*}{m}\simeq 1+\frac{3}{4\pi^2}\,\frac{(X-E_F)^2\delta}{(K_BT)^3\cosh^2\left(\dfrac{X-E_F}{2K_BT}\right)}, \quad (37)$$

where δ is the width of the conduction band arising from the energy dispersion of $\hat{H}_{kinetic}$. Figure 2 shows $C(T)$ from Eq. (37). $C(T)$ thus deduced can be thousands of times larger than that of conventional metals. The main characteristic of this electronic specific heat is that at low temperatures ($\simeq 2$ K) there is a maximum, while for T larger than 4 K, $C(T)$ is linear as any metal. A similar behavior appears in several uranium compounds such as UBe_{13}.[5,26]

Let us analyze the resulting $C(T)$ at low temperatures, within the interval $0<k_BT<10(X-E_F)$. The above T interval can be between $0<T<10$ K if one considers standard values for δ and $X-E_F$ (see Fig. 2). According to the above expression, $C(T)$ presents an inflexion point at roughly $k_BT\simeq\frac{1}{6}(X-E_F)$; a maximum for $k_BT\approx 0.31(X-E_F)$ (in Fig. 2 this maximum is ≈ 1 K); and for $k_BT=10(X-E_F)$, $C(T)\approx C^0(T)$. For temperatures lower than the maximum, the above expression of $C(T)$ can be approximated to a polynomial function. Actually, in the interval $0<K_\beta T<\frac{1}{6}(X-E_F)$ Eq. (37) can be approximated by the following equation:

$$\frac{C(T)}{\gamma T}\approx 1+\frac{0.05\delta}{X-E_F}-\frac{1.75(k_BT)\,\delta}{(X-E_F)^2}+\frac{14.61(k_BT)^2\delta}{(X-E_F)^3}, \quad (38)$$

where the γ parameter is the standard linear coefficient of the specific heat corresponding to $C^0(T)$. In a previous paper,[18] I determined $C(T)$ by means of the first terms of the Sommerfeld theory of the specific heat in metals and I gave a polynomial expression. On the other hand, there is experimental evidence for some U compounds[4] (concretely UBe_{13}) showing how the specific heat at low temperatures increases polynomically with T. From expressions (37) and (38) for $C(T)$ and the results of Fig. 2, one can see that $C(T)$ can be thousands of times larger than in the normal phases of conventional metals. Therefore the main feature of the heavy-fermion state can be explained by the partial occupation of the SCE bands. The methodology described above can also determine $C(T)$ for the phases A, B, and C.

VII. COMPARISION WITH SOME PREVIOUS ANALYSES

Since some years ago, several variational and perturbative analysis of the $s-f$ Hamiltonian in the Kondo limit have been realized.[6,7,28–30] The Kondo limit allows to consider a spin field within a fixed $S=1/2$ spin representation where the spin direction fluctuations generate a boson gas. The interaction of this spin-wave gas with the conduction electrons becomes the reason and the origin of a rich phenomenology: Kondo lattice phenomena, heavy-fermion state, competence and concomitance between antiferromagnetism and superconductivity, etc. Some of the above cited works analyze the electronic gas spectrum[6,30] and others separately determine the fermionic and bosonic gas spectra.[28,29] On the contrary, in our model,[16–18] we approximately determine the many-body eigenstates of the $s-f$ Hamiltonian considering the coupling of the fermionic and bosonic gas forming composite fermionic states which we have named strong correlated states (SCE). The operational kind of the Kondo Hamiltonian suggests this coupling in a natural way, which is used in several other previous papers.[7,9,10] In these papers, similar associations between fermion charged modes and bosonic spin fluctuation states are utilized for obtaining composite fermions as those of the SCE spectra of Fig. 1.

The variational procedures are usually used in heavy-fermion systems[2,3,6,7,30] because with these methods one can approximately obtain a diagonalization of the many-body Hamiltonian eluding some possible convergence problems which the perturbative theories would produce. The variational analyses[6,30] consider many-electron trial wave functions, and they obtain an effective Hamiltonian whose diagonalization yields two effective bands of electrons similar to those of the perturbative study of Ref. 28. These bands can be split by a gap, and are generated by the hybridization of

extended electron bands with the lattice of localized *f* levels. The hybridization implies a certain delocalization of the *f* states which partially contribute to the bands, and therefore the electron hopping among different *f* electron atoms can occur. The probability of appearance of this hopping increases when one of the two bands tends to be more than half filled. As a consequence, the number of double f^2 configurations tends to vary in the electron conduction. These *f* intersite electronic transferences can imply a contradiction in the Kondo limit theory.[7] Therefore the variational calculations are usually considered for band occupations that minimize the effects of these *f* transferences. However, the Kondo effect arises from the thermal occupation of the *f* peaks in the DOS. Therefore this conduction effect should be explained by the movement of the electrons in the part of the band with strong *f* component and, on the contrary, the calculation of these bands is usually obtained fixing the numbers of single f^1 and double f^2 configurations. In our model, the Kondo peaks near E_F arise from the SCE states whose *f* component corresponds to the spin-wave fluctuations developed in the *f* spin field. Therefore the conduction electron movements through the SCE states occur maintaining intact the Kondo limit condition in all phases described in Sec. VI.

Some perturbative analyses of the Kondo lattices apply a mean-field theory to magnetically ordered Kondo lattices.[28] Other studies[29] deal with a ''poor man scaling'' approach[23] for obtaining the renormalized magnetic parameters and band dispersion of magnons. The first study[28] is based on the one-body DOS of the ground state of the interacting system, and, in Ref. 29, the spin-wave spectrum and the renormalized interacting parameters in magnetically ordered systems are given (the paramagnetic spin field is not worked because within perturbative scheme the authors considered complicated this magnetically nonordered case). In our analysis: (i) we determine the ground state and the excited many-body states (the SCE spectra) in the Kondo lattice which are obtained from a variational procedure, and (ii) the SCE spectra correspond to many-body states based on the coupling among charged modes and neutral bosons in paramagnetic and antiferromagnetic spin field structures. However, although the procedures of our analysis and those of Irkhin and Katsnelson (IK) are different, our results seem to be qualitatively compatible with theirs. The Kondo resonance just above E_F given in IK papers[28] could be related with the peaks arising from the SCE states (see Fig. 1) (obviously, this relation cannot be interpreted as a coincidence due to the different nature of this resonance and that of the SCE states). Therefore the electronic structure of phase *D* of Fig. 1, described as normal metallic Kondo lattice phase presents some similarity with the IK results,[28] because in the Fermi level, there are both extended charged modes and states arising from the dynamics of *f*-spin field. The given DOS (Ref. 28) corresponds to a band occupation less than half filling, but it is clear that in the half-filling limit the Δ_c gap of Fig. 1 of my calculation could also appear in these previous calculations.[28] Therefore the insulating Kondo lattice phase of Fig. 1(a), described in Sec. VI, could also be deduced as a consequence of the IK calculation. The heavy-fermion state from perturbative treatments of the Kondo lattice effects could be justified by the thermal occupation of *f* peaks of the DOS just above E_F, and from our variational insight this state is interpreted as depending on the energy location of the SCE states. In addition, in these cited papers[28] it is also concluded that instabilities of the ground state can be reliable. In Sec. VI, I describe several phase transitions which are compatible with this conclusion. On the other hand, a small gap in the magnon spectrum appears in previous calculations[29] in the case of antiferromagnetic spin field. This gap can unequivocally be related with the spin gap (Δ_s) of Fig. 1 because Δ_s arises from the Kondo and RKKY effects in the SCE states which, as said above, do have a neutral boson component of the same nature as the IK magnon structure. On the other hand, I have not been able to find resemblance between the *B* phase, where the electron-hole pairing is more probable, and the pattern yielded by the analyses of previous literature.[7,6,27–30]

VIII. CONCLUDING REMARKS

I have presented here a calculation of the spectrum of the Kondo lattices. This is made considering a model already explained in previous papers.[16–18] The essential difference with those calculations[16–18] is that only the renormalized Kondo term was considered to calculate the SCE spectra, whereas in the present work the SCE spectra is determined by including both the renormalized Kondo term and the induced RKKY Hamiltonian. From the spectra of the SCE bands (one of them corresponding to holes and another of particles) we describe the different phases which can appear when the density of states at E_F and the Kondo coupling parameter *J* of the initial Hamiltonian (1) are modified. For a given D_F four phases can appear. For small *J* values, the system is a small-gap insulator. Increasing *J*, a first insulator-conductor transition occurs. The charge-carrier relaxation times in this conducting phase are governed by the interchange of phonons between strongly correlated SCE states. When increasing *J* further a different insulating phase appears, and for even larger *J* a second insulating-conducting transition can be produced. In the final conducting phase (*D*), the conductivity is standard even in the case of narrow SCE bands. This is so, because in the *D* phase both intraband and interband inelastic processes can be produced. Therefore this *D* phase presents a normal conductivity similar to other normal (nonsuperconducting) heavy-fermion metals. The main heavy-fermion feature, namely, the huge electronic specific heat, is obtained for small SCE bandwidth δ_{SCE}. Thus the temperature evolution and values (in order of magnitude) of the specific heat of paradigmatic heavy-fermion materials such as UBe_{13} and $CeAl_3$ could be justified by the occupation of these SCE states.

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