Low-energy excitation spectra and excitonic condensate state in strong correlated antiferromagnetic systems

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The strongly correlated antiferromagnetic lattices can be the scenario for different states of matter. The interactions causing the different situations within these systems are the Kondo exchange and the Heisenberg interaction within a localized spin field. In this work, we analyze the low-energy excitation states of such lattices in any dimension, considering these two interactions in an antiferromagnetic insulator background. These states can be obtained from the associations of fermionic states with spin fluctuation waves. Such composite states interact via the two types of exchange, and their locations and $E_{\mathbf{k}}$ dispersions allow one to analyze the main features of the system. For certain values of the bandwidth of the noninteracting system (δ) and the Kondo coupling parameter (J_0), these composite states either are located within the antiferromagnetic gap, this implying a decrease in the insulating character, or can cross the Fermi level and a quantum phase transition can appear. Some denominated Kondo insulators and the normal state of some antiferromagnetic superconductors might be explained within this model. On the other hand, the charged-particle–magnon mixed states based on electrons and holes present attractive interactions and can then produce magnetic excitons. When these magnetic exciton states are located in the insulating gap, they constitute the lowest energy excitation spectra of the system. In an extreme case, the attractive interaction between the partners of these excitons can be the cause of the appearance of a new phase that presents structural similitude with an insulating Bose-Einstein condensate and a thermodynamic behavior similar to that of the BCS states. The special conditions for the appearance of this condensate are analyzed.

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I. INTRODUCTION

The determination of the low-lying excitations of strongly correlated (SC) systems has revealed many interesting properties of nonconventional new materials.[1–7] These SC systems present peculiar features concerning electrical conductivity and magnetic ordering behavior in such a way that these physical properties are inextricably mixed, and it is particularly difficult to put forward arguments that can separately explain each of them.[1,3–7] In this paper, we perform an analysis of the low-energy excitation states of a Kondo lattice in which the extended conduction-band electrons are immersed in an antiferromagnetic localized interacting spin field. In this context, the interplay between the Heisenberg correlations and the Kondo exchange allows one to explain the large narrowing of the conduction band, which is the origin of the heavy-fermion behavior in some SC systems.[8–13] The concomitance of these two magnetic interactions allows one to connect, in some of these compounds, the existence of different types of energy condensation states with the heavy-fermion properties.[14] In a second place, we address our attention to the study of different states of matter[12,15–21] that can be produced by the dynamic Kondo lattice acting on an insulating antiferromagnetic background. These many-body states can appear when the excitation single-particle states are close to E_F, implying the proximity of different phase transitions. Some of these phases present anomalous electrical-resistance behaviors:[15–17] they can be exotic superconductors,[22–24] Bose condensate states such as those that appeared in $TlCuCl_3$,[25–27] and other different coherent states whose origin is due to several fermionic couplings. While experiments have been expeditious in finding and characterizing materials that show these phenomena,[8,13,16,17,28–30] a theoretical treatment where the Kondo and RKKY-Heisenberg effects play a competitive role for obtaining these antiferromagnetic energy-condensed states is, nevertheless, far from being well formalized.[8,14,22,23,31] The theoretical analysis of this double exchange and its consequences for the SC systems is the global objective of this paper.

The structure of this paper is as follows. Section II deals with the Hamiltonian model within the electron-hole operators. In Sec. III, we give the trial wave functions for the excitation states of the system whose calculation is the main objective of the first part of this paper. In Sec. IV and in the Appendix, the variational method for determining these states and their spectra is developed. In the following part, we describe the results of the spectra of the electron-magnon mixed states. Section VI deals with the electron-hole interactions of these coupled states, and we define and analyze the magnetic exciton condensate (MEC) that appears when the total energy of the excitonic system becomes less than that of the initial ground state. In this section, we also give the conditions for the appearance of this MEC state, and finally, we summarize the study and give some concluding remarks.

II. HAMILTONIAN MODEL

We start from an insulating Kondo lattice (KL) Hamiltonian in which we consider an extended band of electrons

submerged in an antiferromagnetic spin-1/2 field in a bipartite lattice, where a Heisenberg interaction is concurrent with the Kondo lattice exchange.[11,15,19,32,33] A general expression for this Hamiltonian of the KL system is[15,32,34,35]

$$H = \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + \frac{J_0}{2\sqrt{N}} \sum_{\mathbf{k}\mathbf{k}'\alpha\beta} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}'\beta} \vec{\sigma}_{\alpha\beta} \cdot \vec{S}_{\mathbf{k}'-\mathbf{k}} + \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where the kinetic term corresponds to the extended band, the spin operators $\vec{S}$ correspond to the localized spin field, J_0 is the Kondo exchange energy, J_{ij} are the Heisenberg parameters ($J_{ij}=0$ for $i=j$), and $c^{\dagger}_{\mathbf{k}\alpha}(c_{\mathbf{k}\alpha})$ is the creation (annihilation) operator of the conduction electrons. We can use the particle-hole representation of this Hamiltonian, and this can thus be written as[35–37]

$$\begin{aligned} H &= H_{kinetic} + H_{Kondo} + H_H \\ &= 2\sum_{\mathbf{q}} \varepsilon_{\mathbf{q}} + \sum_{\mathbf{p}\alpha} \varepsilon_{\mathbf{p}} e^{\dagger}_{\mathbf{p}\alpha} e_{\mathbf{p}\alpha} + \sum_{\mathbf{q}\alpha} (-\varepsilon_{\mathbf{q}}) h^{\dagger}_{\mathbf{q}\alpha} h_{\mathbf{q}\alpha} + \frac{J_0}{2N^{1/2}} \sum_{\mathbf{q}\mathbf{q}'} \{(h^{\dagger}_{\mathbf{q}\uparrow} h_{\mathbf{q}'\uparrow} - h^{\dagger}_{\mathbf{q}\downarrow} h_{\mathbf{q}'\downarrow}) S^{z}_{\mathbf{q}'-\mathbf{q}} - h^{\dagger}_{\mathbf{q}\uparrow} h_{\mathbf{q}'\downarrow} S^{-}_{\mathbf{q}'-\mathbf{q}} - h^{\dagger}_{\mathbf{q}\downarrow} h_{\mathbf{q}'\uparrow} S^{+}_{\mathbf{q}'-\mathbf{q}}\} \\ &+ \frac{J_0}{2N^{1/2}} \sum_{\mathbf{p}\mathbf{p}'} \{(e^{\dagger}_{\mathbf{p}\uparrow} e_{\mathbf{p}'\uparrow} - e^{\dagger}_{\mathbf{p}\downarrow} e_{\mathbf{p}'\downarrow}) S^{z}_{\mathbf{p}'-\mathbf{p}} + e^{\dagger}_{\mathbf{p}\uparrow} e_{\mathbf{p}'\downarrow} S^{-}_{\mathbf{p}'-\mathbf{p}} + e^{\dagger}_{\mathbf{p}\downarrow} e_{\mathbf{p}'\uparrow} S^{+}_{\mathbf{p}'-\mathbf{p}}\} + \frac{J_0}{2N^{1/2}} \sum_{\mathbf{p}\mathbf{q}} \{(e^{\dagger}_{\mathbf{p}\uparrow} h^{\dagger}_{\mathbf{q}\downarrow} - e^{\dagger}_{\mathbf{p}\downarrow} h^{\dagger}_{\mathbf{q}\uparrow}) S^{z}_{-\mathbf{p}-\mathbf{q}} + e^{\dagger}_{\mathbf{p}\uparrow} h^{\dagger}_{\mathbf{q}\uparrow} S^{-}_{-\mathbf{p}-\mathbf{q}} \\ &+ e^{\dagger}_{\mathbf{p}\downarrow} h^{\dagger}_{\mathbf{q}\downarrow} S^{+}_{-\mathbf{p}-\mathbf{q}}\} + \frac{J_0}{2N^{1/2}} \sum_{\mathbf{p}\mathbf{q}} \{(h_{\mathbf{q}\downarrow} e_{\mathbf{p}\uparrow} - h_{\mathbf{q}\uparrow} e_{\mathbf{p}\downarrow}) S^{z}_{\mathbf{p}+\mathbf{q}} + h_{\mathbf{q}\downarrow} e_{\mathbf{q}'\downarrow} S^{-}_{\mathbf{p}+\mathbf{q}} + h_{\mathbf{q}\uparrow} e_{\mathbf{p}\uparrow} S^{+}_{\mathbf{p}+\mathbf{q}}\} + \sum_{ij} J_{ij} \left(S^{z}_i S^{z}_j + \frac{1}{2} S^{+}_i S^{-}_j + \frac{1}{2} S^{-}_i S^{+}_j \right), \end{aligned} \tag{2}$$

where $e^{\dagger}_{\mathbf{p}\uparrow\downarrow} = c^{\dagger}_{\mathbf{p}\uparrow\downarrow}$ for $\varepsilon_{\mathbf{p}} > E_F$, $h^{\dagger}_{\mathbf{q}\uparrow\downarrow} = c_{-\mathbf{q}\downarrow\uparrow}$ for $\varepsilon_{\mathbf{q}} \leqslant E_F$, and $S^{\pm}_i = S^{x}_i \pm i S^{y}_i$.

III. ANSATZ FOR EXCITATION STATES

We will analyze the energy excitations produced by removing a single electron (or hole) and one spin-field excitation corresponding to a magnon. The ground state of the mixed system is $|\text{g.s.}\rangle = |\Phi\rangle|\text{AF}\rangle$, where $|\Phi\rangle$ is the vacuum of charged modes and $|\text{AF}\rangle$ is that corresponding to the antiferromagnetic spin field. The third Kondo term of Eq. (2) ($e^{\dagger}h^{\dagger}S$) prevents the possibility of the ground state of $H_{kinetic}+H_{Kondo}$ being the same as that of $H_{kinetic}$. However, to first order, the energies of these two ground states are equal. Therefore, the one-particle excitation charged mode is then defined as $e^{\dagger}_{\mathbf{p}\uparrow\downarrow}|\Phi\rangle$ and $h^{\dagger}_{\mathbf{q}\uparrow\downarrow}|\Phi\rangle$. On the other hand, we assume an antiferromagnetic localized spin-field vacuum state in a double antiferromagnetic structure, which can be written as follows

$$|\text{AF}\rangle = \prod_i |\sigma_i; +\rangle \prod_j |\sigma_j; -\rangle, \tag{3}$$

where

$$|\sigma_i; +\rangle = \cos(\theta_i/2)|1/2; +1/2\rangle + \sin(\theta_i/2) e^{-i\phi_i} |1/2; -1/2\rangle$$

and

$$|\sigma_j; -\rangle = \sin(\theta_j/2)|1/2; +1/2\rangle - \cos(\theta_j/2) e^{-i\phi_j} |1/2; -1/2\rangle.$$

These $\pm$ states are the spin eigenstates of the $\vec{S}\cdot\vec{n}_i$ operator, localized in the i site of a lattice of any dimension, whose eigenvalues are $\pm 1/2$, with $\vec{n}_i$ being an arbitrary quantization direction defined by the vector $\vec{n}_i = (\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i)$ and $\vec{S}$ the vectorial spin operator. Each i site of the $\pm$ sublattices is localized by a real lattice vector $\mathbf{R}_i$. The choice of a determined antiferromagnetic bipartite structure implies to fix the $\mathbf{R}_i$ vectors for each substructure [for instance, a possible simple cubic antiferromagnetic bipartite structure can be constructed by means of the following real vectors: $\mathbf{R}_i = (m\vec{e}_x + n\vec{e}_y + l\vec{e}_z)a$, where a is the cubic lattice parameter and $m+n+l$ is an even (odd) integer number for the sites of the $+$ $(-)$ sublattice, with m, n, and l being positive or negative integer numbers]. On the other hand, we consider that $J_{ij} > 0$ if the indices i and j correspond to different spin sublattices and $J_{ij} < 0$ if i and j are sites belonging to the same sublattice. Taking into account that $\langle \vec{S}_i \rangle = \frac{1}{2}\vec{n}_i$, the average value of $\langle H_H \rangle$ for any spin-1/2 lattice is $\frac{1}{4}\Sigma_{ij} J_{ij} \vec{n}_i \cdot \vec{n}_j$. Therefore, the minimal Heisenberg energy for any bipartite antiferromagnetic structure is $-\frac{1}{4}\Sigma_{ij}|J_{ij}|$ which corresponds to the average value of H_H when the $\vec{n}_i$ quantum directions of all i sites are equal. Therefore, henceforth we consider an only quantization direction for all i sites defined by the angles θ and ϕ (obviously in each $\pm$ substructure, the spin states is $\pm\frac{1}{2}$ measured in the $\vec{n}$ quantization direction). Within this spin field, the low-energy excitations are given by the one-magnon creation such as $S^{\pm}_{\mathbf{k}}|\text{g.s.}\rangle = N^{-1/2}\Sigma_j e^{i\mathbf{k}\cdot\mathbf{R}_j} S^{\pm}_j |\text{AF}\rangle$.

The charged modes, defined above, and the neutral magnetic bosons interact via Kondo and Heisenberg exchange. Therefore, we can construct an ansatz for these excitation

states of the system that is treated as a trial wave function which can be determined by a variational method.[15,33,36,37] Here, we only consider the excitations produced by removing a single electron of the charged part of the vacuum state and its coupling with the one-magnon state wave function. These trial wave functions can be written as

$$\alpha^{\dagger}_{\mathbf{k}\uparrow}|\mathrm{g.s.}\rangle = |\alpha^{(e)}_{\mathbf{k}\uparrow}\rangle = N^{-1/2}\sum_{\mathbf{p}} a_{\mathbf{p}} e^{\dagger}_{\mathbf{p}\downarrow} S^{+}_{\mathbf{k}-\mathbf{p}}|\mathrm{g.s.}\rangle, \tag{4}$$

$$\beta^{\dagger}_{\mathbf{k}\uparrow}|\mathrm{g.s.}\rangle = |\alpha^{(h)}_{\mathbf{k}\uparrow}\rangle = N^{-1/2}\sum_{\mathbf{q}} a_{\mathbf{q}} h^{\dagger}_{\mathbf{q}\downarrow} S^{+}_{\mathbf{k}-\mathbf{q}}|\mathrm{g.s.}\rangle, \tag{5}$$

$$\alpha^{\dagger}_{\mathbf{k}\downarrow}|\mathrm{g.s.}\rangle = |\alpha^{(e)}_{\mathbf{k}\downarrow}\rangle = N^{-1/2}\sum_{\mathbf{p}} a_{\mathbf{p}} e^{\dagger}_{\mathbf{p}\uparrow} S^{-}_{\mathbf{k}-\mathbf{p}}|\mathrm{g.s.}\rangle, \tag{6}$$

$$\beta^{\dagger}_{\mathbf{k}\downarrow}|\mathrm{g.s.}\rangle = |\alpha^{(h)}_{\mathbf{k}\downarrow}\rangle = N^{-1/2}\sum_{\mathbf{q}} a_{\mathbf{q}} h^{\dagger}_{\mathbf{q}\uparrow} S^{-}_{\mathbf{k}-\mathbf{q}}|\mathrm{g.s.}\rangle. \tag{7}$$

These states can be seen as associations of the spin fluctuations that appear in the localized spin field along with one electron (or hole) in a such a way that the intensity of their coupling is given by the $a_{\mathbf{p}}$ ($a_{\mathbf{q}}$) parameters and the signature of these associations is the fact that the quasimoment of the $\alpha_{\mathbf{k}}$ state is shared between the electron (or hole) and the magnon state. The calculation of the energies and wave functions corresponding to the $|\alpha^{(e)}_{\mathbf{k}\sigma}\rangle$ and $|\alpha^{(h)}_{\mathbf{k}\sigma}\rangle$ states along with the energy of $|\mathrm{g.s.}\rangle$ allows one to obtain an effective quasidiagonalization of the Hamiltonian in the Hilbert subspace formed from the α states.

IV. CALCULATIONS

The $a_{\mathbf{p}}$ ($a_{\mathbf{q}}$) parameters and the $E_{\mathbf{k}}$ spectra of the different α states of Eqs. (4)–(7) can be calculated by means of a variational method. The variational calculation of the total energies of the states is obtained by

$$E_{\mathbf{k}} = \frac{\langle \alpha_{\mathbf{k}\uparrow\downarrow}|H_{kinetic} + H_{Kondo} + H_H|\alpha_{\mathbf{k}\uparrow\downarrow}\rangle}{\langle \alpha_{\mathbf{k}\uparrow\downarrow}|\alpha_{\mathbf{k}\uparrow\downarrow}\rangle}. \tag{8}$$

First, we calculate $\langle H_{Kondo}\rangle$ (we give in the Appendix details of the intermediate steps of the calculation):

$$\begin{aligned}\langle \alpha_{\mathbf{k}\uparrow}|H_{Kondo}|\alpha_{\mathbf{k}\uparrow}\rangle &= -\frac{1}{2N^3}\sum_{\mathbf{p}\mathbf{p}'} a^{*}_{\mathbf{p}} a_{\mathbf{p}'} J_0 \sum_{\mu\nu\alpha} e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{\mu}} \\ &\times e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{R}_{\nu}} e^{i(\mathbf{k}-\mathbf{p}')\cdot\mathbf{R}_{\alpha}} \langle \mathrm{AF}|S^{-}_{\mu} S^{z}_{\nu} S^{+}_{\alpha}|\mathrm{AF}\rangle \\ &= -\frac{1}{8N^2}\sum_{\mathbf{p}\mathbf{p}'} a^{*}_{\mathbf{p}'} J_0 a_{\mathbf{p}} (2\cos^2\theta - \sin^2\theta),\end{aligned} \tag{9}$$

where the θ angle corresponds to the quantization direction of the spin field.

In a second place, we calculate $\langle H_H\rangle$ (see details in the Appendix) and the result is

$$\begin{aligned}\langle H_H\rangle &= \frac{1}{8N}\sum_{\mathbf{p}} a^2_{\mathbf{p}} \sum_{ij} |J_{ij}| \left(-1 + \frac{1}{2}\sin^2\theta\right) + \frac{1}{2N^2}\sum_{\mathbf{p}} a^2_{\mathbf{p}} \sum_{ij} |J_{ij}| \\ &\times \left(1 + \frac{1}{4}\sin^2\theta\right) + \frac{1}{8N^2}\sum_{\mathbf{p}} a^2_{\mathbf{p}} \sum_{ij} |J_{ij}| \cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}] \\ &\times \left(-1 + \frac{1}{2}\sin^2\theta\right).\end{aligned} \tag{10}$$

The average value of $H_{kinetic}$ is

$$\langle \alpha_{\mathbf{k}\uparrow}|H_{kinetic}|\alpha_{\mathbf{k}\uparrow}\rangle = \frac{1}{2N}\sum_{\mathbf{p}} a^{*}_{\mathbf{p}} \left(\varepsilon_{\mathbf{p}} + \sum_{\mathbf{q}} 2\varepsilon_{\mathbf{q}}\right) a_{\mathbf{p}} \left(1 - \frac{1}{2}\sin^2\theta\right). \tag{11}$$

The normalization of α states, $\langle \alpha_{\mathbf{k}}|\alpha_{\mathbf{k}}\rangle$, is

$$\langle \alpha_{\mathbf{k}}|\alpha_{\mathbf{k}}\rangle = \frac{1}{2N}\sum_{\mathbf{p}} |a_{\mathbf{p}}|^2 \left(1 - \frac{1}{2}\sin^2\theta\right). \tag{12}$$

Bearing in mind that

$$E_{\mathrm{g.s.}} = \langle \mathrm{g.s.}|H_{kinetic} + H_{Kondo} + H_H|\mathrm{g.s.}\rangle = \sum_{\mathbf{q}} 2\varepsilon_{\mathbf{q}} - \frac{1}{4}\sum_{ij} |J_{ij}|, \tag{13}$$

Eq. (8) can be written as

$$\begin{aligned}\sum_{\mathbf{p}\mathbf{p}'} a^{*}_{\mathbf{p}} \Bigg[\Bigg\{ E_{\mathbf{k}} - E_{\mathrm{g.s.}} - \varepsilon_{\mathbf{p}} - \frac{1}{N}\sum_{ij} f_1(\theta) \ |J_{ij}| \\ + \frac{1}{4N}\sum_{ij} |J_{ij}| \cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}] \Bigg\} \delta_{\mathbf{p}\mathbf{p}'} \\ + \frac{1}{4N} J_0 f_2(\theta) \Bigg] a_{\mathbf{p}'} = 0,\end{aligned} \tag{14}$$

where $f_1(\theta) = (1 + \frac{1}{4}\sin^2\theta)/(1 - \frac{1}{2}\sin^2\theta)$ and $f_2(\theta) = (1 + \cos^2\theta - 2\sin^2\theta)/(1 - \frac{1}{2}\sin^2\theta)$. The minimization of the energy $E_{\mathbf{k}}$ with respect to all $a_{\mathbf{p}}$ variational parameters of the trial wave functions leads to the following equation:

$$a_{\mathbf{p}} = \frac{\Delta_{\mathbf{p}}}{E_{\mathbf{k}} - E_{\text{g.s.}} - \varepsilon_{\mathbf{p}} - \frac{1}{N}\sum_{ij}|J_{ij}|f_1(\theta) + \frac{1}{4N}\sum_{ij}|J_{ij}|\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]}, \tag{15}$$

where $\Delta_{\mathbf{p}}$ is given by

$$\Delta_{\mathbf{p}} = -\frac{1}{4N}\sum_{\mathbf{p}'}\frac{J_0 f_2(\theta)\Delta_{\mathbf{p}'}}{E_{\mathbf{k}} - E_{\text{g.s.}} - \varepsilon_{\mathbf{p}'} - \frac{1}{N}\sum_{ij}f_1(\theta)|J_{ij}| + \frac{1}{4N}\sum_{ij}|J_{ij}|\cos[(\mathbf{p}'-\mathbf{k})\cdot\mathbf{R}_{ij}]}. \tag{16}$$

We notice that the cosine term of the above equation and Eq. (16) ($\cos[(\mathbf{p}'-\mathbf{k})\cdot\mathbf{R}_{ij}]$) can be considered as a small perturbation with respect to the remaining terms. As a consequence, an alternative simplified way to obtain $E_{\mathbf{k}}$ is to consider $E_{\mathbf{k}}$ at a first stage without accounting for these cosine Heisenberg effects and then to calculate these effects from the $a_{\mathbf{p}}$ parameters attained in this simplified calculation. This alternative procedure can be summarized by the following mathematical relations:

$$\Delta_{\mathbf{p}} = -\frac{J_0 f_2(\theta)}{4N}\sum_{\mathbf{p}'}\frac{\Delta_{\mathbf{p}'}}{E'_{\mathbf{k}} - \varepsilon_{\mathbf{p}'}},$$

where $E'_{\mathbf{k}} = E_{\mathbf{k}} - E_{\text{g.s.}} - (1/N)\Sigma_{ij}|J_{ij}|f_1(\theta)$. From these latter expressions, one can deduce that $\Delta_{\mathbf{p}} = \Delta_0$, and the equation for $\Delta_{\mathbf{p}} = \Delta_0$ can be written as

$$1 = -\frac{J_0 f_2(\theta)}{4N}\sum_{\mathbf{p}'}\frac{1}{E'_{\mathbf{k}} - \varepsilon_{\mathbf{p}'}}.$$

Considering a rectangular density of states with an effective bandwidth for the initial band and a half-filling occupation, we obtain that

$$E'_{\text{k}} = \Delta_{\text{AF}}/2 - \frac{\delta}{2}\exp\left(-\frac{2\delta}{J_0 f_2(\theta)}\right)$$

for $2 \geqslant f_2(\theta) \geqslant 0$, $E'_{\mathbf{k}} = \Delta_{\text{AF}}/2$ for $f_2(\theta) = 0^+$, and $E'_{\mathbf{k}} = \Delta_{\text{AF}}/2 + \delta/2$ for $0^- \geqslant f_2(\theta) \geqslant -2$, where Δ_{AF} is the antiferromagnetic gap included, as an input datum, in the $\varepsilon_{\mathbf{p}}$ band structure and δ is the initial effective bandwidth of the conduction band.

As a consequence, we deduce that for positive values of $f_2(\theta)$, the spectrum $E_{\mathbf{k}}$ corresponding to the α states is

$$E_{\mathbf{k}} = E_{\text{g.s.}} + \frac{\Delta_{\text{AF}}}{2} - \frac{1}{N}\sum_{ij}f_1(\theta)|J_{ij}| - \delta/2\exp\left(-\frac{2\delta}{J_0 f_2(\theta)}\right) + \Delta H_H. \tag{17}$$

Considering the normalization of the α states and including ΔH_H in Eq. (17), we have the following result for the $E_{\mathbf{k}}$ energy:

$$E^{(e)}_{\mathbf{k}} = E^{(h)}_{\mathbf{k}} = E_{\text{g.s.}} + \frac{\Delta_{\text{AF}}}{2} - \Omega + \frac{1}{N}\sum_{ij}|J_{ij}|f_1(\theta) - \frac{1}{4N}\sum_{\mathbf{p}}\frac{\Delta_0^2}{(\Omega+\varepsilon_{\mathbf{p}})^2}\frac{1}{N}\sum_{ij}|J_{ij}|\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}], \tag{18}$$

where

$$\Omega = \frac{\delta}{2}\exp\left(-\frac{2\delta}{J_0 f_2(\theta)}\right).$$

The α states based on hole excitations present an identical expression of their energies if the initial band satisfies the half-filling condition.

The analytical results of the $a_{\mathbf{p}}$ ($a_{\mathbf{q}}$) parameters and the $E_{\mathbf{k}}$ spectra are

$$E^{(e)}_{\mathbf{k}} = E_{\text{g.s.}} + \frac{\Delta_{\text{AF}}}{2} - \Omega + \frac{1}{N}\sum_{ij}f_1(\theta)|J_{ij}| - \frac{1}{4N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}|J_{ij}|\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}], \tag{19}$$

$$E^{(h)}_{\mathbf{k}} = E_{\text{g.s.}} + \frac{\Delta_{\text{AF}}}{2} - \Omega + \frac{1}{N}\sum_{ij}f_1(\theta)|J_{ij}| - \frac{1}{4N^2}\sum_{\mathbf{p}}a^2_{\mathbf{q}}\sum_{ij}|J_{ij}|\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}], \tag{20}$$

$$a_{\mathbf{p}} = \frac{\Delta_0}{\Omega + \varepsilon_{\mathbf{p}} - \frac{\Delta_{\text{AF}}}{2}}, \tag{21}$$

$$a_{\mathbf{q}} = \frac{\Delta_0}{\Omega - \varepsilon_{\mathbf{q}} - \frac{\Delta_{\text{AF}}}{2}}, \tag{22}$$

where Δ_0 is calculated from the normalization condition of α states (see below).

By inspection of this spectrum, we can draw the following conclusions.

(i) The Kondo exchange effects produce an exponential term $(-\Omega)$ which decreases the excitation energy of the α

states. The maximum value of the $f_2(\theta)$ factor is equal to 2, which corresponds to the "classical" solution—i.e., for $\theta=0$. The value of this factor is $2 \geqslant f_2(\theta) \geqslant -2$ for θ values between $\theta=0$ and $\theta=\pi/2$. This implies a sign change of the Kondo effects in the α states at $\theta=\arcsin\left(\sqrt{\frac{2}{3}}\right)$. These Kondo effects acquire at $\theta=\pi/2$ the maximum positive value $-\Omega \approx \delta/2$, which is obtained for the maximum negative value of $f_2(\theta)=-2$. Consequently, in order to consider the α states as the low-energy excitations of the system, only negative values of $-\Omega$ have a true physical meaning. Therefore, the quantum directions of the localized spins that allow the locations of the α states within the gap of the initial H_0 are in the interval $0 \leqslant \theta < \arcsin\left(\sqrt{\frac{2}{3}}\right)$. On the other hand, the spectra (19) and (20) are invariant before rotations of the spin quantization directions with respect to the z axis, since both the Kondo effects and the Heisenberg contributions in these spectra are independent of the azimuthal angle.

(ii) The term $(1/N)\Sigma_{ij} f_1(\theta)|J_{ij}|$ is a positive energy and is quantitatively the main contribution of the Heisenberg interaction to the spectra of the α states. This term leads to an increase of the antiferromagnetic gap between the occupied and unoccupied α states and, therefore, it can contribute to the enhancement of the insulating phase. This term takes the minimum value in the "classical" local spin states of the bipartite antiferromagnetic field and the maximum value is attained at $\theta=\pi/2$. When the Heisenberg interaction is considered to be induced by the Kondo interaction, the maximum value of the J_{ij} parameters is[38,39] $\propto J^2$. In this case, the Heisenberg effects in α states can directly compete with Kondo effects accounted for the Ω exponential term because these two effects can have different sign. Between these two terms along with the antiferromagnetic gap Δ_{AF} produce the different phases, since, in certain conditions, these contributions can lead the $E_{\mathbf{k}}$ spectra to be negative. In this case, another ground state and a new metallic phase appear.

(iii) The cosine term $(1/4N^2)\Sigma_{\mathbf{p}} a_{\mathbf{q}}^2 \Sigma_{ij}|J_{ij}|\cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}]$ gives a band character to the α states arising from the magnon structure. On the other hand, the functional dependence of the cosine term does not change with the quantization direction of the local spin states. This band can be narrow in the cases where the J_{ij} terms are small and short ranged. In these cases, the contribution to $E_{\mathbf{k}}$ of this term becomes less than that commented on in the former item. However, this contribution acquires importance when the other Heisenberg effects $[(1/2N)\Sigma_{ij} f_1(\theta)|J_{ij}|]$ and the exponential Kondo contribution Ω tend to compensate the antiferromagnetic gap. This importance arises from that, in these conditions, the band structure of the α states crosses the Fermi level and, consequently, this cosine term allows one to define the Fermi surface.

(iv) When $E_{\mathbf{k}}^{(e,h)} > E_{\mathrm{g.s.}}$ and the contribution corresponding to the J_{ij} terms of the $E_{\mathbf{k}}^{(e,h)}$ spectra is less in absolute value than Ω, the $\alpha_{\mathbf{k}}$ states are more accessible than the simple $e^{\dagger}|\Phi_0\rangle$ states of H_0. Obviously, we should also consider as low-energy excitations those states arising from the simple magnon states without contribution of charged modes. However, we are fundamentally interested in those states that can take part in the conduction properties; therefore, a specific analysis of the independent and noncoupled magnon spectra is not performed in this work. The pattern offered in the conducting scheme by this model is in qualitative agreement with other recent analyses,[18,40,41] since a third group of low-energy excitations could be constituted by α excitons composed by an $\alpha_{\mathbf{k}}^{(e)} - \alpha_{-\mathbf{k}}^{(h)}$ pair which is composed by two magnon plus a normal electron-hole pair. The exploration and analysis of this third group of low-energy pair states in these systems is one of the main objectives of the second part of this paper.

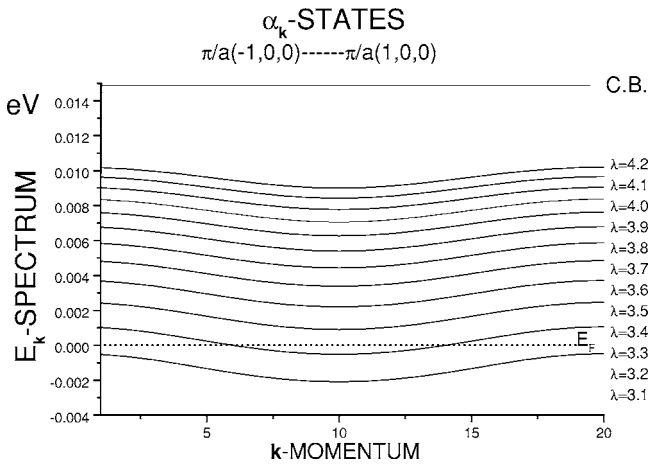

FIG. 1. Band structure of the α states corresponding to Eq. (28), for the $(\pm\pi/a,0,0)$-symmetry direction, considering a free-electron band for H_0. The calculations are performed by 21 points in each direction in such a way that for $k=1$ the corresponding point is $(-\pi/a,0,0)$ and for $k=20$ the point is the limit of the symmetry direction $(\pi/a,0,0)$. C.B. stands for the conduction-band bottom; E_F is the zero energy.

V. ANALYSIS OF THE $E_{\mathbf{k}}^{(e,h)}$ SPECTRA

The states (4)–(7) are completely determined by the spectra (19) and (20) and the $a_{\mathbf{p}}$ parameters, which depend on Δ_0. For an isotropic renormalized Kondo interaction, Δ_0 has to be calculated from the normalization condition of the α states. Bearing in mind Eq. (15), the value of Δ_0 is given by

$$\Delta_0^2 = 2\left(f_3(\theta)\int_0^{\delta/2} \frac{N_0(\varepsilon)d\varepsilon}{(\Omega+\varepsilon)^2}\right)^{-1}, \tag{23}$$

where $f_3(\theta)=1-\frac{1}{2}\sin^2\theta$. As a consequence of Eq. (23), Δ_0 depends on the different density of states yielded by each band structure $\varepsilon_{\mathbf{p}}$. Two extremes can be considered.

(i) The free-electron model ($\varepsilon_{\mathbf{p}}=\hbar p^2/2m^*$) for the starting noninteracting system of Hamiltonian (2). The strong correlation system properties seem to be contradictory with this simplified model. However, this assumption of including the free-electron model in Eq. (23) can be legitimated because the concatenation of the Kondo and RKKY-Heisenberg interactions are the causes that produce the heavy-fermion nature of the system (see Figs. 1–4), which is independent of the extended band condition for the kinetic part of the initial Hamiltonian.

(ii) The heavy-fermion band structure for the same kinetic part of Eq. (2). The narrow-band condition is not required in

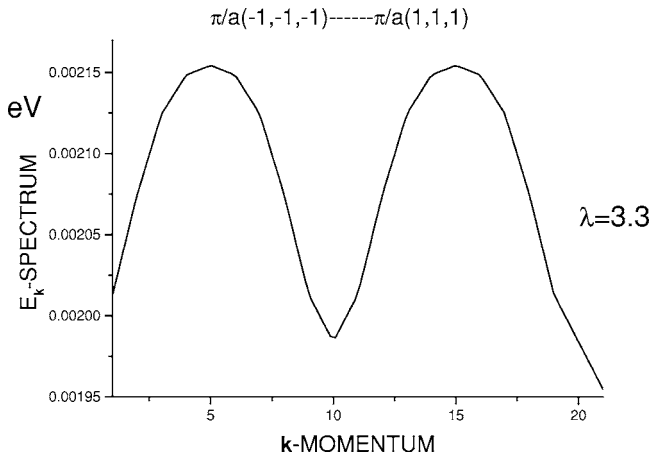

FIG. 2. Band structures for the $(\pi/a, \pi/a, \pi/a)$ direction corresponding to the free-electron band of H_0.

the starting kinetic Hamiltonian; however, in a certain sense it is another limit different from that of item (i). Therefore, we can consider that all realistic cases can be found between these two cases. In the cases of heavy-fermion systems, we can consider $\varepsilon_{\mathbf{p}}=\hbar\mathbf{v}_{\mathbf{p}}\cdot\mathbf{p}$ (Ref. 42) as an initial kinetic part of Eq. (2); even for the sake of simplicity we can consider that $\varepsilon_{\mathbf{p}}=\hbar v_F p$, v_F being the velocity of the particles at E_F.

In the case of a tridimensional free-electron system, we have the following expression:

$$\Delta_0^2=\frac{\pi^2\hbar^3\delta^{1/2}\exp\left(-\frac{2\delta}{J_0 f_2(\theta)}\right)}{f_3(\theta)m^{*3/2}a^3}, \tag{24}$$

where δ is the bandwidth of the initial extended band structure of H_0.

For a band structure appropriate for the heavy-fermion electron gas,[42] Δ_0 is given by

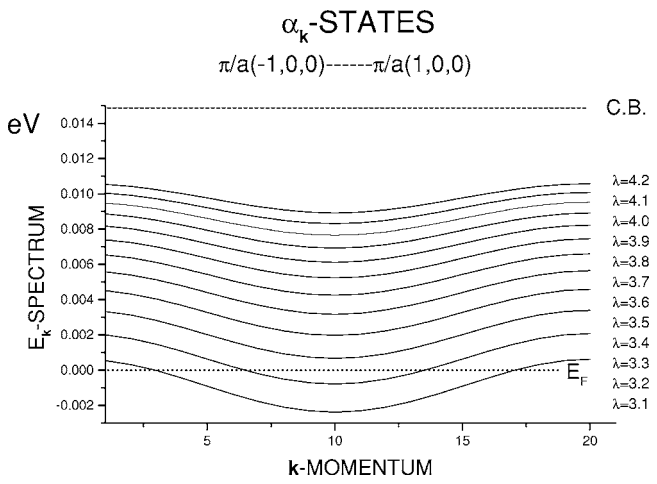

FIG. 3. As in Fig. 1 but for a Tomonaga-Luttinger band structure for H_0.

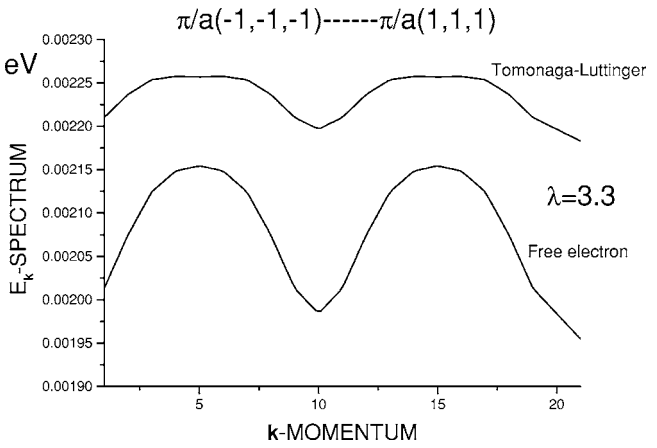

FIG. 4. Band structure of the α states in the (1,1,1)-symmetry direction (a) for free electrons and (b) Tomonaga-Luttinger band structure of the initial Hamiltonian H_0.

$$\Delta_0^2=\frac{4\pi\hbar^3 v_F^3\exp\left(-\frac{2\delta}{J_0 f_2(\theta)}\right)}{f_3(\theta)a^3\delta}. \tag{25}$$

With the determination of Δ_0 and the $a_{\mathbf{p}}$ and $a_{\mathbf{q}}$ coefficients, the low-energy states of the Hamiltonian (1) are determined for any dimension of the antiferromagnetic Kondo lattice.

The $E_{\mathbf{k}}^{(e,h)}$ spectra have four different components: Δ_{AF}, $\Omega=(\delta/2)\exp[-2\delta/f_2(\theta)J_0]$, $(1/2N)\Sigma_{ij}|f(\theta)|J_{ij}|$, and the cosine-term which is responsible for the appearance of the band structure of the $E_{\mathbf{k}}^{(e,h)}$ spectra. The true gap corresponding to the band structure of the α-excited states is given by $E_{\mathbf{k}}^{(e)}+E_{\mathbf{k}}^{(h)}$. The evaluation of the gap requires a knowledge of the J_{ij} terms corresponding to the antiferromagnetic structure which in the cases of heavy-fermion systems becomes short ranged: in some cases, extremely so. These J_{ij} parameters should then obey the law[43] $(1/N)\Sigma_{ij}|J_{ij}||\mathbf{R}_i-\mathbf{R}_j|^2<\infty$. Many expressions can be considered which satisfy this law; one of them for bipartite antiferromagnatic simple cubic structures could be $J_{ij}=-J(-1)^{m+n+l}\exp\{\gamma(1-\sqrt{m^2+n^2+l^2})\}$, where J is the nearest-neighbor RKKY-Heisenberg exchange parameter and γ a constant $\geqslant 1$. These J_{ij} parameters imply a determined antiferromagnetic structure; however, in any other antiferromagnetic case, an equivalent expression can easily be deduced by analogy. The methodology of our model is independent of the geometry of the bipartite antiferromagnetic structure, although the results, logically, depend on the distribution of J_{ij} parameters. If we consider the H_H Hamiltonian as induced by the Kondo effect over the localized spin field, it is well known that J of the J_{ij} expression is proportional to J_0^2, where J_0 is the initial Kondo exchange parameter.[38,39] Thus, it is easy to deduce that $(1/N)\Sigma_{ij}|J_{ij}|=cJ_0^2\delta$, where c is a positive constant and J_0 is a dimensionless parameter which is given in bandwidth (δ) units.

The band nature of the α states is, as indicated above, due to the cosine term, which can be written as

$$\hbar\omega_{\mathbf{k}} = -\frac{1}{4N^2}\,\mathrm{Re}\sum_j{}'|J_j|\exp(-i\mathbf{k}\cdot\mathbf{R}_j)\sum_{\mathbf{p}}\frac{\Delta_0^2\exp(i\mathbf{p}\cdot\mathbf{R}_j)}{(\varepsilon_{\mathbf{p}}+\Omega)^2}, \tag{26}$$

where J_j is the RKKY-Heisenberg interaction parameter between two spin states that are distanced by a $\mathbf{R}_j$ vector. $\hbar\omega_{\mathbf{k}}$ is the product of two different terms; the $\Sigma_{\mathbf{p}}$ term includes dependence on the charged-mode part of the composite states, while the $\Sigma_{\mathbf{k}}$ accounts for the dynamic of the magnon dispersion into $\hbar\omega_{\mathbf{k}}$. The calculation of the $\Sigma_{\mathbf{p}}$ of Eq. (26) depends on, as the case of the Δ_0 calculation, the initial extended band structure ($\varepsilon_{\mathbf{p}}$), and, for the cases in which the band structure only depends on the $\mathbf{p}$ modulus, it can be written as follows:

$$\frac{1}{4N}\sum_{\mathbf{p}}\frac{\Delta_0^2\exp(i\mathbf{p}\cdot\mathbf{R}_j)}{(\varepsilon_{\mathbf{p}}+\Omega)^2} = \frac{a^3\Delta_0^2}{8\pi^2R_iP_M^2}\int_0^1\frac{x\sin(xP_MR_i)}{(-x^2+A)^2}dx, \tag{27}$$

where a is the primitive cell parameter of the cubic crystal, $A=1+\exp(-2\delta/J_0f_2(\theta))$, and x is a dimensionless variable defined by $x=p/p_M$, where p_M is the $|\mathbf{p}|$ modulus of the largest wave vector. In the free-electron model it can be calculated by the following two equivalent expressions: $p_M=(3\pi^2n)^{1/3}$ and $p_M=(2m^*\delta)^{1/2}/\hbar$, with n being the density of charged particles. In the heavy-fermion-like band structure $p_M=\delta/2\hbar v_F$.

Including Eq. (27) in Eq. (26) and joining all expressions calculated in the former section, we can compose the band structure of the α states whose expression is given by

$$E_{\mathbf{k}}^{(e,h)} = \Delta_{\mathrm{AF}}/2 - \frac{\delta}{2}\exp\left(-\frac{2\delta}{J_0f_2(\theta)}\right) + cJ_0^2\delta - \sum_{m,n,l}I(m,n,l) \times|J_{m,n,l}|\cos(\mathbf{k}\cdot\mathbf{R}_{m,n,l}), \tag{28}$$

where $\mathbf{R}_{m,n,l}=(m\mathbf{e}_x+n\mathbf{e}_y+l\mathbf{e}_z)a$ and $|J_{m,n,l}|$ is the absolute value of the Heisenberg parameter between two spin-field states whose coordinates differ from a real vector defined by the integer numbers $m,n\ y\ l$. $I(m,n,l)$ in the case of free-electron band structure for $\varepsilon_{\mathbf{p}}$, is given by

$$I(m,n,l) = \frac{\sin(3.09\sqrt{m^2+n^2+l^2})}{6.18f_3(\theta)\sqrt{m^2+n^2+l^2}} - \frac{1}{2f_3(\theta)}\exp\left(-\frac{2\delta}{J_0f_2(\theta)}\right) \times\int_0^1\frac{\cos(3.09x\sqrt{m^2+n^2+l^2})dx}{1-x^2+\exp\left(-\frac{2\delta}{J_0f_2(\theta)}\right)}. \tag{29}$$

In the case of heavy electron band structure for $\varepsilon_{\mathbf{p}}$ it is given by

$$I(m,n,l) = \frac{\exp\left(-\frac{2\delta}{J_0f_2(\theta)}\right)}{3.09f_3(\theta)\sqrt{m^2+n^2+l^2}} \times\int_0^1\frac{x\sin(3.09x\sqrt{m^2+n^2+l^2})dx}{\left[1-x+\exp\left(-\frac{2\delta}{J_0f_2(\theta)}\right)\right]^2}. \tag{30}$$

The band center of Eq. (28) is fixed by the $\mathbf{k}$-independent terms, and the balance of the four contributions can lead to either the α states being excitations of the system or else being present in the ground state. The band nature provided by the $\mathbf{k}$-dependent term presents a narrow-band character (see Figs. 1–4). In Fig. 1, we give the $E_{\mathbf{k}}^{(e,h)}$ energy band of Eq. (28) for the symmetry directions $(\pm1,0,0)$ and different values of $\lambda=\delta/J_0$. The bandwidths arising from these α states are approximately 0.002 eV. These α bandwidths are obtained considering 0.37 eV for the effective initial band structure (δ) and 0.03 eV for the antiferromagnetic gap. Therefore, the narrow-band condition of the α states is clearly displayed in these results. In these figures, one can see that the widths of these band structures are dependent on λ in such a way that for increasing λ values one obtains decreasing bandwidths for $E_{\mathbf{k}}$. The $E_{\mathbf{k}}$-band structures present similar shapes for all λ values; however, the energies of the gravity centers of these bands increase with increasing values of λ. On the other hand, all band structures of Figs. 1 and 3 are within of this gap (the zero in Figs. 1–4 is the g.s. energy) for $\lambda\geqslant3.25$, and for λ values less than this value the α band crosses the Fermi level. Therefore, the bands of Eq. (28) for λ values larger than 3.25 are the lowest excitation states of Hamiltonian (1), and for values of this parameter less than this critical value, the α states are components of a new ground state of the system.

The spectra of Eq. (28) has different expressions for the $I_{m,n,l}$ functions according to the chosen band structure model for H_0. However, the final results arising from the free-electron model [Eq. (29)] are similar to those coming from the Luttinger-Tomonaga model, Eq. (30) (see Figs. 3 and 4). In both cases the heavy-fermion narrowness is obtained since the widths of these α bands are two orders less than that of the initial band structure.

VI. α EXCITONS AND EXCITON CONDENSATE STATE

The mechanisms of spin symmetry changes via dimerization and/or coupling of fermions, which allow one to avoid the constraints of the exclusion Pauli principle, have always been an issue largely dealt with by both theoretical and experimental points of view.[26,27,44–47] The possible consequences of these couplings are the energy condensates. These condensates can appear when the corresponding excitation vacuums of the systems are coherentlike states in which the average value of the creation pair operator is equal to that of the corresponding annihilation pair operator and different from zero.[25] In this case, a Bose-Einstein condensate arising from the fermionic gas of the solid is attained, which presents certain similitudes with the fermionic pair condensates

such as that recently observed in cooled true gases.[48]

In this section, we deal with the attractive interaction between α and β states. The α-β pairs can constitute excitons that, due to their mixed nature of charged modes and magnons, can be named magnetic excitons. The interaction between the partners of the magnetic exciton, $V_{\mathbf{kk}}$, can be attractive and therefore decreases the energy of an electron-hole α pair, $E^{(e)}_{\mathbf{k}}+E^{(h)}_{\mathbf{k}}$, which can be positive or negative (see Figs. 1 and 3).

A. Excitonic pair interaction

When an electron is excited to an $\alpha^{(e)}_{\mathbf{k}\sigma}$ state another $\alpha^{(h)}_{-\mathbf{k}-\sigma}$ state has to be occupied in order to conserve the total quasimomentum, spin, and charge. The Coulombian interaction between electron and holes α states is given by

$$V^{c}_{\mathbf{kk}'}=\langle\alpha^{(e)}_{\mathbf{k}\uparrow}\alpha^{(h)}_{-\mathbf{k}\downarrow}|V_{eh}|\alpha^{(e)}_{\mathbf{k}'\uparrow}\alpha^{(h)}_{-\mathbf{k}'\downarrow},$$

where

$$V_{eh}=-\sum_{\mathbf{p}_1\mathbf{q}_1\mathbf{q}}\sum_{\sigma}V_{\mathbf{q}}e^{\dagger}_{\mathbf{p}_1\sigma}h^{\dagger}_{(-\mathbf{q}_1-\mathbf{q})-\sigma}h_{-\mathbf{q}_1-\sigma}e_{(\mathbf{p}_1-\mathbf{q})\sigma}.$$

We then obtain

$$\begin{aligned}V^{c}_{\mathbf{kk}'}=&\sum_{\mathbf{p}_1\mathbf{q}_1\mathbf{q}}\frac{V_{\mathbf{q}}}{N^2}\sum_{\mathbf{p}_2\mathbf{p}_2'\mathbf{q}_2\mathbf{q}_2'}a^{*}_{\mathbf{p}_2}a_{\mathbf{p}_2'}a^{*}_{\mathbf{q}_2}a_{\mathbf{q}_2'}\\&\times\langle h_{\mathbf{q}_2\uparrow}e_{\mathbf{p}_2\downarrow}e^{\dagger}_{\mathbf{p}_1\uparrow}h^{\dagger}_{(\mathbf{q}_1-\mathbf{q})\downarrow}h_{\mathbf{q}_1\downarrow}e_{\mathbf{p}_1-\mathbf{q}\uparrow}e^{\dagger}_{\mathbf{p}_2'\downarrow}h^{\dagger}_{\mathbf{q}_2'\uparrow}\rangle\\&\times\langle S^{+}_{\mathbf{k}+\mathbf{q}_2}S^{-}_{\mathbf{p}_2-\mathbf{k}}S^{+}_{\mathbf{k}'-\mathbf{p}_2'}S^{-}_{-\mathbf{k}'-\mathbf{q}_2'}\rangle,\end{aligned}\tag{31}$$

where the spin average term is the two-magnon scattering induced by the Coulomb interaction. This magnon scattering depends on the quantization direction of the spin eigenstates of the two antiferromagnetic sublattices. We consider the quantum direction that implies a minimum value of the energies of the two components of the exciton (i.e., $E^{(e)}_{\mathbf{k}}+E^{(h)}_{-\mathbf{k}}$). This direction is $\vec{n}=(0,0,1)$, which *a priori* is the most favorable for obtaining the exciton condensate when considering the Coulombian interaction. In these conditions, in an antiferromagnetic bipartite lattice of $s=1/2$, the evaluation of the Coulombian interaction $V^{c}_{\mathbf{kk}}$ is relatively simple, though tedious, and the result is

$$\begin{aligned}V^{c}_{\mathbf{kk}'}=-\frac{1}{N^2}\Bigg[&\sum_{\mathbf{pq}}V_{\mathbf{q}}\sum_{j}a^{*}_{\mathbf{p}}a_{\mathbf{p}-\mathbf{q}}a^{*}_{\mathbf{Q}_j-\mathbf{p}}a_{\mathbf{Q}_j-\mathbf{p}+\mathbf{q}}\\&+\sum_{\mathbf{pq}}\sum_{j}e^{i\mathbf{Q}_j\cdot\mathbf{a}}V_{(\mathbf{k}-\mathbf{k}'-\mathbf{Q}_i)}a^{*}_{\mathbf{p}}a^{*}_{\mathbf{q}}a_{\mathbf{p}-\mathbf{k}+\mathbf{k}'+\mathbf{Q}_i}a_{\mathbf{q}-\mathbf{k}'+\mathbf{k}-\mathbf{Q}_i}\Bigg].\end{aligned}\tag{32}$$

The j index runs over the $\mathbf{Q}_j$ vectors, these vectors being either the origin ($\mathbf{Q}_j=0$) or any reciprocal vector obtained by means of the application of a punctual-group symmetry operation of the crystal to the magnetic $\mathbf{Q}$ vector,[49] the vector $\mathbf{a}$ is any minimal vector of the real primitive cell, and the factor $e^{i\mathbf{Q}_j\cdot\mathbf{a}}$ is $+1$ when $\mathbf{Q}_j$ is the origin and -1 when $\mathbf{Q}_j$ is any other vector defined above. This factor $e^{i\mathbf{Q}_j\cdot\mathbf{a}}$ is due to the bipartite antiferromagnetic structure of the spin field in such a way that $e^{i\mathbf{Q}\cdot\mathbf{R}_j}=+1$ (-1) for the $\mathbf{R}_j$ belonging to the up (down) antiferromagnetic sublattice. The concrete analysis of Eq. (32) should be completed by considering the $a_{\mathbf{p}}$ parameters which have been calculated in the variational calculation of the $E^{(e)}_{\mathbf{k}}$ and $E^{(h)}_{\mathbf{k}}$ spectra of Eqs. (19) and (20). The parameter $a_{\mathbf{p}}$ corresponds to states whose energy is larger than E_F, and therefore the energies ($\varepsilon_{\mathbf{Q}_i-\mathbf{p}}$) of the states whose parameters are $a_{\mathbf{Q}_i-\mathbf{p}}$ are less than E_F. Consequently, these parameters $a_{\mathbf{Q}_i-\mathbf{p}}$ should correspond to $\alpha^{(h)}$ states of Eqs. (5) and (7).

The first term of Eq. (32) vanishes when the j index corresponds to $\mathbf{Q}_j=0$ and the second term is only negative for $\mathbf{Q}_j=0$. The coupling of magnons and charged particles in the α states implies that the magnon scattering explained above modifies the Coulombian attractive interaction. $V^{c}_{\mathbf{kk}'}$ contains a contribution, which is independent of $\mathbf{k}$ and $\mathbf{k}'$, therefore is isotropic and negative, and another is dependent on $\mathbf{k}$ and $\mathbf{k}'$ and can be either positive or negative.

B. Conditions for the MEC appearance

In Figs. 1 and 3, we show the different locations of the $|\alpha^{(e)}_{\mathbf{k}\sigma}\rangle$ and $|\alpha^{(h)}_{-\mathbf{k}-\sigma}\rangle$ band states with respect to E_F. When the total energy of the global many-body system arising from the attractive interaction among the α states plus those coming from their $E_{\mathbf{k}}$ spectra of Eqs. (19) and (20) is less than zero, the appearance of a new ground state is ensured. The ground state can be a global magnetic exciton condensate $|\Phi_{MEC}\rangle$, which consists of excitons in a many-body state such as that of the BCS theory, and then, the following wave function can be proposed[44,45,50,51]:

$$|\Phi_{EC}\rangle=\prod_{\mathbf{k}\sigma}(u_{\mathbf{k}}+v_{\mathbf{k}}\alpha^{\dagger}_{\mathbf{k}\sigma}\beta^{\dagger}_{-\mathbf{k}-\sigma})|0\rangle,\tag{33}$$

where $\alpha^{\dagger}_{\mathbf{k}\sigma}$ and $\beta^{\dagger}_{-\mathbf{k}\sigma}$ are operators such that $\alpha^{\dagger}_{\mathbf{k}\sigma}|0\rangle=|\alpha^{(e)}_{\mathbf{k}\sigma}\rangle$ and $\beta^{\dagger}_{-\mathbf{k}-\sigma}|0\rangle=|\alpha^{(h)}_{-\mathbf{k}-\sigma}\rangle$, and the $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ parameters are determined by the BCS variational procedure.

The BCS-like Hamiltonian for this phase with excitonic pairing is

$$\begin{aligned}H_{eff}=&\sum_{\mathbf{k}\sigma}E^{(e)}_{\mathbf{k}}\alpha^{\dagger}_{\mathbf{k}\sigma}\alpha_{\mathbf{k}\sigma}+\sum_{\mathbf{k}\sigma}E^{(h)}_{\mathbf{k}}\beta^{\dagger}_{\mathbf{k}\sigma}\beta_{\mathbf{k}\sigma}\\&+\sum_{\mathbf{kk}'\sigma}V^{c}_{\mathbf{kk}'}\alpha^{\dagger}_{\mathbf{k}\sigma}\beta^{\dagger}_{-\mathbf{k}-\sigma}\beta_{-\mathbf{k}'-\sigma}\alpha_{\mathbf{k}'\sigma},\end{aligned}\tag{34}$$

where the $\mathbf{k}$ index runs over the magnetic first Brillouin zone and $V^{c}_{\mathbf{kk}'}$ is the attractive interaction given by Eq. (32).

Following the same methodology of the BCS theory, the energy of the MEC ground state of Eq. (33) is

$$E_{MEC}=4\sum_{\mathbf{k}}E_{\mathbf{k}}v^{2}_{\mathbf{k}}+2\sum_{\mathbf{kk}'}V_{\mathbf{kk}'}u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'},\tag{35}$$

where $E_{\mathbf{k}}$ is the spectrum of the α states given by Eqs. (19) and (20). By minimizing the above expression, one can obtain the standard BCS relations between the $v_{\mathbf{k}}$ and $u_{\mathbf{k}}$ parameters with the coherent gap ($g_{\mathbf{k}}=-\Sigma_{\mathbf{k}'}V^{(c)}_{\mathbf{kk}'}u_{\mathbf{k}'}v_{\mathbf{k}'}$) and with the $E_{\mathbf{k}}$ spectrum. The only differences with the BCS theory are the nature of the α pairs and the attractive inter-

action of Eq. (32). In the case of the dominant isotropic term of Eq. (32), the MEC gap is constant—i.e., $V^{(c)}_{\mathbf{kk'}}=V_0$—and it implies that $g_{\mathbf{k}}=g_0$. In this case, we have

$$V^c_{\mathbf{kk}}=V_0=-\frac{1}{N^2}\sum_{\mathbf{pq}}V_{\mathbf{q}}\sum_j a^{*(e)}_{\mathbf{p}}a^{(e)}_{\mathbf{p-q}}a^{*(h)}_{\mathbf{Q}_j-\mathbf{p}}a^{(h)}_{\mathbf{Q}_j-\mathbf{p+q}}, \quad (36)$$

where the coefficients $a^{*(h)}_{\mathbf{Q}_j-\mathbf{p}}$ and $a^{(h)}_{\mathbf{Q}_j-\mathbf{p+q}}$ correspond to holes and the others to electrons. Using the symmetry between electrons and holes, we have the following relations: $a^{*}_{\mathbf{Q}_j-\mathbf{p}}=a^{*}_{\mathbf{p}}$ and $a_{\mathbf{Q}_j-\mathbf{p+q}}=a_{\mathbf{p-q}}$.

$V_{\mathbf{q}}$ of Eqs. (32) and (36) can have several expressions according to the localization of the states of the initial noninteracting band of H_0. The most unfavorable initial condition for our study is to take into account plane waves for these initial band states and thus $V_{\mathbf{q}}=e^2(1-\delta_{\mathbf{q},0})/\epsilon\tau(q^2+\eta^2)$, τ being the system volume. Other expressions for $V_{\mathbf{q}}$ arising from other more localized wave functions for the initial band states of H_0 would yield other results. However, we prefer to consider in this part of the analysis the same conditions as those considered in the spectra of α states [Eqs. (19) and (20)]. As a consequence, we obtain that

$$V_0=-\frac{n\tau}{(2\pi)^6\epsilon N^2}\int\int\frac{e^2}{(\mathbf{p}-\mathbf{p'})^2+\eta^2}\frac{\Delta_0^2}{(\varepsilon_{\mathbf{p}}+\Omega)^2}\times\frac{\Delta_0^2}{(\varepsilon_{\mathbf{p'}}+\Omega)^2}d^3pd^3p', \quad (37)$$

where n represents the number of $\mathbf{Q}_i$ vectors, obviously depending on the dimension of the magnetic lattice. Equation (37) is converted into a double single integral if one considers band structures depending on $|\mathbf{p}|$. For free-electron band structures for $\varepsilon_{\mathbf{p}}$ we obtain that

$$V_0=-\frac{60.8}{N\varepsilon_r\exp(-2\lambda)}\int_0^1\frac{ydy}{[-y^2+1+\exp(-\lambda)]^2}\times\int_0^1\frac{x\ln\left|\frac{(x-y)^2+\kappa^2}{(x+y)^2+\kappa^2}\right|dx}{[-x^2+1+\exp(-\lambda)]^2}, \quad (38)$$

where x and y are dimensionless integration variables and $\kappa\approx\eta/p_M$, $\lambda=2\delta/J_0f_2(\theta)$, and ε_r is the dielectric constant. The results of NV_0 of Eq. (38) are given in eV.

The E_{MEC} energy of Eq. (35) for totally unoccupied α bands is

$$E_{MEC}=2\sum_{\mathbf{k}}\left(E_{\mathbf{k}}+\frac{E^2_{\mathbf{k}}}{(E^2_{\mathbf{k}}+g_0^2)^{1/2}}\right)-\frac{2g_0^2}{|V_0|}, \quad (39)$$

where g_0 is the isotropic coherent gap, which is given by $g_0=|V_0|\Sigma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}$; V_0 is the isotropic part of the interaction given in Eq. (32). The MEC state appearance requires that $g_0>0$ along with the energy of Eq. (39) be negative. A characteristic feature of Eq. (39) is that when $g_0=0$, this energy is equal to that of two independent α bands without constituting α excitons. On the other hand, we show in Figs. 1–4 that

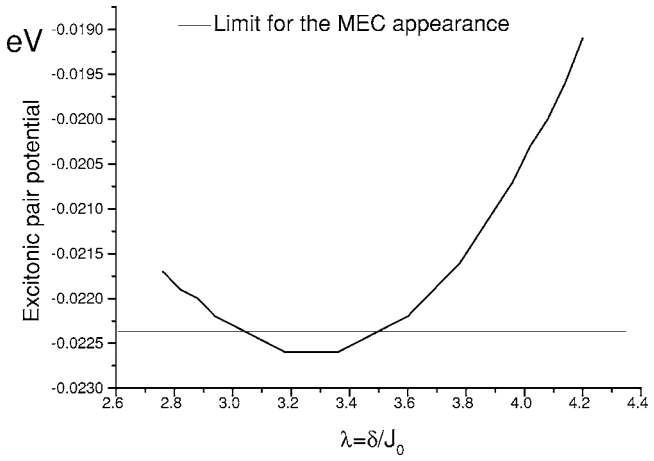

FIG. 5. Energy interaction among the electron and hole α states that compose the excitons. In the interval of the λ parameter between $3.0<\delta/J_0<3.4$ the condition (40) is satisfied and therefore the exciton condensate is possible.

the α-band states are narrow; therefore, we can substitute $E_{\mathbf{k}}$ by the constant value of its band gravity center, E_0. Thus, the conditions for the appearance of the MEC state are

$$E_{MEC}=2N\left(E_0+\frac{E_0^2}{(E_0^2+g_0^2)^{1/2}}\right)-\frac{2g_0^2}{|V_0|}<0, \quad (40)$$

$$g_0=\frac{1}{2}[(N|V_0|)^2-4E_0^2]^{1/2}>0, \quad (41)$$

N being the number of magnetic sites in each antiferromagnetic sublattice. Consequently, the energy of Eq. (35) belongs to a MEC ground state when the following relation is satisfied:

$$N|V_0|>6E_0. \quad (42)$$

In the case of a totally occupied α band, the E_{MEC} energy of Eq. (39), taking into account the same conditions that those for obtaining Eq. (40), is

$$E_{MEC}=2N\left(E_0-\frac{E_0^2}{(E_0^2+g_0^2)^{1/2}}\right)-\frac{2g_0^2}{|V_0|}<0, \quad (43)$$

where g_0 is also given by Eq. (41). In this case, the condition of negative energy of Eq. (39) is always satisfied whenever g_0 is larger than zero—i.e., when $N|V_0|>2|E_0|$.

In Fig. 5, we represent $N|V_0|$ versus λ considering Eq. (38). For values within the interval between 3.0 and 3.4, the above relations [Eqs. (40)–(43)] may be satisfied. These conditions for the MEC existence seem to be possible for realistic values of the initial parameter of Hamiltonian (1) whenever we use a excitonic pair potential such as that of Eq. (38).

However, we want to remark that the calculation of V_0 of Eq. (38) is obtained from a first-order perturbation potential. Consequently, it is reasonable to question if the results of Fig. 5 and the corresponding conclusions arising from this

"bare" interaction can be maintained when one considers the renormalization of the excitonic pair potential or if the physical consequences deduced from Eq. (40) should be modified when one considers a larger perturbation order in this interaction. Any infinite perturbation series appropriate for our case[52–54] can be useful for the renormalization analysis, since our purpose is to analyze the dependence of the MEC appearance with the pair potential. We can apply, therefore, the T-matrix formalism to the case of the α electron-hole pair potential. Thus, the renormalized effective interaction for $T=0$ coming from the "bare" interaction V_0 becomes

$$\begin{aligned}\langle \alpha_{\mathbf{k}'\uparrow}\beta_{-\mathbf{k}'\downarrow}|V_{eff}|\alpha_{\mathbf{k}\uparrow}\beta_{-\mathbf{k}\downarrow}\rangle &= \langle \alpha_{\mathbf{k}'\uparrow}\beta_{-\mathbf{k}'\downarrow}|V_0|\alpha_{\mathbf{k}\uparrow}\beta_{-\mathbf{k}\downarrow}\rangle \\ &+ \frac{(-i)}{2\pi}\sum_{\mathbf{q}}\int G_{\mathbf{k}+\mathbf{q}}(\omega+\omega')G_{-\mathbf{k}-\mathbf{q}}(-\omega-\omega')d\omega' \\ &\times \langle \alpha_{\mathbf{k}'\uparrow}\beta_{-\mathbf{k}'\downarrow}|V_0|\alpha_{\mathbf{k}+\mathbf{q}\uparrow}\beta_{-\mathbf{k}-\mathbf{q}\downarrow}\rangle \\ &\times \langle \alpha_{\mathbf{k}+\mathbf{q}\uparrow}\beta_{-\mathbf{k}-\mathbf{q}\downarrow}|V_{eff}|\alpha_{\mathbf{k}\uparrow}\beta_{-\mathbf{k}\downarrow}\rangle, \end{aligned} \tag{44}$$

where $G_{\mathbf{k}+\mathbf{q}}$ and $G_{-\mathbf{k}-\mathbf{q}}$ are the noninteracting system Green functions corresponding to the α states. The effective interaction equation, when $\langle \alpha_{\mathbf{k}'\uparrow}\beta_{-\mathbf{k}'\downarrow}|V_0|\alpha_{\mathbf{k}+\mathbf{q}\uparrow}\beta_{-\mathbf{k}-\mathbf{q}\downarrow}\rangle$ is a constant such as that of Eq. (38), can be written in the following summarized expression:

$$V_{eff} = V_0 - V_0\Pi V_{eff}, \tag{45}$$

where $\Pi=[(-i)/2\pi N]\Sigma_{\mathbf{kq}}\int G_{\mathbf{k}+\mathbf{q}}(\omega+\omega')G_{-\mathbf{k}-\mathbf{q}}(-\omega-\omega')d\omega'$. For both totally occupied and totally unoccupied α bands, Π is given by $\Pi\approx -N/2|E_0|$, E_0 being the gravity center of the α bands (for obtaining this expression for Π, we have considered the extreme narrowness property of $E_{\mathbf{k}}^{(e)}$ and $E_{\mathbf{k}}^{(h)}$ bands corresponding to the α and β states).

According to Eq. (45), the value of NV_{eff} for either totally occupied or totally unoccupied α bands is

$$NV_{eff} \simeq \frac{-N|V_0|}{1+\dfrac{N|V_0|}{2|E_0|}}.$$

Consequently, in these conditions, when considering NV_{eff} instead of NV_0, Eqs. (40) and (43) cannot be satisfied since $N|V_{eff}|<2|E_0|$. Therefore, for both totally occupied and unoccupied α bands, the MEC-state appearance depends on the perturbation order of the pair potential and the α bandwidths. This fact leads us to think that for these α-band occupations the MEC quantum transition is dubious and it should be analyzed in each given case.

For a partially occupied α band (see Figs. 1 and 3), whose occupation ratio is $0<n=(1/N)\Sigma_{\mathbf{k}}n_{\mathbf{k}}<1$, the corresponding conditions, equivalent to Eqs. (40)–(43), which ensure the MEC state, are given by

$$\begin{aligned}E_{MEC} \approx N\Bigg(&(1-2n)t - n(n^2t^2+g_0^2)^{1/2} - (1-n)[(1-n)^2t^2 \\ &+ g_0^2]^{1/2} + + \frac{g_0^2}{t}\ln\left[\frac{(1-n)t+\sqrt{(1-n)^2t^2+g_0^2}}{-nt+\sqrt{n^2t^2+g_0^2}}\right]\Bigg) \\ &- \frac{2g_0^2}{|V|} < 0, \end{aligned} \tag{46}$$

$$t = N|V|\left[\sinh^{-1}\left(\frac{(1-n)t}{g_0}\right)+\sinh^{-1}\left(\frac{nt}{g_0}\right)\right], \tag{47}$$

where t is the bandwidth of the α bands. Equations (46) and (47) are valid for any n value different from 1 and 0. In addition, V can be either the "bare" interaction of Eq. (38) or any renormalized pair interaction appropriate for partially occupied bands. Equation (47) relates the main parameters which govern the dynamic of this system, t, g_0, and $N|V|$. Equation (46) allows one to obtain the total energy of system in function of t and $N|V|$, which are physical variables that have been calculated in former sections of this work. When this energy of Eq. (46) is less than zero, the MEC state is possible. These equations can be simplified in some illustrative case such as the half filling for the α bands (i.e., for $n=1/2$). In this case, Eqs. (46) and (47) are

$$\begin{aligned}E_{MEC} = N\Bigg\{ &-0.5(t^2+4g_0^2)^{1/2} + \frac{g_0^2}{2t}\ln\left[\frac{t+\sqrt{t^2+4g_0^2}}{-t+\sqrt{t^2+4g_0^2}}\right]\Bigg\} \\ &- \frac{2g_0^2}{|V|} < 0, \end{aligned} \tag{48}$$

$$g_0 = \frac{t}{2\sinh\left(\dfrac{t}{2N|V|}\right)}. \tag{49}$$

Besides, if we assume that $2N|V| \gg t$ due to the narrowness of the α bands displayed in Figs. 1–4, Eqs. (48) and (49) become

$$g_0 = \frac{24(N|V|)^3}{24(N|V|)^2+t^2} \simeq N|V|, \tag{50}$$

$$E_{MEC} = -\frac{N}{2}[t^2+4(N|V|)^2]^{1/2} - 2Ng_0, \tag{51}$$

which imply that the MEC state is possible for realistic systems *independently of the pair potential* that we consider.

In short, we want emphasize that *the MEC state can be obtained in the cases of extremely narrow α bands whose occupations are either n=0 or n=1 whenever one considers first-order pair potentials. On the contrary, for renormalized pair potentials this possibility may disappear. However, when the α band crosses E_F (see Figs. 1 and 3), the MEC-state*

transition is possible with both mean-field interactions and renormalized pair potentials.

VII. SUMMARY AND CONCLUDING REMARKS

We have variationally obtained the low-energy excitations of a combined Kondo-Heisenberg antiferomagnetic insulating system. The resulting spectra are narrow bands whose states are associations of charged modes and magnons and whose $E_{\mathbf{k}}$ dispersion is coherent with their magnetic nature. The narrowness of these spectra is independent of the features of the initial conduction electron band; i.e., the heavy-fermion-like properties are present due to the concomitance of the Heisenberg interaction with the Kondo lattice exchange, especially when H_H is short ranged. Therefore, the narrowness of these magnon-charged mode states can complete the explanation of the heavy-fermion behavior of the cases in which the renormalization of the *e-e* interaction does not totally explain it. On the other hand, in our model, the spectra of Eq. (28) lead to the possibility that the heavy-fermion metal features can be due to a quantum criticality, since for λ values less than 3.25, the α bands cross E_F. The main cause for the appearance of this critical point is that the states close to E_F, belonging to a Kondo-Heisenberg lattice, are formed between excitations of local fields and conduction electrons. Coleman *et al.*[14] have discussed the quantum critical behavior in the heavy-fermion materials, focusing their analysis on the breakdown of the Fermi liquid of electron quasiparticles when the antiferromagnetic correlation leads to magnetic ordering in the system. Although our objectives, starting points, and methodology are different from those of Coleman *et al.*,[14] our results and conclusions, written above, contain no relevant disagreement and present basic concordances with the "strong-coupling" alternative of these authors.[14] On the other hand, our model can be valid for any lattice, independently of its dimension. Therefore, we can also conclude that the existence of quantum critical points when the heavy-fermion behavior is present can be independent of the lattice dimension and it does not seem to be an exclusive property of the low (two) dimensionality. This point is, in our opinion, complementary of the analysis of Coleman *et al.* and gives a reasonable route for answering some questions posed in the remarks of their paper.

Another consequence precipitated by the nature of these α states within the Heisenberg-Kondo lattice is that these are located within the gap of the insulating band structure of H_0. In addition, we have shown in Figs. 1–4 that in certain conditions (for certain values of the λ parameter), the α bands can be partially and totally located below E_F. This situation induces new possibilities for the ground state of the system when one considers the electron-hole interaction within the α states. In the second part of this work, we analyze the Coulombian interaction among α states based on these electrons and holes. This interaction is influenced by the magnon components of the α states and this attractive interaction modifies the total energy of the corresponding exciton. For determined and restricted conditions [see Eqs. (40)–(51)] of the governing parameters of Hamiltonian (1), the total attractive interaction of the global system of α excitons can lead to the total energy of the system being less than that of the initial ground state. In these conditions, the vacuum of the system can be a coherent energy-condensed state, which is thermodynamically similar to that of the BCS theory, although its electromagnetic behavior can correspond to a narrow-gap system that has the features of a Bose condensate. The appearance of this MEC state depends fundamentally on the $E_{\mathbf{k}}$ spectra [given Eqs. (19) and (20) and Figs. 1–4] and the strength of the pair potential. For a bare pair potential arising from the Coulombian interaction between the components of the excitons, the MEC is possible even for α bands located above E_F. For renormalized versions of this pair potential, this possibility can vanish; however, for partially occupied α bands, the MEC state is possible with both bare interactions and renormalized electron-hole pair potentials. Therefore, we want to remark that in our results of Figs. 1–4, three different phases are described, which represent three different situations within the nonsuperconducting strongly correlated antiferromagnetic systems: insulating, metallic, and excitonic condensed phases. The main parameter whose variations produce the quantum phase transitions is λ, the ratio between the bandwidths of the initial extended band and the J_0 Kondo exchange.

Concerning the future perspectives of this model, an important point could be the behavior of these phases before the magnetic field action. The details of this study will be the objective of a next analysis. For values $\lambda > 3.4$, the α states reduce the initial gap and constitute the low-energy in-gap states. In this insulating phase, a constant magnetic field with the corresponding Zeeman $s=1/2$ splitting leads to that the $s_z=-1/2$ band energies are less than those of the $s_z=1/2$ ones. This energy shift approaches the lower α band to E_F, modifying the optical properties of the system concerning the frequency-dependent conductivity. Some exotic magnetic behaviors provided by constant magnetic field have been observed in some Kondo insulators.[55] However, the most interesting effect that the magnetic field may produce in this system is that the Zeeman splitting can locate the corresponding lower-energy α bands within the energy interval in which the fermion coupling can induce the MEC transition according to Eq. (43). In this case a bosonic condensed state is provoked by a constant magnetic field. This situation would present in a certain sense some similarities with the magnetic BEC transition recently observed in $TlCuCl_3$,[26,27] although, obviously, these are two different situations, since, in TlCuCl, the Bose condensation is produced by dimerization of $s=1/2$ spin states. On the other hand, we want to emphasize that for high fields the own magnon charged-mode association can be energetically unfavorable and, as a consequence, the condensate can evaporate.

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APPENDIX

Developing the term of Eq. (9), $\Sigma_{\mu\nu\alpha} e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_\mu} e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{R}_\nu} e^{i(\mathbf{k}-\mathbf{p}')\cdot\mathbf{R}_\alpha} \langle \mathrm{AF}|S_\mu^- S_\nu^z S_\alpha^+|\mathrm{AF}\rangle$, we obtain that

$$\langle \alpha_{\mathbf{k}\uparrow\downarrow}|H_{Kondo}|\alpha_{\mathbf{k}\uparrow\downarrow}\rangle = -\frac{1}{2N^3}\sum_{\mathbf{p}p'} a^*_{\mathbf{p}}a_{\mathbf{p}'}J_0\sum_{\mu\nu\alpha} e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_\mu}e^{i(\mathbf{p}'-\mathbf{p})\cdot\mathbf{R}_\nu}e^{i(\mathbf{k}-\mathbf{p}')\cdot\mathbf{R}_\alpha}(\langle S^-_\mu\rangle\langle S^+_\alpha\rangle\langle S^z_\nu\rangle(1-\delta_{\mu\nu}-\delta_{\mu\alpha}-\delta_{\alpha\nu}-\delta_{\mu\nu}\delta_{\alpha\nu})$$
$$+\langle S^-_\mu S^z_\nu\rangle\langle S^+_\alpha\rangle\delta_{\mu\nu}(1-\delta_{\nu\alpha})+\langle S^-_\mu\rangle\langle S^z_\nu S^+_\alpha\rangle\delta_{\alpha\nu}(1-\delta_{\mu\alpha})+\langle S^-_\mu S^+_\alpha\rangle\langle S^z_\nu\rangle\delta_{\mu\alpha}(1-\delta_{\nu\alpha})+\langle S^-_\mu S^+_\alpha S^z_\nu\rangle\delta_{\alpha\mu}\delta_{\nu\alpha}), \tag{A1}$$

where all $\langle\cdots\rangle$ average values are calculated in the $|\mathrm{AF}\rangle$ state defined by Eq. (3). And using that

$$\langle S^-_\mu S^z_\mu S^+_\mu\rangle_+ = \frac{1}{2}\sin^2(\theta/2); \langle S^-_\mu S^z_\mu S^+_\mu\rangle_+ = \frac{1}{2}\cos^2(\theta/2),$$

$$\langle S^-_\mu S^z_\nu S^+_\alpha\rangle = \langle S^-_\mu\rangle_\pm\langle S^z_\mu\rangle_\pm\langle S^+_\mu\rangle_\pm = (\pm\sin\theta e^{-i\phi})(\pm\cos\theta)(\pm\sin\theta e^{i\phi}),$$

$$\langle S^-_\mu S^z_\mu\rangle_\pm = \pm\frac{1}{2}\sin\theta e^{-i\phi}; \langle S^z_\mu S^+_\mu\rangle_\pm = \pm\frac{1}{2}\sin\theta e^{i\phi},$$

$$\langle S^-S^+\rangle_+ = \sin^2(\theta/2); \langle S^-S^+\rangle_- = \cos^2(\theta/2), \tag{A2}$$

we obtain the following:

$$\langle \alpha_{\mathbf{k}\uparrow\downarrow}|H_{Kondo}|\alpha_{\mathbf{k}\uparrow\downarrow}\rangle = -\frac{1}{8N^2}\sum_{\mathbf{p}\mathbf{p}'} a^*_{\mathbf{p}}J_0a_{\mathbf{p}}(2\cos^2\theta-\sin^2\theta). \tag{A3}$$

The average value of Heisenberg Hamiltonian H_H is obtained as follows:

$$\langle H_H\rangle = -\frac{1}{N}\sum_{\mathbf{p}}|a_{\mathbf{p}}|^2\sum_{ij}{}'J_{ij}\delta_{\mathbf{p}\mathbf{p}'}\langle S^-_{\mathbf{p}-\mathbf{k}}\vec{S}_i\cdot\vec{S}_jS^+_{\mathbf{k}-\mathbf{p}}\rangle = \frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}\sum_{\mu\nu}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_\mu}e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{R}_\nu}\langle S^-_\mu\vec{S}_i\cdot\vec{S}_jS^+_\nu\rangle$$
$$=\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}\sum_{\mu\nu}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_\mu}e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{R}_\nu}\langle S^-_\mu\rangle\langle\vec{S}_i\rangle\cdot\langle\vec{S}_j\rangle\langle S^+_\nu\rangle(1-\delta_{\mu i}-\delta_{\mu j}-\delta_{\nu i}-\delta_{\nu j}-\delta_{\mu\nu}-\delta_{\mu i}\delta_{\mu\nu}-\delta_{\mu j}\delta_{\mu\nu}-\delta_{\mu i}\delta_{\nu j}-\delta_{\mu i}\delta_{\nu i})$$
$$+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}\sum_{\nu}e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{R}_\nu}\langle S^-_i\vec{S}_i\rangle\cdot\langle\vec{S}_j\rangle\langle S^+_\nu\rangle(1-\delta_{\nu i}-\delta_{\nu j})+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}\sum_{\mu}e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{R}_\nu}\langle S^-_j\vec{S}_j\rangle\cdot\langle\vec{S}_i\rangle\langle S^+_\nu\rangle(1-\delta_{\nu i}-\delta_{\nu j})$$
$$+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}\sum_{\mu}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_\mu}\langle S^-_\mu\rangle\langle\vec{S}_iS^+_i\rangle\cdot\langle\vec{S}_j\rangle(1-\delta_{\mu j}-\delta_{\mu i})+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}\sum_{\mu}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_\mu}\langle S^-_\mu\vec{S}_i\rangle\cdot\langle\vec{S}_jS^+_j\rangle(1-\delta_{\mu j}-\delta_{\mu i})$$
$$+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}\sum_{\mu}\langle S^-_\mu S^+_\mu\rangle\langle\vec{S}_i\cdot\vec{S}_j\rangle(1-\delta_{\mu i}-\delta_{\mu j})+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}(\langle S^-_i\vec{S}_iS^+_i\rangle\cdot\langle\vec{S}_j\rangle+\langle\vec{S}_i\rangle\cdot\langle S^-_j\vec{S}_jS^+_j\rangle)$$
$$+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_i}e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{R}_j}\langle S^-_i\vec{S}_i\rangle\cdot\langle\vec{S}_jS^+_j\rangle+\frac{1}{N^2}\sum_{\mathbf{p}}a^2_{\mathbf{p}}\sum_{ij}{}'J_{ij}e^{i(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_j}e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{R}_i}\langle S^-_j\vec{S}_j\rangle\cdot\langle\vec{S}_iS^+_i\rangle \tag{A4}$$

In Eq. (A4) the average values are calculated in a given i-site lattice. In order to calculate Eq. (A4), we can use Eq. (A2) along with the following relations:

$$\langle S^-_\mu\vec{S}_\mu\rangle_+ = \frac{1}{2}\sin^2(\theta/2)\vec{e}_x-\frac{i}{2}\sin^2(\theta/2)\vec{e}_y+\frac{1}{4}\sin(\theta)e^{-i\phi}\vec{e}_z,$$

$$\langle S^-_\mu\vec{S}_\mu\rangle_- = \frac{1}{2}\cos^2(\theta/2)\vec{e}_x+\frac{i}{2}\cos^2(\theta/2)\vec{e}_y-\frac{1}{4}\sin(\theta)e^{-i\phi}\vec{e}_z,$$

$$\langle\vec{S}_\mu S^+_\mu\rangle_+ = \frac{1}{2}\sin^2(\theta/2)\vec{e}_x+\frac{i}{2}\sin^2(\theta/2)\vec{e}_y+\frac{1}{4}\sin(\theta)e^{i\phi}\vec{e}_z,$$

$$\langle\vec{S}_\mu S^+_\mu\rangle_- = \frac{1}{2}\cos(\theta/2)\vec{e}_x+\frac{i}{2}\cos^2(\theta/2)\vec{e}_y-\frac{1}{4}\sin(\theta)e^{i\phi}\vec{e}_z,$$

$$\langle S^-_\mu\vec{S}_\mu S^+_\mu\rangle_- = \frac{1}{2}\sin^2(\theta/2)\vec{e}_z, \quad \langle S^-_\mu\vec{S}_\mu S^+_\mu\rangle_- = \frac{1}{2}\cos^2(\theta/2)\vec{e}_z,$$

$$\langle\vec{S}_i\rangle_- = \frac{1}{2}\vec{n}_i, \quad \langle\vec{S}_i\rangle_+ = -\frac{1}{2}\vec{n}_i. \tag{A5}$$

Taking into account Eqs. (A1)–(A5) we obtain the following expression for $\langle H_H\rangle$:

$$\langle H_H \rangle = \frac{1}{8N}\sum_{\mathbf{p}} a_{\mathbf{p}}^2 \sum_{ij} |J_{ij}| \left(-1 + \frac{1}{2}\sin^2\theta \right) + \frac{1}{2N^2}\sum_{\mathbf{p}} a_{\mathbf{p}}^2 \sum_{ij} |J_{ij}| \left(1 + \frac{1}{4}\sin^2\theta \right) + \frac{1}{8N^2}\sum_{\mathbf{p}} a_{\mathbf{p}}^2 \sum_{ij} |J_{ij}| \cos[(\mathbf{p}-\mathbf{k})\cdot\mathbf{R}_{ij}] \left(-1 + \frac{1}{2}\sin^2\theta \right). \tag{A6}$$

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