Magnetic and lattice polaron in the Holstein t-J model

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We investigate the interplay between the formation of a lattice and magnetic polaron in the case of a single hole in the antiferromagnetic background. We present an exact analytical solution of the Holstein t-J model in infinite dimensions. The ground-state energy, electron-lattice correlation function, spin bag dimension as well as spectral properties are calculated. The magnetic and hole-lattice correlations sustain each other, i.e., the presence of antiferromagnetic correlations favors the formation of the lattice polaron at lower values of the electron-phonon coupling while the polaronic effect contributes to reduce the number of spin defects in the antiferromagnetic background. The crossover towards a spin-lattice small polaron region of the phase diagram becomes a discontinuous transition in the adiabatic limit.

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I. INTRODUCTION

A single hole in an antiferromagnetic background represents a widely studied problem in solid-state physics due to its relevance to the problem of high-T_c superconductivity.[1,2] High-T_c compounds indeed show an antiferromagnetic undoped phase, which is gradually degraded and finally destroyed by doping. The electronic properties at low doping are therefore often described in terms of the Hubbard or t-J model.[3,4]

The problem of the motion of a single hole, far from being a pure academic issue, can be representative of the extreme low doping case of these materials. It is worth noting that even in the case of a single hole the problem of intermediate/strong magnetic interaction with an antiferromagnetic background is a nontrivial many-body problem. The difficulty consists in describing the dressing of the hole by a cloud of spin background excitations (the magnetic or spin polaron), which can coherently move as a quasiparticle.[5–7] The situation is similar to that of a small lattice polaron, i.e., the case of an electron moving together with a phonon cloud, which represents the lattice deformation induced by the presence of the charge.[8]

The connection between lattice and magnetic polarons goes, however, beyond a methodological interest. There are indeed several observations of a sizable interplay between electron-phonon and magnetic interaction in cuprates[9] as well as in manganites.[10] The purpose of this paper is to explore in detail the physical consequences of this interplay, in particular, with regard to the lattice and magnetic polaron properties. To this aim a nonperturbative way is clearly needed.

We present an exact analytical solution of the Holstein t-J model for a single hole in infinite dimension. The ground-state energy, electron-lattice correlation function, spin bag dimension as well as spectral properties are calculated. We find that the lattice (spin) polaron formation depends strongly on the magnetic (hole-phonon) interaction. We identify thus regions of the phonon-assisted magnetic polaron as well as the magnetic induced lattice polaron. The extension of these regions is strongly dependent on the adiabatic ratio. In the adiabatic regime, lattice and magnetic polaron formation are strictly tied each other. These general results could help to explain the strong interplay between lattice and spin degrees of freedom in cuprates and manganites. Finally we discuss the major drawback of our approximation and give some ideas to overcome it.

II. THE HOLSTEIN T-J MODEL AND ITS INFINITE-DIMENSION SOLUTION

Let us consider the Holstein t-J model defined by the Hamiltonian[11,12]

$$H=-\frac{t}{2}\sum_{\langle ij\rangle\sigma}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c.})+\frac{J}{2}\sum_{\langle ij\rangle}\left[\left(S^z_iS^z_j-\frac{n_in_j}{4}\right)+\frac{1}{2}(S^+_iS^-_j+S^-_iS^+_j)\right]+g\sum_i n_i(b_i+b^{\dagger}_i)+\omega_0\sum_i b^{\dagger}_ib_i, \qquad (1)$$

where $\tilde{c}^{\dagger}_{i\sigma}$ are the electron operators in the presence of an infinite on-site repulsion that prevents double occupancy $[\tilde{c}^{\dagger}_{i\sigma}=c^{\dagger}_{i\sigma}(1-n_{-\sigma})]$, $b^{\dagger}_i$ are the phonon operators, and S^z_i, S^+_i, and S^-_i, respectively, the z component, the raising, and lowering spin operators. The first term in Eq. (1) describes the hopping of the electrons on nearest neighbors of a square lattice, the second one the direct and the exchange interaction, the third one the local electron-phonon interaction coupled to charge density, and the fourth one the Einstein phonon frequency. The choice of a hopping matrix element equal to $t/2$ gives rise to a band with bare bandwidth t. The model can be straightforwardly generalized in infinite dimensions by using the usual rescaling: $t\to t/\sqrt{z}$, $J\to J/z$, where z

is the coordination number. For a hypercubic lattice, the coordination number is $z=2d$, while for a Bethe lattice $z=d$.

Throughout this paper we shall consider one hole created on the antiferromagnetic half-filled state. The antiferromagnetic state is described in terms of a *classical* Néel ground state. A convenient approach to this aim is the spin-wave theory applied to the lattice model as can be found, e.g., in Refs. 5,6, and 11. A useful effective Hamiltonian can be thus derived by mainly following the discussion in Ref. 11, generalized now in the presence of a Holstein electron-phonon interaction. The Hamiltonian is first transformed by a canonical transformation into a ferromagnetic one. Then "hole" and "spin" defect operators are introduced, respectively, as fermionic h and bosonic a operators on the antiferromagnetic ground state. The resulting Hamiltonian reads, thus,

$$
\begin{aligned}
H=&\frac{t}{2\sqrt{z}}\sum_{\langle ij\rangle}(h_j^\dagger h_i a_j+\text{H.c.})-g\sum_i h_i^\dagger h_i(b_i+b_i^\dagger)\\
&+\omega_0\sum_i b_i^\dagger b_i+\frac{J}{4z}\sum_{\langle ij\rangle}[a_i^\dagger a_i+a_j^\dagger a_j+a_i^\dagger a_j^\dagger+a_ia_j]\\
&-\frac{J}{2z}\sum_{\langle ij\rangle}h_i^\dagger h_i a_j^\dagger a_j-\frac{J}{2z}\sum_{\langle ij\rangle}a_i^\dagger a_i a_j^\dagger a_j\\
&+\frac{J}{2}\sum_i h_i^\dagger h_i-\frac{J}{4},
\end{aligned}
\tag{2}
$$

where we have neglected the hole-hole terms since we are interested in a single hole in an antiferromagnetic background.

Equation (2) can be significantly simplified in infinite dimension. In that limit indeed the two terms of the fourth line can be shown to be negligible since they contribute only at $O(1/d)$. In addition, in the absence of any boson condensate $\langle a\rangle$, $\langle a^\dagger\rangle$, which should destroy the antiferromagnetic background and which is forbidden in our context, also the last two terms of the third line can be dropped. We end up thus with the effective Hamiltonian of the Holstein t-J model valid in infinite dimension:

$$
\begin{aligned}
H=&\frac{t}{2\sqrt{z}}\sum_{\langle ij\rangle}(h_j^\dagger h_i a_j+\text{H.c.})-g\sum_i h_i^\dagger h_i(b_i+b_i^\dagger)\\
&+\omega_0\sum_i b_i^\dagger b_i+\frac{J}{4z}\sum_{\langle ij\rangle}[a_i^\dagger a_i+a_j^\dagger a_j]+\frac{J}{2}\sum_i h_i^\dagger h_i .
\end{aligned}
\tag{3}
$$

The first term of Eq. (3) describes the kinetic hopping of one hole on the antiferromagnetic background, which is accompanied by the creation (destruction) of a spin defect which breaks (restores) $2z$ magnetic bonds with individual energy $J/4z$. In addition, we have the usual local electron-phonon interaction which couples the hole density to the local phonon. The last term in Eq. (3) can be absorbed in the definition of the hole chemical potential which, for the single-hole case here considered, has to be set at the bottom of the hole band. It is important to note that, although written in terms of hole operators, the phonon part (free phonon part + hole-phonon interaction) is formally identical to the Holstein model. This is not a trivial result since in a half-filling case all the electrons are coupled with the phonons and one should, in principle, deal with a many-body problem. As a consequence we are thus able to reduce the many-body problem to a single-particle (one-hole) system interacting with phonons and with spin defects through Eq. (3).

Although the Hamiltonian (3) looks much more affordable than (1), the analytic study of its properties is still quite a hard task at finite dimension. The problem can be much simplified, however, in infinite dimensions, where, as we are going to see, the limit of infinite coordination number $z\rightarrow\infty$,[13–16] all together with the retraceable path constraint enforced by the antiferromagnetic background,[17] provides an *exact* solution. An explicit derivation can be found in Appendix A. In this section we only summarize the final equations which determine in a self-consistent way the hole Green's function.

A crucial point is the possibility of writing the self-energy of the local propagator as the sum of two contributions, labeled as $\Sigma_{\text{hop}}(\omega)$ and $\Sigma_{\text{el-ph}}(\omega)$, which closely resemble the functional expressions of the hopping and phonon self-energy, respectively, in the pure t-J and Holstein models, but *which are now evaluated in the presence of both exchange and phonon interactions*. We can write, thus,

$$G(\omega)=\frac{1}{\omega-\Sigma_{\text{hop}}(\omega)-\Sigma_{\text{el-ph}}(\omega)}, \tag{4}$$

where the hopping contribution is given by[17]

$$\Sigma_{\text{hop}}(\omega)=\frac{t^2}{4}G(\omega-J/2), \tag{5}$$

and the phonon self-energy can be expressed by means of a continued fraction:[16]

$$\Sigma_{\text{el-ph}}(\omega)=\cfrac{g^2}{G_t^{-1}(\omega-\omega_0)-\cfrac{2g^2}{G_t^{-1}(\omega-2\omega_0)-\cfrac{3g^2}{G_t^{-1}(\omega-3\omega_0)-\cdots}}}, \tag{6}$$

where

$$G_t^{-1}(\omega)=\omega-\frac{t^2}{4}G(\omega-J/2). \tag{7}$$

It should be stressed again that both $\Sigma_{\text{hop}}(\omega)$ and $\Sigma_{\text{el-ph}}(\omega)$ are functions of the *total* Green's function G [Eqs. (5)–(7)], which contains the full dynamics (hopping, exchange, electron-phonon) of the system. This nottrivial self-consistency accounts thus for the complex interplay between the phonon and spin degrees of freedom.

Equations (4)–(7) represent a closed self-consistent system, which we can numerically solve by iterations to obtain the explicit *exact* expression of the local Green's function $G(\omega)$, and hence any local one-particle relevant property of the system.

The formal scheme looks quite similar to the dynamical mean-field theory in infinite dimension for a Bethe lattice, applied, for instance, at the purely electron-phonon system.[16] However, due to the antiferromagnetic background, the physical interpretation is quite different.

Due to the orthogonality of the initial and final antiferromagnetic background, the nonlocal component of the Green's function in the Holstein t-J model for $J=0$ is strictly zero $G_{ij}(\omega)=G(\omega)\delta_{i,j}$,[17] whereas for the pure Holstein model $G_{i\neq j}(\omega)$ is finite and provides information about the non-local dynamics: $G(\mathbf{k},\omega)=1/[\omega-\epsilon_{\mathbf{k}}-\Sigma(\omega)]$.

In addition, the magnetic ordering has important consequences also on the local Green's function $G_{ii}(\omega)$. In the Néel state of the Holstein t-J model the hole must follow indeed a retraceable path in order to restore the antiferromagnetic background.[17] A Bethe-like dynamics is thus enforced by the magnetic ordering regardless of the actual real-space lattice. The object made up by the hole plus the local modification of the spin configuration due to the presence of the hole is the "spin polaron."

The local constraint $G_{ij}(\omega)=G(\omega)\delta_{i,j}$ induced at $d=\infty$ in the Holstein t-J model by the antiferromagnetic background can appear to be quite a strong simplification. However, it should be noted that it holds true as long as the antiferromagnetic spin configuration can be assumed to be frozen, in particular, as long as the Hamiltonian does not induce spin dynamics. This is the case of the effective Holstein t-J Hamiltonian (3) in infinite dimension where spin fluctuations are neglected.[17] The existence of the spin polaron itself could be questioned at finite dimension where spin fluctuations are operative. However, several numerical and analytic studies have shown that the restoring of spin fluctuations does not destroy the spin polaron object, but opens coherent channels of hole propagation.[5–7] In this situation the spin polaron can thus propagate as a whole through the crystal.

Many studies have investigated the motion of the spin polaron and determined its **k** dispersion and optical conductivity, both in the absence[11,18–20] and in the presence of electron-phonon interaction.[12,21–25] However, apart from few exceptions,[21,26,27] the internal degrees of freedom of the spin (lattice) polaron object have not so far been investigated much. In the present work we mainly focus on the formation of the spin polaron and on its internal structure properties (size, binding energy, etc.). These quantities are local features which, we believe, are only weakly affected by the itinerant nature of the spin polaron. In this perspective we think that the infinite-dimension approach considered here provides valuable information on the spin polaron formation and on its interplay with the local (Holstein) electron-phonon interaction.

III. SPECTRAL PROPERTIES

In order to have a complete description of the physical properties of the Holstein t-J model, it is useful to identify three independent dimensionless parameters:[28] the adiabatic ratio ω_0/t, the electron-phonon coupling $\lambda=g^2/\omega_0 t$, and the exchange interaction J/t. Another important parameter to be defined is the multiphonon constant $\alpha=g/\omega_0$, which is a local quantity that does not involve electron hopping t. The limiting cases are $\lambda=0$, where the system reduces to the t-J model, and $J/t=0$, where the Holstein model *on an antiferromagnetic background* is recovered.

At a first look this problem could be regarded as a simple interplay between two energy scales: the exchange J/t, which rules the magnetic properties, and λ related to the electron-phonon coupling. The dominance of one of them would therefore determine the overall properties of the system, while the weaker one could be considered as a perturbation. However, as we are going to see, this picture is too simplistic. A more accurate description of the physics must take into account first of all the role of the adiabatic ratio (ω_0/t), which in the pure Holstein model rules also the polaron crossover.[29] In particular, we can expect that the magnetic (lattice) polaron formation induces a drastic renormalization of the effective kinetic-energy scale t^* ($t^*\ll t$). The "effective" adiabatic ratio will depend in an implicit way on the electron-phonon and magnetic interactions. Then the magnetic (lattice) polaron formation induces a drastic renormalization of the kinetic-energy scale, which in its turn affects the phonon (magnetic) properties and eventually leads toward intermediate/strong hole-phonon couplings. It is interesting to note that the multiphonon parameter $\alpha=g/\omega_0$ does not depend on t, so that it can be considered unaffected by local hopping renormalization (we recall that phonon frequency ω_0 is not screened by electron-phonon interaction for the single-hole case).

Let us now first discuss spectral properties by studying the spectral density defined as $A(\omega)=-(1/\pi)\text{Im}[G(\omega)]$ directly accessible by the knowledge of the Green function.

All through this paper we consider a Bethe lattice and a standard semicircular density of states with bandwidth $2t$. It should be noted however that, since the antiferromagnetic background enforces a retraceable path approximation,[17] a semicircular density of states is recovered independently of the chosen crystal lattice, i.e., also for a hypercubic lattice. In other words Eqs. (4)–(7) are valid for any lattice structure, provided the coordination number is infinite. The assumption of a nonretraceable Bethe lattice however allows to classify explicitly all the hopping processes, which leads to the magnetic polaron formations.[17] Moreover in the Bethe lattice,

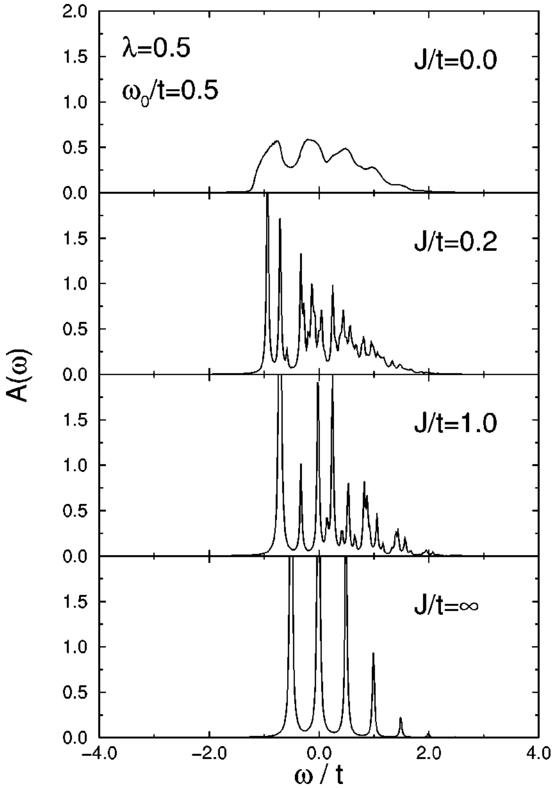

FIG. 1. Spectral density $A(\omega)$ for different values of exchange energy: $J/t=0,0.2,1.0,\infty$ and $\lambda=0.5$, $\omega_0/t=0.5$. We use a finite broadening $(0.02t)$.

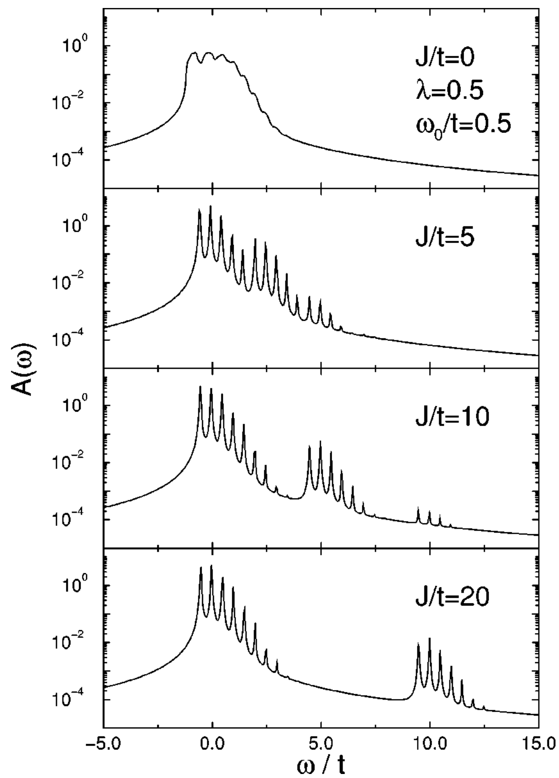

FIG. 2. Spectral density $A(\omega)$ for different values of exchange energy: $J/t=0,5,10,20$ and $\lambda=0.5$, $\omega_0/t=0.5$.

contrary to hypercubic infinite bandwidth case, the single-polaron problem can be well defined.[16] To obtain the spectral function we have iterated Eqs. (4)–(7) up to numerical convergence by using a truncation in the continued fraction Eq. (6) according to the procedure outlined in Ref. 16, i.e., we truncate the continued fraction Eq. (6) at a stage $N_{\mathrm{ph}}\gg\alpha^2$. Moreover, we notice that a continued fraction arises also in the absence of hole-phonon interaction[17] once G_t [Eq. (7)] is substituted in Eq. (4). We have found that in order to properly generate a certain number M of the magnetic poles of the spectrum we have to choose a truncation $N_J\gg M$.

In Fig. 1 we show the evolution of the spectral density for moderate values of J/t and $\lambda=0.5$, $\omega_0/t=0.5$. For $J/t=0$ the spectral density is made by a continuum with incipient structures due to the electron-phonon coupling. This shape is characteristic of weak electron-phonon coupling in a small-intermediate adiabatic regime $\omega_0/t\lesssim 1$, with no well-defined polaron peak.[16] By switching on the exchange interaction $J/t=0.2$ the continuum spectrum is split into a set of magnetic peaks. This trend is quite similar to what happens in the infinite-dimensional t-J model[17] with an additional modulation due to the underlying electron-phonon features. We can thus think of the resulting spectral function as ruled by different couplings on different scales, where the gross structure on scale t is determined by the pure electron-phonon interaction superimposed by the fine structure on scale J given by the magnetic peaks spaced as $(J/t)^{2/3}$ (for small J/t). By further increasing J/t we pass an intermediate regime where magnetic and phonon peaks are mixed together and eventually we have a purely phononic spectrum with a set of peaks starting from $-g^2/\omega_0$ and equally spaced by ω_0. This is indeed just the characteristic spectrum of the atomic Holstein model with $\alpha^2=0.5$.[30] As discussed above, the origin of such a behavior is the strong hopping amplitude renormalization due to the magnetic polaron formation for $J>1$, which drives the system from an almost adiabatic case to an effective antiadiabatic regime $\omega_0/t^*\gg 1$. It is however surprising that a strong magnetic interaction $J/t\gg\lambda$ yielded a purely phononic spectrum.

In order to better understand the global evolution of the spectral function it is interesting to look at what happens on a larger energy scale. In Fig. 2 we have thus plotted the behavior of $A(\omega)$ on a linear-log scale for $J/t=0,5,10,20$. We see that the spectrum for finite J/t is roughly determined by replicas of the $J/t=0$ spectrum equally spaced by J and with vanishing spectral weight. On a closer look we find that the structure can be derived from the spectrum of the pure t-J model, made for $J/t\gg 1$ by equally spaced magnetic peaks $\Sigma_n a_n \delta(\omega-nJ/2)$, by broadening each peak according the electron-phonon interaction as in $J/t=0$ case. The inverse occurs for $J/t<\lambda$. In this case we found magnetic structures on a small energy scale J coexisting with a phonon structure spread on energy t. On the contrary the spectral function for large J/t can be thought of as built by a pure magnetic structure for large energy superimposed on a finer phononic structure made by peaks separated by the bare phonon frequency ω_0. This feature resembles the ''interband'' transitions found in Ref. 23 in the antiadiabatic regime. Of course when the magnetic coupling strictly goes to infinity,

$J/t\rightarrow\infty$, the high-energy magnetic peaks are shifted to infinite energy and completely loose their spectral weight. The spectral function reduces in this case to what shown in the lower panel of Fig. 1.

IV. GROUND-STATE PROPERTIES

Ground-state properties can be derived in a direct way by the knowledge of the Green's function, which allows the evaluation of the ground-state energy E_0 through the determination of the lowest band edge or the lowest pole.

The nature of the ground state can be determined by the knowledge of several relevant quantities that can be evaluated using the Hellman-Feynman theorem as[31] follows: (i) The mean number of phonons $N_{ph}=\langle b^\dagger b\rangle$, $N_{ph}=\partial E_0/\partial\omega_0$; (ii) The mean hole-phonon correlation function $C_0=\langle h^\dagger h(b+b^\dagger)\rangle$, $C_0=-\partial E_0/\partial g$; (iii) The mean number of spin defects $N_{s.d.}=\langle a^\dagger a\rangle$, $N_{s.d.}=2\partial E_0/\partial J$; (iv) The effective hopping amplitude t^*, $t^*/t=2\partial|E_0|/\partial t$.[32]

Quantities (i) and (ii) shed light on the lattice polaron formation process. A sharp increase of C_0 (N_{ph}) is expected around some intermediate value of the hole-phonon coupling λ in the adiabatic regime. C_0 increase from zero to its strong-coupling limit 2α (α^2). The transition becomes a crossover, which becomes smoother and smoother upon approaching the antiadiabatic case.[16,29]

Quantity (iii) provides information on the size of the magnetic polaron.[26,27] In fact, since the retraceable path approximation is enforced by the antiferromagnetic background in infinite dimension, it is clear that $N_{s.d.}$ gives the *length* of the string of spin defects,[7,17,33] which, in the Bethe lattice, is also the *size* of the magnetic polaron. In the zero-exchange limit $J\rightarrow 0$ no energy cost is associated with a spin defect and the size of the magnetic polaron diverges (large-magnetic-polaron limit). In the $J\rightarrow\infty$ case, instead spin defects are unfavored and the magnetic polaron becomes almost local (small-magnetic-polaron limit). It could appear surprising that information of nonlocal quantities, as the magnetic polaron size, could be available in the local approach we are using. However it should be reminded that this is only a mean quantity. The price we are paying by using the local approximation exactly in infinite dimensions is the impossibility of having information on the probability distribution to find a path with a given length n, as it was done in Ref. 27. We shall see later that a careful inspection of the dependence of $N_{s.d.}$ on the magnetic coupling J can nevertheless provide valuable information about the rough shape of the magnetic polaron size distribution.

In order to establish, however, a criterion for the large-small magnetic polaron formation, we define the value $N_{s.d.}=0.5$ as the conventional transition between large and small magnetic polaron. We can indeed think that for $N_{s.d.}>0.5$ the probability to find paths with length $n\geqslant 1$ is larger that the probability to have a completely magnetically trapped hole ($n=0$), and we are therefore dealing with "large" magnetic polarons.

Finally the tendency to localization that can be due either to magnetic or hole-phonon interaction can be deduced from the behavior of the effective hopping (iv).

Returning to the analysis of the lattice polaron case we could certainly use as well the criterion $N_{ph}\geqslant 1$ or $C_0\geqslant 1$ to identify the lattice polaron formation.[16,21,25,28,29] However, because of the local nature of the electron-phonon interaction, we can gain a deeper insight by looking at the *probability distribution* of the phonon numbers.[21,23] The probability distribution of phonon numbers is defined as

$$P(n)=|\langle n|h|0\rangle|^2, \tag{8}$$

where $|n\rangle$ is a state with zero holes and n phonons and $|0\rangle$ is the ground state of the single hole. It can be obtained as a residue at the ground-state energy $\omega=E_0$ of $G^{nn}(\omega)$ [Eq. (A3)]. From the same procedure outlined in Appendix A (see also Ref. 16) one obtains[34]

$$G^{nn}(\omega)=\frac{1}{\omega-n\omega_0-\Sigma_{hop}(\omega-n\omega_0)-\Sigma_{em}(\omega)-\Sigma_{abs}(\omega)}, \tag{9}$$

where $\Sigma_{em}(\omega)$ represents the processes related to the emission of a phonon from the state $|n\rangle$,

$$\Sigma_{em}(\omega)=\cfrac{(n+1)g^2}{G_t^{-1}(\omega-n\omega_0-\omega_0)-\cfrac{(n+2)g^2}{G_t^{-1}(\omega-n\omega_0-2\omega_0)-\cfrac{(n+3)g^2}{G_t^{-1}(\omega-n\omega_0-3\omega_0)-\cdots}}}, \tag{10}$$

and $\Sigma_{abs}(\omega)$ takes into account the absorption processes which are allowed also at zero temperature by the initial n-phonon state,

$$\Sigma_{abs}(\omega)=\cfrac{ng^2}{G_t^{-1}(\omega-n\omega_0+\omega_0)-\cfrac{(n-1)g^2}{G_t^{-1}(\omega-n\omega_0+2\omega_0)-\cfrac{(n-2)g^2}{\ddots-\cfrac{g^2}{G_t^{-1}(\omega)}}}}. \tag{11}$$

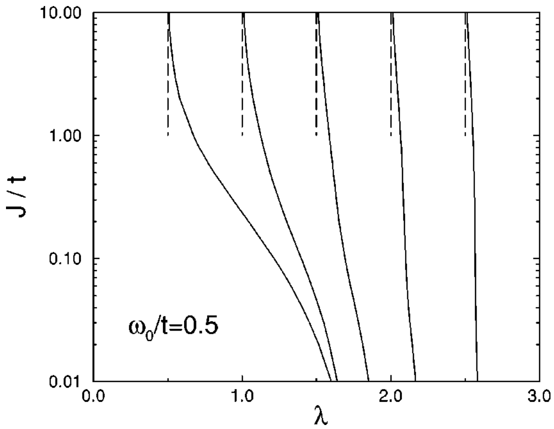

FIG. 3. Multiphonon processes in the λ-(J/t) space for $\omega_0/t = 0.5$. From the left to the right the lines correspond to $P(n=1) \geqslant P(n=0)$, $P(n=2) \geqslant P(n=1)$, $P(n=3) \geqslant P(n=2)$, etc. Dashed lines indicate the antiadiabatic limit, $\alpha^2 = 1,2,3$, etc.

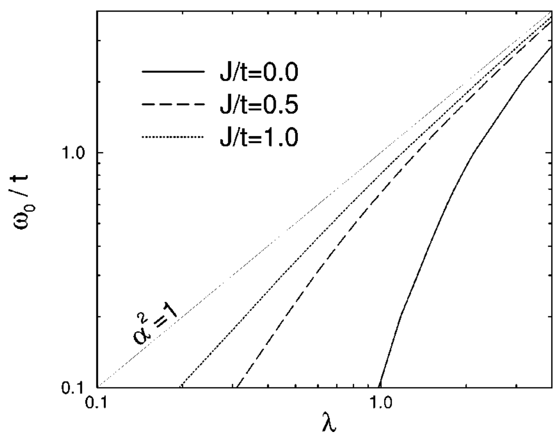

FIG. 4. Lattice polaron transition as determined by Eq. (13) in the λ-(ω_0/t) space for different exchange couplings: $J/t = 0.0$ (solid line), $J/t = 0.5$ (dashed line), $J/t = 1.0$ (dotted line).

The propagator $G_t^{-1}(\omega)$ is defined in Eq. (7), so that $G^{nn}(\omega)$ is a direct by-product of the self-consistent solution of Eqs. (4)–(7). From that we immediately obtain the phonon number distribution as

$$P(n) = \left(\frac{\partial [G^{nn}(\omega)]^{-1}}{\partial \omega} \right)^{-1}_{\omega = E_0}. \tag{12}$$

For a noninteracting system ($g = 0$) the phonon distribution contains only a δ peak at $n = 0$: $P(n) = \delta_{n,0}$. Switching on the electron-phonon interaction, the onset of local lattice distortions are reflected in a shift of total weight towards higher multiphonon peaks. We can now unambiguously identify the lattice polaron formation with the condition

$$P(n=0) \leqslant P(n=1). \tag{13}$$

It is easy to check that this definition reproduces the well-known results for the Holstein model, namely, the criterion $\lambda \geqslant \lambda_c$ in the adiabatic limit ($\lambda_c = 0.844$), and $\alpha \geqslant 1$ in the antiadiabatic one.[16,28,29] It could be worth remarking that the polaron transition occurs, however, in a different way in the two limits. In the nonadiabatic regime the most probable phonon number $\overline{n}$ evolves in a smooth way by increasing λ from $\overline{n} = 0$ to higher numbers $\overline{n} \sim \alpha^2$. The dependence on λ becomes sharper and sharper by decreasing the adiabatic ratio ω_0/t, and in the adiabatic limit $\omega_0/t = 0$, $\overline{n}$ jumps in a discontinuous way from $\overline{n} = 0$ for $\lambda < \lambda_c$ to $\overline{n} = \infty$ for for $\lambda > \lambda_c$.

In Fig. 3 we plot the transition curves corresponding, respectively, to $P(n=1) \geqslant P(n=0)$, $P(n=2) \geqslant P(n=1)$, $P(n=3) \geqslant P(n=2)$, etc. in the λ-(J/t) phase diagram for $\omega_0/t = 0.5$. Lattice polaron formation occurs on the left line corresponding to $P(n=1) = P(n=0)$. We notice a strong dependence of the lattice polaron formation on the magnetic energy. In particular, by increasing the exchange coupling J/t the lattice polaron formation is shifted to smaller values of λ until at $J/t \to \infty$ lattice polaron formation is ruled by the antiadiabatic criterion $\alpha^2 = 1$.

The role of the magnetic interaction in driving the system towards an effective antiadiabatic limit is even more evident when we draw the lattice polaron phase diagram in the λ-(ω_0/t) space (Fig. 4). For zero exchange coupling $J/t = 0.0$ (solid line) it is possible to distinguish an adiabatic regime, where the lattice polaron formation is ruled by the condition $\lambda \gtrsim 1$, and an antiadiabatic regime where the polaron occurs for $\alpha^2 \geqslant 1$ By switching on the magnetic interaction the polaron crossover approaches the line $\alpha^2 = 1$ and the validity of the antiadiabatic criterion is extended for smaller values of ω_0/t.

We can now address the open issue concerning the modification of the lattice polaron criterion in the presence of electronic correlation. The point is to determine whether the simple relation $\lambda < \lambda_c$ in the adiabatic regime could be generalized by introducing properly scaled parameters. Two alternative pictures have been debated in literature. According to the first one[25] the relevant parameter in the presence of electron-electron and magnetic interaction is the ratio between the lattice polaron energy g^2/ω_0 and the purely electronic ground-state energy in the absence of hole-phonon interaction $E_{0,\mathrm{mg}} \equiv E_0(\lambda = 0)$,

$$\lambda_1^* = \frac{g^2}{\omega_0 |E_{0,\mathrm{mg}}|}. \tag{14}$$

An alternative point of view[21] regards the effective hopping amplitude $t^*_{\mathrm{mg}} = t^*(\lambda = 0)$ as the main renormalization effect of the exchange coupling

$$\lambda_2^* = \frac{g^2}{\omega_0 |t^*_{\mathrm{mg}}|}. \tag{15}$$

According to these two ideas the relation $\lambda = \lambda_c$ should be replaced in the presence of magnetic interaction by $\lambda^* = \lambda_c$.

We have carefully checked the validity of these two criteria within our exact solution in infinite dimension. We found that both of them fail to locate correctly the polaron crossover in the presence of magnetic coupling, because the effective adiabatic ratio is increased by the decrease of kinetic energy ($t^*_{\rm mg}$) due to magnetic localization. This drives the system toward an antiadiabatic regime in which the polaron crossover is ruled by the multiphonon constant α which is not renormalized by magnetic coupling. A naive way to take into account the reduction of the kinetic energy is to renormalize also the adiabatic ratio ω_0/t in a similar way with Eqs. (14) and (15), respectively, $\omega_0/|E_{0,\rm mg}|$ and $\omega_0/|t^*_{\rm mg}|$. We have also checked this criteria and found that the lattice polaron crossover in the presence of magnetic interaction cannot be described in a satisfactory way even within this scheme, although it provides a better agreement than the simple renormalization of λ. This just means that the magnetic and lattice degrees of freedom cannot be separated, namely, that the single-hole Holstein *t-J* here considered here cannot be mapped in a simple Holstein model with renormalized parameters.

After having analyzed the process of lattice polaron formation, we can now investigate the properties of the spin polaron in the presence of hole-phonon interaction. We have just seen that the hole-phonon and magnetic interactions are not in competition. On the contrary the exchange coupling favors the lattice polaron formation. On the same footing we can expect that similar arguments hold for magnetic polaron formation, namely, that the electron-phonon trapping favors small spin polarons.

In Fig. 5 we show the mean number of spin defects $N_{\rm s.d.}$ as a function of the exchange coupling J/t for various electron-phonon couplings λ and different adiabatic ratios ω_0/t. In the pure *t-J* model (solid line) the small-large magnetic polaron crossover is denoted by a change of slope at about $J/t=1$, which separates a $N_{\rm s.d.}\propto J^{-1}$ from a $N_{\rm s.d.}\propto J^{-1/3}$ regime.[26,27]

This trend is qualitatively unaffected in the antiadiabatic regime $\omega_0/t=2.0$ for the electron-phonon coupling considered here, $\lambda\leqslant 2$. In this situation the lattice polaron formation occurs as a smooth crossover with negligible localization. Large-small spin polaron formation is driven therefore only by the magnetic interaction without any significant interplay between lattice and spin degrees of freedom. We can schematize this scenario as a two-phase transition, large magnetic polaron/small magnetic polaron.

The scenario changes upon approaching the adiabatic limit. In the intermediate regime $\omega_0/t=0.5$ we can distinguish a weak electron-phonon coupling regime ($\lambda\leqslant 1$), where the magnetic interaction is still the only relevant energy scale for the large-small spin polaron transition, and the strong-coupling regime ($\lambda>1$), where lattice polaron formation interferes with the magnetic one. The case $\lambda=2$ (dot-dashed line) is representative of this regime. For very small $J/t\to 0$ we recover the usual $N_{\rm s.d.}\simeq cJ^{-1/3}$ behavior, characteristic of the large magnetic polaron. Effective electron-phonon coupling is not sufficient to give the lattice polaron localization and it solely gives a reduction of the prefactor c

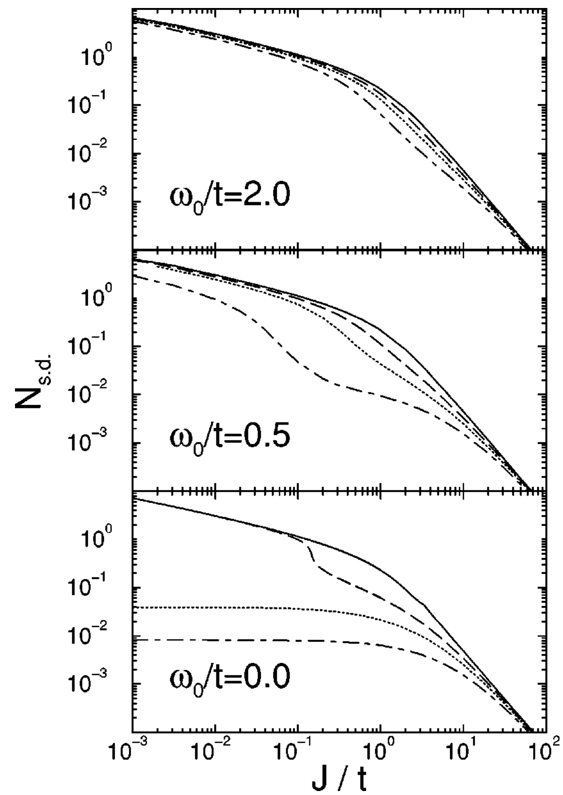

FIG. 5. Mean number of spin defects $N_{\rm s.d.}$ as a function of the exchange coupling J/t for different adiabatic parameters: $\omega_0/t=0.0,0.5,2.0$ and $\lambda=0$ (solid lines), $\lambda=0.5$ (dashed lines), $\lambda=1.0$ (dotted lines), $\lambda=2.0$ (dot-dashed lines).

due to the renormalization of the local hopping amplitude. For larger J, $0.05\lesssim J/t\lesssim 5$, we find a remarkable decrease of the mean number of spin defects $N_{\rm s.d.}$. The origin of such a decrease is not magnetic since in this region $N_{\rm s.d.}$ depends only weakly on the exchange coupling J. We can identify this regime as a small magnetic polaron *induced* by lattice polaron trapping. Finally, for larger interaction, $J/t>5$, the magnetic energy becomes strong enough to overcome the lattice polaron localization and we recover a pure magnetic trapping. The overall evolution from a large magnetic polaron to a small magnetic polaron can be described as two crossovers: large magnetic polaron/small (magnetic) polaron induced by lattice polaron localization/small magnetic polaron.

Crossovers become even sharper upon approaching the adiabatic regime and become a *discontinuous* transition in the adiabatic limit ($\omega_0/t=0.0$ in Fig. 5). Detailed calculations for this particular limit (static lattice distortions) have been explicitly carried out in Appendix B. The dependence of $N_{\rm s.d.}$ on J/t is drastically different in the weak $\lambda<\lambda_c$ and in the strong $\lambda>\lambda_c$ coupling cases. In this latter case, in particular, the particles are almost perfectly trapped and the intermediate region of the small magnetic polaron induced by lattice trapping extends towards $J/t=0$. In the adiabatic limit, for $\lambda>0.844$, we have always the small lattice/magnetic polaron (see Appendix B).

In the above discussion particular care needs to be paid in distinguishing between the character (small/large) and the

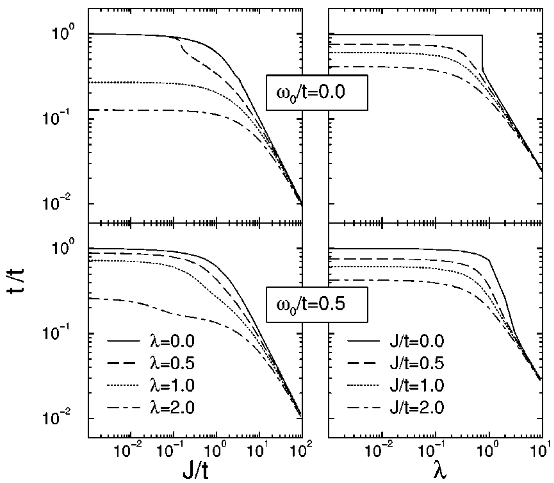

FIG. 6. Effective hopping amplitude t^*/t as a function of the exchange coupling and of the electron-phonon coupling λ.

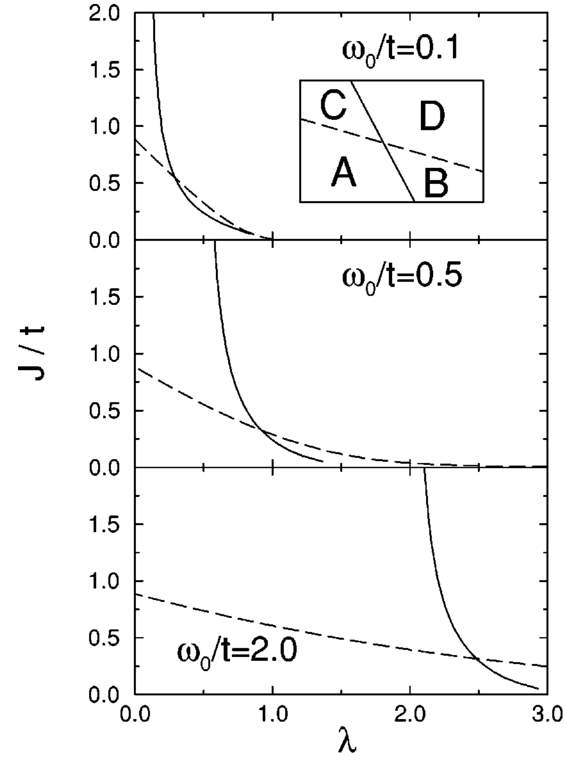

FIG. 7. Polaron phase diagram of the Holstein *t-J* model for different values of the adiabatic ratio ω_0/t. Solid lines denote the lattice polaron formation, dashed lines the large/small spin polaron transition. Inset: pictorial sketch of the generic phase diagram.

nature (magnetic of phononic) of the polaron transition. We can find a similarity between the small/large magnetic polaron and the small/large lattice polaron transition: both of them depend on the local probability of the hole to hop from a site *i* to another site *j*. A suitable quantity to express this concept is the effective hopping amplitude t^*.[16,21,28] Small values of t^*/t denote strong localization of the hole, *regardless of its specific origin* (lattice polaron trapping or small magnetic polaron).

In Fig. 6 we plot t^*/t as a function of the exchange coupling J/t (left panel) and of the electron-phonon coupling λ (right panel) for the cases $\omega_0/t=0.0$ and $\omega_0/t=0.5$. Comparing the left panel of Fig. 6 with the corresponding cases in Fig. 5 we can clearly identify the trends discussed above. For $\lambda\lesssim 1$ the electron-phonon interaction induces only a weak reduction of t^*/t, while the localization transition is essentially driven by the magnetic coupling J/t. When the electron-phonon coupling is strong enough ($\lambda\gtrsim 1$), however, the hole dynamics is strongly suppressed already at $J/t=0$ by lattice polaron trapping, and higher values of J/t are needed to further decrease the effective hopping amplitude by magnetic effects.

This behavior is quite similar when we plot t^*/t as function of λ for different exchange coupling J/t (left panel). We note, however, that the decrease of the kinetic energy at $\omega_0/t=0.5$ is steeper when induced by lattice polaron formation than by the magnetic one. This difference is amplified by approaching the adiabatic regime $\omega_0/t\ll 1$. In the adiabatic limit $\omega_0/t=0$ a discontinuous transition occurs at a small value of J/t around a critical value of the coupling, which in the limit $J/t=0$ approaches the value found in the Holstein model[16] (see Appendix B).

We can now summarize the above study in a global polaronic phase diagram for the Holstein *t-J* model, shown in Fig. 7. The solid line denotes the lattice polaron formation according to the criterion (13) and the dashed line denotes the small/large spin polaron transition with $N_{\mathrm{s.d.}}=0.5$. The dependence of the lattice polaron formation on the magnetic exchange J/t (solid line) and of the spin polaron transition on electron-phonon coupling λ (dashed line) points out the strong interplay between the two kind of processes. In particular, they are not competing but sustaining each other. We can distinguish four regions characterized as follows (see inset in Fig. 7): (*A*) no lattice polaron, large spin polaron; (*B*) lattice polaron, large spin polaron; (*C*) no lattice polaron, small spin polaron; (*D*) lattice polaron, small spin polaron.

It is interesting to compare the evolution of the phase diagram with respect to the adiabatic ratio ω_0/t. For large ω_0/t the lattice polaron formation is not accompanied by a strong hole trapping but appears as a smooth crossover just like the magnetic transition. We can thus identify finite regions (*B*) and (*C*) where lattice and spin polaron can be established independently of each other. Approaching the adiabatic regime ($\omega_0/t=0.1$) the phases (*B*) and (*C*) gradually shrink.

Particular care is needed in the strict adiabatic limit $\omega_0/t=0$. The criterion described, Eq. (13), states the existence of a multiphonon state as a small polaron key feature. Due to the localized nature of the system, lattice distortions with vanishing quantum fluctuation are always present for any finite λ (see Appendix B). This classical lattice state is indeed constituted by an infinite number of phonons giving $\lambda_c=0$ by using the criterion of Eq. (13). Nevertheless we can always identify a discontinuous transition from very small to large lattice distortions, which survives up to $J/t\simeq 0.132$. Explicit results are shown in Fig. 8. It is thus this transition that strongly reduces the electron local hopping t^* and enforces the spin polaron. For larger J/t, such a sharp transi-

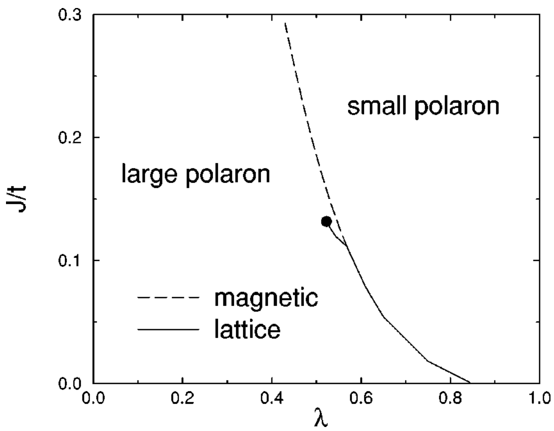

FIG. 8. Adiabatic phase diagram obtained at $\omega_0/t=0$. The solid line denotes the large/small lattice polaron discontinuous transition, the dashed line the large/small spin polaron transition. The sharp large/small lattice polaron transition disappears at $J_c/t \simeq 0.132$ (marked by the filled circle) where it becomes a continuous crossover.

tion disappears and also the small magnetic polaron formation becomes a smooth crossover (dashed line in Fig. 8).

It should be stressed, however, that the extension of the strict adiabatic to the realistic finite adiabatic ratio is relevant as far as quantum fluctuations are small with respect to the average lattice distortion. In the case of $\omega_0/t=0.1$, for instance, quantum fluctuations are larger than the small average lattice distortion found in the adiabatic limit. In this case the multiphonon criterion as described by Eq. (13) denotes as well the small polaron crossover.

V. CONCLUSIONS

We have mapped the half-filled Holstein t-J model on an antiferromagnetic background into a one-particle Hamiltonian (hole interacting with phonons and spin defects), which can be exactly solved in infinite dimension in terms of a continued fraction. The method immediately gives access to the hole spectral density and ground-state properties. The main results of our work can be summarized as follows:

(i) Magnetic and phononic excitations are well separated in the antiadiabatic regime and/or in the strong magnetic regime. In this case phononic peaks are separated by the bare phonon frequency ω_0.

(ii) Magnetic and lattice correlations sustain each other. Not only is polaron crossover shifted to lower coupling by magnetic correlations as noticed in Refs. 21 and 25, but also spin defects are reduced by polaronic effects.

(iii) Phonon retardation is affected for large J/t by magnetic correlations leading the system towards antiadiabatic conditions in which the relevant electron-phonon coupling changes from λ to α. Therefore it is not sufficient to scale λ with the renormalized electron kinetic energy to locate the polaron crossover.

(iv) We identify a crossover region between the regions of parameter space in which magnetic and lattice polarons occur independently (B,C) and the regions $(A$–$D)$ in which they are mutually dependent. We find the rigorous adiabatic regime to be quite peculiar wherein the small magnetic polaron formation is always accompanied by a small polaron formation.

The main drawback of our $d=\infty$ method lies in neglecting the dispersion of spin waves, which leads to hole coherent motion. This is evident in our spectra, which are constituted by **k**-independent peaks. As a starting point to overcome this difficulty we explicitly included in Eq. (2) terms which would lead to hole delocalization as well as to spin-wave dispersion in the next order in $1/z$. A controlled way to include this process is currently under investigation. We expect that taking into account the coherent quasiparticle motion of the hole due to the quantum spin fluctuation would modify the low-energy features of the spectral function by giving rise to finite bands. However we think that the gross features of the spectral weight would not be strongly affected. In addition, the existence of spin fluctuations could lead to the delocalization of the large polaron found in the adiabatic limit at weak coupling.

ACKNOWLEDGMENTS

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APPENDIX A: EXACT SOLUTION OF THE ONE-HOLE HOLSTEIN *T-J* MODEL IN INFINITE DIMENSION

Let us consider the Hamiltonian in Eq. (3), which we write as $H=H_t+H_L$. Here H_t contains the hopping terms and H_L all the other *local* contribution. In the absence of any hole, the ground state is just the antiferromagnetic one, which can be written as $|AF\rangle=|0;0\rangle$, where $|0;0\rangle$ represents the antiferromagnetic background with no phonon and no spin defect on any site. In a similar way we can introduce the notation

$$|n_{(i)},m_{(j)},\ldots;l,k,\ldots\rangle \equiv \left[\frac{(b_i^\dagger)^n}{\sqrt{n}}\frac{(b_j^\dagger)^m}{\sqrt{m}}\ldots\right] \times [a_l^\dagger a_k^\dagger \cdots]|0;0\rangle \qquad \text{(A1)}$$

to express the state with *n* phonons on the site *i*, *m* phonons on the site *j*, and defects of spin on the site *l*, *k*, ...

The aim of investigation is this appendix will be the Green's function[35]

$$G_{ii}(\omega)=\left\langle 0;0\left|h_i\frac{1}{\omega-H}h_i^\dagger\right|0;0\right\rangle, \qquad \text{(A2)}$$

which can be considered as the (0,0) element $[G(\omega)=G^{00}(\omega)]$ of the generalized Green's function

$$G_{ii}^{nm}(\omega)=\left\langle 0;n_i\left|h_i\frac{1}{\omega-H}h_i^\dagger\right|m_i;0\right\rangle. \qquad \text{(A3)}$$

In addition, we introduce the *atomic* propagator

$$g_{ii}^{nm}(\omega)=\left\langle 0;n_i\left|h_i\frac{1}{\omega-H_L}h_i^\dagger\right|m_i;0\right\rangle, \qquad \text{(A4)}$$

which satisfies the following properties ($i\neq j$):

$$\left\langle 0;n_i,m_j\left|h_j\frac{1}{\omega-H_L}h_j^\dagger\right|p_j,n_i;0\right\rangle =\left\langle 0;m_j\left|h_j\frac{1}{\omega-H_L-n\omega_0}h_j^\dagger\right|p_j;0\right\rangle =g_{jj}^{mp}(\omega-n\omega_0) \tag{A5}$$

and

$$\left\langle s_i;p_i\left|h_j\frac{1}{\omega-H_L}h_j^\dagger\right|q_i;s_i\right\rangle =\left\langle 0;p_i\left|h_j\frac{1}{\omega-J/2-H_L}h_j^\dagger\right|q_i;0\right\rangle\delta_{p,q} =\left\langle 0;0\left|h_j\frac{1}{\omega-J/2-H_L-p\omega_0}h_j^\dagger\right|0;0\right\rangle\delta_{p,q} =g_{jj}^{00}(\omega-J/2-p\omega_0)\delta_{p,q}. \tag{A6}$$

Equations (A5) and (A6) stem from the fact that the electron-phonon coupling in H_L is operative only on the site on which the hole stays.

Let us now expand in Eq. (A2) the resolvent $1/(\omega-H)$ in powers of H_t:

$$\frac{1}{\omega-H}=\frac{1}{\omega-H_L}+\frac{1}{\omega-H_L}H_t\frac{1}{\omega-H_L}+\frac{1}{\omega-H_L}H_t\frac{1}{\omega-H_L}H_t\frac{1}{\omega-H_L}+\cdots. \tag{A7}$$

It is easy to see that all the odd powers do not contribute in Eq. (A2) since they create or destroy an odd number of spin defects. More generally, since the initial and final states do not contain spin defects, it is clear that all the spin defects created in the dynamics must be destroyed on each site before reaching the final state. In infinite dimension this constraint selects only the retraceable paths. Each "step forward" is thus ruled by the term $t/(2\sqrt{z})\Sigma_{\langle\alpha\beta\rangle}h_\alpha^\dagger a_\alpha h_\beta$ and each "step backward" by its complex conjugate.

At the second order in t we have, for instance,

$$[G_{ii}^{(2)}(\omega)]^{nm} =\left\langle 0;n_i\left|h_i\frac{1}{\omega-H_L}H_t\frac{1}{\omega-H_L}H_t\frac{1}{\omega-H_L}h_i^\dagger\right|m_i;0\right\rangle =\sum_{\langle\alpha,\beta\rangle}\sum_{\langle\gamma,\delta\rangle}\left\langle 0;n_i\left|h_i\frac{1}{\omega-H_L}\frac{t}{2\sqrt{z}}h_\alpha^\dagger a_\alpha h_\beta\frac{1}{\omega-H_L}\times\frac{t}{2\sqrt{z}}h_\gamma^\dagger a_\delta^\dagger h_\delta\frac{1}{\omega-H_L}h_i^\dagger\right|m_i;0\right\rangle. \tag{A8}$$

Equation (A8) can be expressed in terms of the atomic propagator g by introducing the identity operator in each hopping term: $h_\alpha^\dagger a_\alpha h_\beta=\Sigma_M h_\alpha^\dagger a_\alpha|M\rangle\langle M|h_\beta$, $h_\gamma^\dagger a_\delta^\dagger h_\delta=\Sigma_N h_\gamma^\dagger|N\rangle\langle N|a_\delta^\dagger h_\delta$, where $|M\rangle$, $|N\rangle$ are complete sets of states. It is easy to check that only the states $\Sigma_M|M\rangle\langle M|=\Sigma_p|p_i;s_i\rangle\langle s_i,p_i|$ and $\Sigma_N|N\rangle\langle N|=\Sigma_q|q_i;s_i\rangle\langle s_i,q_i|$ give a nonzero contribution. Using the properties Eqs. (A5) and (A6) we have, thus,

$$[G_{ii}^{(2)}(\omega)]^{nm}=-g_{ii}^{np}(\omega)\frac{t}{2}g_{jj}^{00}(\omega-J/2-p\omega_0)\frac{t}{2}g_{ii}^{pm}(\omega). \tag{A9}$$

Applying a similar procedure for all the orders of the expansion (A7) we obtain a perturbative expression for the Green's function G:

$$G_{ii}^{nm}(\omega)=g_{ii}^{nm}(\omega)-g_{ii}^{np}(\omega)\frac{t}{2}g_{jj}^{00}(\omega-J/2-p\omega_0)\frac{t}{2}g_{ii}^{pm}(\omega)+g_{ii}^{np}(\omega)\frac{t}{2}g_{jj}^{00}(\omega-J/2-p\omega_0)\times\frac{t}{2}\left[g_{ii}^{pq}(\omega)\frac{t}{2}g_{kk}^{00}(\omega-J/2-q\omega_0)\frac{t}{2}g_{ii}^{qm}(\omega)\right]+g_{ii}^{np}(\omega)\frac{t}{2}\left[g_{jj}^{0q}(\omega-J/2-p\omega_0)\frac{t}{2}g_{kk}^{00}(\omega-2J/2-p\omega_0-q\omega_0)\times\frac{t}{2}g_{jj}^{q0}(\omega-J/2-p\omega_0)\right]\frac{t}{2}g_{ii}^{pm}(\omega)+\cdots, \tag{A10}$$

which can be resummed in the compact form (we drop now the site indices),

$$G^{nm}(\omega)=g^{nm}(\omega)-g^{np}(\omega)\frac{t}{2}G^{00}(\omega-J/2-p\omega_0)\frac{t}{2}G^{pm}(\omega), \tag{A11}$$

or in the matricial form,

$$[\mathbf{G}^{-1}(\omega)]^{nm}=[\mathbf{g}^{-1}(\omega)]^{nm}-\delta_{n,m}\frac{t^2}{4}G^{00}(\omega-n\omega_0-J/2). \tag{A12}$$

In particular, the terms in square brackets in Eq. (A10) correspond to the iteration up to the second order, respectively, of $G^{pm}(\omega)$ and of $G^{00}(\omega-J/2-p\omega_0)$ according to Eq. (A11).

Note that the contribution of the hopping processes [second term in Eq. (A12)] is diagonal in the phonon space. This is due to the property (A6), which relies on the locality of the electron-phonon interaction.

From the explicit solution of the atomic problem,

$$[\mathbf{g}^{-1}(\omega)]^{nm}=(\omega-n\omega_0)\delta_{n,m}+gX^{nm}, \tag{A13}$$

where

$$X^{nm}=\sqrt{m+1}\,\delta_{n,m+1}+\sqrt{m}\,\delta_{n,m-1}, \tag{A14}$$

we end up finally with the following self-consistent equation for the Green's function in the multiphonon space:

$$[\mathbf{G}^{-1}(\omega)]^{nm} =gX^{nm}+\delta_{n,m}\left[\omega-n\omega_0-\frac{t^2}{4}G^{00}(\omega-n\omega_0-J/2)\right]. \tag{A15}$$

The solution of Eq. (A15) reduces to the inversion problem of a tridiagonal matrix.[16,36] The diagonal elements G^{nn} can be expressed as continued fractions[16] obtaining Eqs. (4)–(7) and (9)–(11). Equation (A15) looks similar to Eq. (34) of Ref. 16 with the important difference that G_0^{-1} depends now on the exchange energy *J*. The same result can be obtained for G^{00} using diagrammatic techniques as in Ref. 17.

APPENDIX B: ADIABATIC LIMIT

In this appendix we will solve the problem of an electron moving in an infinite coordination *static* lattice. Here we follow the derivation of the adiabatic limit done in the Holstein model in Ref. 16 and we use the same notations. The adiabatic limit is achieved as $M\rightarrow\infty$ keeping $k=M\omega_0^2$ constant. The coupling constant of Hamiltonian Eq. (3) is given in terms of g' by $g=g'/\sqrt{2M\omega_0}$. The polaron energy $\epsilon_p=-g^2/\omega_0=-g'^2/2k$ is then a well-defined quantity in the adiabatic limit. Minimizing the ground-state energy of the Holstein model with respect to the lattice deformation X_i around a given site *i* we have

$$X_i=\frac{g'}{M\omega_0^2}\langle n_i\rangle. \tag{B1}$$

Therefore charge localization around a given site means also a localization of lattice deformations.

The infinite coordination limit together with Eq. (B1) implies that, for a single hole, only one site is appreciably distorted. Around a localization center (site 0) the nearest-neighbor deformation is $O(1/z)$, the next-nearest-neighbor deformation is $[O(1/z^2)]$ and so on, so that the total charge can be spread over several shells of neighbors even in the $z\rightarrow\infty$ limit, but the deformations around a localization center vanishes in the $z\rightarrow\infty$ limit.

From the equation of motion we can derive a hole propagator for a *given* set of lattice deformations.[16] The main simplification of the $d\rightarrow\infty$ limit is then that the elastic energy *is solely determined by the* 0*-site deformation*, for it depends on X_i^2. Consequently we have two kinds of local propagators: one which describes the motion of the electron from site 0 back to site 0 and which depends upon the deformation,

$$G_{00}(\omega)=\frac{1}{\omega+g'X_0-\Sigma_{\rm hop}(\omega)}; \tag{B2}$$

and a second propagator which enters in $\Sigma_{\rm hop}(\omega)$ [Eq. (5)], which does not depend on lattice deformation but *depends on exchange J*,

$$G(\omega)=\frac{1}{\omega-\dfrac{t^2}{4}G(\omega-J/2)}. \tag{B3}$$

It is worth noting that Eqs. (B2 and (B3) can be obtained within the t-J-v_i model of Ref. 17 with on-site energy $v_1=g'X_0$ and zero neighbor energy.

The lowest-energy pole of $G_{0,0}$ gives the electronic energy $E_{\rm el}$ for a given 0-site deformation X_0:

$$E_{\rm el}+g'X_0-\frac{t^2}{4}\mathrm{Re}\left[G\left(E_{\rm el}-\frac{J}{2}\right)\right]=0. \tag{B4}$$

Equation (B4) also defines X_0 as a function of $E_{\rm el}$. By defining properly scaled deformation $X_0=g'u/k$ and energies $E_{\rm el}=t\epsilon$, $E_{\rm tot}=t\epsilon_{\rm tot}$ and exploiting the continued fraction structure[17] of Eq. (B3), we have

$$u(\epsilon)=\frac{1}{2\lambda}\left(\frac{1/4}{\epsilon-J/2-\dfrac{1/4}{\epsilon-J-\dfrac{1/4}{\epsilon-3J/2-\cdots}}}-\epsilon\right). \tag{B5}$$

By adding the elastic contribution we have the total energy which has to be minimized with respect to ϵ:

$$\epsilon_{\rm tot}(\epsilon)=\lambda u^2(\epsilon)-\epsilon. \tag{B6}$$

The total-energy minimization can be carried out explicitly in the strong-coupling limit, i.e., when $J/t\gg 1$ or when $\lambda\gg 1$. In these limits the continued fraction appearing in Eq. (B5) can be neglected giving a linear dependence for *u* ($u=-\epsilon/2\lambda$). The minimization of Eq. (B6) gives $\epsilon=-2\lambda$ and $\epsilon_{\rm tot}=-\lambda$. This limit corresponds to a small lattice/magnetic polaron regime. In this case the deformation "saturates" the charge deformation relation of Eq. (B1) and the hole is perfectly localized on a given site.

Another interesting case is the $J/t\rightarrow 0$ limit. An analytical calculation can be done in this limit following the lines of Ref. 16. We have in this case a solution with vanishing deformation which gives the lowest energy for $\lambda<0.844$. In this case the Green function is the same of Ref. 17 and consists of a semicircular band of *localized* states, and a solution with nonzero deformation which gives the lowest energy for $\lambda>0.844$. In this case a pole emerges out of the band at low energies.

The transition at $\lambda_c=0.844$ is found to be discontinuous. It is important to notice that even if it is possible to follow the formal steps of Ref. 16 to recover these solutions, the physical interpretation of the case with vanishing deformation is quite different. In particular, we may understand this solution as describing a *localized* large lattice/magnetic polaron in the limit of infinitely large polaronic radius in contrast to the case of the pure Holstein model, where in this case the motion of the electron is *coherent* through the lattice.[16] Instead a solution associated with a nonvanishing deformation has the same character in both models, i.e., it describes a localized small polaron.

In the general case the minimization of Eq. (B6) can be easily carried out numerically. Derivatives of the ground-state energy with respect to g' and J gives, respectively, the hole-phonon and the exchange (mean number of spin defects) contributions to the total energy, the hole kinetic energy being obtained by subtraction. These derivatives of the ground-state energy are discontinuous at the transition found for $J/t=0$ at $\lambda_c=0.844$. The discontinuous large to small lattice/magnetic polaron transition exists up to $J/t=0.132$. For larger magnetic couplings a smooth crossover takes place.

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