Polaron features for long-range electron-phonon interaction

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The polaron features for long-range electron-phonon interaction are investigated by extending a variational approach previously proposed for the study of systems with local coupling. The ground-state spectral weight, the average kinetic energy, the mean number of phonons, and the electron-lattice correlation function are discussed for a wide range of model parameters focusing on the adiabatic regime and comparing the results with the short-range case (Holstein model). A strong mixing of electronic and phononic degrees of freedom for small values of the electron-phonon coupling constant is found in the adiabatic case due to the long-range interaction. Finally a polaron "phase diagram" is proposed.
I. INTRODUCTION

In the last years many experimental results have pointed out the presence of strong electron-phonon (el – ph) coupling and polaronic effects in several compounds, such as high-temperature cuprate superconductors and colossal magnetoresistance manganites.\textsuperscript{1,2} This large amount of experimental data has renewed the interest in studying simplified el – ph coupled systems of the Holstein\textsuperscript{3} or Fröhlich\textsuperscript{4} type and in proposing more realistic interaction models.\textsuperscript{5,6}

The Holstein molecular crystal model is the prototype for short-range (SR) el – ph interaction since it takes into account local coupling of a tight-binding electron to optical local phonon modes. Till now an exact solution for this model has not been found and perturbative expansions are not able to describe the most interesting region characterized by intermediate el – ph couplings and electron and phonon energy scales not well separated. In this regime, as shown by several numerical studies\textsuperscript{7–11} and variational approaches,\textsuperscript{12–14} the system undergoes a crossover from a weakly dressed electron to a massive localized polaronic quasiparticle, the small Holstein polaron (SHP), with increasing the strength of interaction. All the ground state properties of the Holstein model can be described with great accuracy by a variational approach\textsuperscript{13,14} based on a linear superposition of Bloch states that describe weak and strong coupling polaron wave functions. Indeed this method provides an immediate physical interpretation of the intermediate regime and is in excellent agreement with numerical results.

Recently a quite general el – ph lattice Hamiltonian with a ”density-displacement” type interaction has been introduced in order to understand the role of long-range (LR) coupling on the polaron formation.\textsuperscript{5,15} The model for a single particle is described by the Hamiltonian

\begin{equation}
H = -t \sum_{<i,j>} c_i^\dagger c_j + \omega_0 \sum_i \left( a_i^\dagger a_i + \frac{1}{2} \right) + \alpha \omega_0 \sum_{i,j} f(||\vec{R}_i - \vec{R}_j||) c_i^\dagger c_i \left( a_j + a_j^\dagger \right).
\end{equation}

The units are such that \( \hbar = 1 \). In Eq.(1) \( c_i^\dagger (c_i) \) denotes the electron creation (annihilation)
operator at site $i$, whose position vector is indicated by $\vec{R}_i$, and the symbol $<>$ denotes nearest neighbours linked through the transfer integral $t$. The operator $a_i^\dagger$ ($a_i$) represents the creation (annihilation) operator for phonon on the site $i$, $\omega_0$ is the frequency of the optical local phonon modes, $\alpha$ controls the strength of $el-ph$ coupling, and $f(|\vec{R}_i - \vec{R}_j|)$ is the interacting force between an electron on the site $i$ and an ion displacement on the site $j$.

The Hamiltonian (1) reduces to the Holstein model if $f(|\vec{R}_i - \vec{R}_j|) = \delta_{\vec{R}_i, \vec{R}_j}$, while in general it contains $LR$ interaction. In particular when one attempts to mimic the nonscreened coupling between doped holes and apical oxygen in some cuprates, the interaction force is given by

$$f(|\vec{R}_i - \vec{R}_j|) = \left(|\vec{R}_i - \vec{R}_j|^2 + 1\right)^{-\frac{3}{4}},$$

(2)

if the distance $|\vec{R}_i - \vec{R}_j|$ is measured in units of lattice constant. Considering the general $el-ph$ matrix element $M_{\vec{q}}$

$$M_{\vec{q}} = \frac{\alpha \omega_0}{\sqrt{L}} \sum_m f(|\vec{R}_m|) e^{i \vec{q} \cdot \vec{R}_m},$$

(3)

with $L$ number of lattice sites, we can define the polaronic shift $E_p$

$$E_p = \sum_{\vec{q}} \frac{M_{\vec{q}}^2}{\omega_0},$$

(4)

and the coupling constant $\lambda = E_p/zt$, with $z$ lattice coordination number, that represents a natural measure of the strength of the $el-ph$ interaction in both $SR$ and $LR$ case. Clearly for $LR$ interaction forces the matrix element $M_{\vec{q}}$ is peaked around $\vec{q} = 0$. Since it has been claimed that the enhancement of the forward direction in the $el-ph$ scattering could play a role in explaining several anomalous properties of cuprates as the linear temperature behaviour of the resistivity and the $d$-wave symmetry of the superconducting gap, the study of lattice polaron features for $LR$ interactions is important in order to clarify the role of the $el-ph$ coupling in complex systems.

When the interaction force is given by Eq. (2), the model has been investigated applying a path-integral Monte-Carlo ($PIMC$) algorithm efficient in the thermodynamic limit. The
first investigations have been mainly limited to the determination of the polaron effective mass pointing out that, due to the $LR$ coupling, the polaron is much lighter than the $SHP$ with the same binding energy in the strong coupling regime. Furthermore it has been found that this effect due to the weaker band renormalization becomes smaller in the antiadiabatic regime. Then the quasi-particle properties have been studied by an exact Lanczos diagonalization method$^{18}$ on finite one-dimensional lattices (up to 10 sites) making a close comparison with the corresponding properties of $HP$. As a result of the $LR$ interaction, the lattice deformation induced by the electron is spread over many lattice sites in the strong coupling region giving rise to the formation of a large polaron ($LP$) as in the weak coupling regime. All numerical and analytical results have been mainly obtained in the antiadiabatic and non-adiabatic regime. Only recently the behavior of the effective mass of a two-site system$^{19}$ in the adiabatic regime has been studied within the nearest-neighbor approximation for the $el – ph$ interaction confirming that the $LP$ is lighter than the $SHP$ at strong coupling.

In this paper we pursue the study of the ground state of the model with the interaction force given by Eq. (2) in the thermodynamic limit. We employ a variational approach previously proposed for the study of systems with $el – ph$ local coupling$^{13,14}$ and based on a linear superposition of Bloch states that describe weak and strong coupling polaron wave functions. Although the method is valid for any spatial dimension, we limit our study to the one-dimensional case. It has been found that the variational approach provides an estimate of the ground state energy in good agreement with $PIMC$ results. The evolution of the ground-state spectral weight, the average kinetic energy, the mean number of phonons, and the electron-lattice correlation function with respect to the adiabaticity ratio $\omega_0/t$ and the $el – ph$ coupling constant is discussed focusing on the adiabatic regime. Indeed, in the adiabatic case, there is a range of values of the $el – ph$ coupling where the ground state is well described by a particle with a weakly renormalized mass but a spectral weight much smaller than unity. Furthermore, with increasing the strength of interaction in the same regime, the renormalized mass gradually increases, while the average kinetic energy is not
strongly reduced. Finally regions of the model parameters are distinguished according to the values assumed by the spectral weight. The resulting "phase diagram"\textsuperscript{20} shows strong mixing of electronic and phononic degrees of freedom for small values of the $el-ph$ coupling constant in the adiabatic case.

II. VARIATIONAL WAVE FUNCTION

The variational approach is summarized following the lines of previous works.\textsuperscript{13,14}

We consider as trial wave functions translational invariant Bloch states obtained by taking a superposition of localized states centered on different lattice sites:

$$ |\psi^{(i)}(i\vec{k})(\vec{R}_n)\rangle = \frac{1}{\sqrt{L}} \sum_{\vec{R}_n} e^{i\vec{k} \cdot \vec{R}_n} |\psi^{(i)}(i\vec{k})(\vec{R}_n)\rangle, \quad (5) $$

where

$$ |\psi^{(i)}(i\vec{k})(\vec{R}_n)\rangle = e^{\sum_{\vec{q}} \left[h^{(i)}(\vec{k})a_{\vec{q}} e^{i\vec{q} \cdot \vec{R}_n + h.c.}\right] \sum_{m} \phi^{(i)}(i\vec{k}\vec{R}_m) c^\dagger_m|0\rangle. \quad (6) $$

In Eq. (5) the apex $i = w, s$ indicates the weak and strong coupling polaron wave function, respectively, $|0\rangle$ denotes the electron and phonon vacuum state, and $\phi^{(i)}(i\vec{k}\vec{R}_m)$ are variational parameters defining the spatial broadening of the electronic wave function. The phonon distribution functions $h^{(i)}(\vec{q})(\vec{k})$ are chosen in order to reproduce the description of polaron features in the two asymptotic limits.\textsuperscript{13} Therefore the weak coupling phonon distribution function $h^{(w)}(\vec{q})(\vec{k})$ is assumed as

$$ h^{(w)}(\vec{q})(\vec{k}) = \frac{M_{\vec{q}}}{\omega_0 + E_b(\vec{k} + \vec{q}) - E_b(\vec{k})}, \quad (7) $$

where $E_b(\vec{k})$ is the free electron band energy, while the strong coupling phonon distribution function $h^{(s)}(\vec{q})(\vec{k})$ as

$$ h^{(s)}(\vec{q})(\vec{k}) = \frac{M_{\vec{q}}}{\omega_0} \sum_m |\phi^{(i)}(\vec{k}\vec{R}_m)|^2 e^{i\vec{q} \cdot \vec{R}_m}. \quad (8) $$

A careful inspection of weak and strong coupling wave functions shows that in the intermediate regime they are not orthogonal and the off-diagonal matrix elements of the
Hamiltonian are not zero. Hence the ground state energy is determined by considering as trial state a linear superposition of the weak and strong coupling wave functions:

\[ |\psi_{\vec{k}}^{\bar{\bar{w}}} \rangle = \frac{A_{\vec{k}} |\psi^{(w)}_{\vec{k}} \rangle + B_{\vec{k}} |\psi^{(s)}_{\vec{k}} \rangle}{\sqrt{A_{\vec{k}}^2 + B_{\vec{k}}^2 + 2A_{\vec{k}}B_{\vec{k}}S_{\vec{k}}}}, \]

where

\[ |\psi^{(w)}_{\vec{k}} \rangle = \frac{|\psi^{(w)}_{\vec{k}} \rangle}{\sqrt{\langle \psi^{(w)}_{\vec{k}} | \psi^{(w)}_{\vec{k}} \rangle}}, \quad |\psi^{(s)}_{\vec{k}} \rangle = \frac{|\psi^{(s)}_{\vec{k}} \rangle}{\sqrt{\langle \psi^{(s)}_{\vec{k}} | \psi^{(s)}_{\vec{k}} \rangle}}, \]

and

\[ S_{\vec{k}} = \frac{\langle \psi^{(w)}_{\vec{k}} | \psi^{(s)}_{\vec{k}} \rangle + h.c.}{2} \]

is the overlap factor of the two wave functions \( |\psi^{(w)}_{\vec{k}} \rangle \) and \( |\psi^{(s)}_{\vec{k}} \rangle \). In Eq.(9) \( A_{\vec{k}} \) and \( B_{\vec{k}} \) are two additional variational parameters which provide the relative weight of the weak and strong coupling solutions of the system for any particular value of \( \vec{k} \).

We perform the minimization procedure with respect to the parameters \( \phi^{(w)}_{\vec{k}} (\vec{R}_m) \), \( \phi^{(s)}_{\vec{k}} (\vec{R}_m) \), \( A_{\vec{k}} \) and \( B_{\vec{k}} \), assuming

\[ \phi^{(i)}_{\vec{k}} (\vec{R}_m) = \alpha^{(i)}_{\vec{k}} \delta_{\vec{R}_m,0} + \beta^{(i)}_{\vec{k}} \sum_{\delta} \delta_{\vec{R}_m,\delta} + \gamma^{(i)}_{\vec{k}} \sum_{\delta'} \delta_{\vec{R}_m,\delta'} + \eta^{(i)}_{\vec{k}} \sum_{\delta''} \delta_{\vec{R}_m,\delta''}, \]

where the quantities \( \alpha^{(i)}_{\vec{k}} \), \( \beta^{(i)}_{\vec{k}} \), \( \gamma^{(i)}_{\vec{k}} \), and \( \eta^{(i)}_{\vec{k}} \) denote variational parameters, and the symbols \( \delta \), \( \delta' \), \( \delta'' \) indicate, respectively, the nearest, the next-nearest neighbors and so on. This choice takes into account the broadening of the electron wave functions up to third neighbors and provides an accurate description of the polaron features for any value of the parameters of the Hamiltonian. The ground state energies obtained with this choice are slightly higher than PIMC mean energies, being the difference less than 0.5% in the worst case of intermediate regime. We note that these wave functions can be improved adding further terms in Eq. (12), so it is possible to obtain better and better estimates of the energy.

**III. RESULTS**

In this paper we study the properties of the ground-state in the one-dimensional case.
In Fig. 1(a) we report the polaron ground state energy for different values of the adiabaticity ratio as a function of the \(el - ph\) constant coupling \(\alpha\). We have checked that our variational proposal recovers the asymptotic perturbative results and improves significantly these asymptotic estimates in the intermediate region. Moreover, our data for the ground-state energy in the intermediate region are in very good agreement with the results of the \textit{PIMC} approach\textsuperscript{5} shown as diamonds in Fig. 1(a). The consistency of the results with a numerically more sophisticated approach indicates that the true wave function is very close to a superposition of weak and strong coupling states.

Another property of interest is the ground state spectral weight \(Z\)

\[
Z = Z_{k=0} = |<\psi_{k=0}|c_{k=0}^\dagger|0>|^2, \tag{13}
\]

that gives the fraction of the bare electron state in the polaronic trial wave function. It measures how much the quasiparticle is different from the free electron \((Z = 1)\), and a small value of \(Z\) indicates a strong mixing of electronic and phononic degrees of freedom. As plotted in Fig. 1(b), the increase of the \(el - ph\) coupling strength induces a decrease of the spectral weight that is smooth also in the adiabatic regime. The reduction of \(Z\) is closely related to the decrease of the Drude weight obtained by exact diagonalizations\textsuperscript{18} pointing out a gradual suppression of coherent motion. We note that the behavior of \(Z\) is different from that of the local Holstein model. In fact for the latter \(Z\) results to be very close to the ratio \(m/m^*\), with \(m\) and \(m^*\) bare electron and effective polaron mass, respectively,\textsuperscript{18} while for \(LR\) couplings \(Z < m/m^*\) in the intermediate to strong coupling adiabatic regime. This relation is confirmed by the results shown in Fig.1 (b), where the dash-dotted line and the squares on a similar line indicate the spectral weight \(Z\) and the ratio \(m/m^*\) obtained within the variational approach, respectively, as a function of the coupling constant \(\alpha\) at \(\omega_0/t = 0.25\).\textsuperscript{15}

Actually there is a large region of the parameters in the adiabatic regime where the ground state is well described by a particle with a weakly renormalized mass but a spectral weight \(Z\) much smaller than unity. While the electron drags the phonon cloud coherently through the lattice, with increasing the \(el - ph\) coupling in the adiabatic case, a band collapse occurs
in the $SR$ case, while the particle undergoes a weaker band renormalization in the case of $LR$ interactions. Therefore in the $LR$ case the polaron results lighter than the $SHP$ in the intermediate to strong coupling adiabatic regime.

Insight about the electron state is obtained by calculating its kinetic energy $K$ in units of the bare one. Since the average kinetic energy gives the total weight of the optical conductivity, $K$ includes both coherent and incoherent transport processes.\textsuperscript{18} As reported in Fig. 1(b) and Fig. 1(c), in the strong coupling adiabatic region before the electron is selftrapped ($K \ll 1$), the average kinetic energy is weakly renormalized, the ratio $m/m^*$ is reduced and the spectral weight is nearly zero. Furthermore, in Figs. 1(c) and 1(d), within the adiabatic regime, the average kinetic energy and the mean number of phonons do not show any sharp change by increasing the $el$ $-$ $ph$ coupling.

Another quantity associated to the polaron formation is the correlation function $S(R_l)$

$$S(R_l) = S_{k=0}(R_l) = \frac{\sum_n <\psi_{k=0}|c_{n}^{\dagger}c_{n}(a_{n+l}^{\dagger} + a_{n+l})|\psi_{k=0}>}{<\psi_{k=0}|\psi_{k=0}>}$$

or equivalently the normalized correlation function $\chi(R_l) = S(R_l)/N$, with $N = \sum_l S(R_l)$. In Fig. 2(a) we report the correlation function $S(R_l)$ at $\omega_0/t = 1$ for several values of the $el$ $-$ $ph$ interaction. The lattice deformation is spread over many lattice sites giving rise to the formation of $LP$ also in the strong coupling regime where really the correlation function assumes the largest values. In the inset of Fig. 2(a) the normalized electron-lattice correlation function $\chi$ shows consistency with the corresponding quantity calculated in a previous work.\textsuperscript{18} While in the weak coupling regime the amplitude $\chi$ is smaller than the quantum lattice fluctuations, increasing the strength of the interaction, it becomes stronger and the lattice deformation is able to generate an attractive potential that can trap the charge carrier. Clearly, even if the correlations between electron and lattice are large, the resulting polaron is delocalized over the lattice due to the translational invariance. Finally the variation of the lattice deformation as a function of $\omega_0/t$ shown in Fig. 2(b) can be understood as a retardation effect. In fact, for small $\omega_0/t$, the less numerous phonons excited by the passage of the electron take a long time to relax, therefore the lattice deformation
increases far away from the current position of the electron.

In Fig. 3 we propose a "phase diagram" based on the values assumed by the spectral weight in analogy with the Holstein polaron.\textsuperscript{14} Analyzing the behavior of $Z$ it is possible to distinguish three different regimes: (1) quasi-free-electron regime ($0.9 < Z < 1$) where the electron has a weakly renormalized mass and the motion is coherent; (2) crossover regime ($0.1 < Z < 0.9$) characterized by intermediate values of spectral weight and a mass not strongly enhanced; (3) strong coupling regime ($Z < 0.1$) where the spectral weight is negligible and the mass is large but not enormous. We note that for LR interactions in the adiabatic case there is strong mixing of electronic and phononic degrees of freedom for values of the coupling constant $\lambda$ (solid lines) smaller than those characteristic of local Holstein interaction (dashed lines). Furthermore in this case, entering the strong coupling regime, the charge carrier does not undergo any abrupt localization, on the contrary, as indicated also by the behavior of the average kinetic energy $K$, it is quite mobile.

In order to study the effects of different $el - ph$ interactions, we have evaluated the average kinetic energy for both LR and SR cases. As reported in Fig. 4(a), in excellent agreement with a previous study,\textsuperscript{18} for LR interactions $K$ decreases very gradually with increasing $\lambda$. Furthermore, if the regime of parameters where the spectral weight $Z = 0.1$ is considered, as shown in Fig. 4(b), in the adiabatic case the average kinetic energy is larger for LR interactions (solid line) with respect to local Holstein ones (dashed line). The comparison emphasizes that due to LR interactions in the adiabatic regime $K$ is slightly renormalized even if the coherent motion is small.

\textbf{IV. CONCLUSIONS}

In this paper we have extended a previous variational approach in order to study the polaronic ground-state features of a one dimensional $el - ph$ model with long-range interaction. The trial function is based on a linear superposition of Bloch states that describe weak and strong coupling polaron wave functions and it provides an estimate of the ground state
energy in good agreement with numerical methods. The results relative to spectral weight, the average kinetic energy, the mean number of phonons, and the electron-lattice correlation function have been discussed mainly in the adiabatic regime. It has been possible to identify a range of intermediate values of the "el – ph" coupling constant in the adiabatic case where the system is well described by a particle characterized with a weakly renormalized mass but a small spectral weight. In the same regime, further increasing the "el – ph" coupling, the renormalized mass shows a smooth increase, while the average kinetic energy is not strongly reduced. Finally we have proposed a "phase diagram" according to the values assumed by the spectral weight. It is found that there is strong mixing between electronic and phononic degrees of freedom for small values of the "el – ph" coupling constant in the adiabatic case.

The variational approach can be easily generalized to high dimensions, and it has been recently applied to study the three dimensional continuum Fröhlich model giving a very good description of ground state features. In any case the results discussed in this paper are not limited to the one-dimensional case as confirmed by the behavior of some properties on the square lattice.

**FIGURE CAPTIONS**

Fig.1 The ground state energy $E_0$ in units of $\omega_0$ (a), the spectral weight $Z$ (b), the average kinetic energy $K$ (c) and the average phonon number $N$ (d) as a function of the coupling constant $\alpha$ for different values of the adiabatic ratio: $\omega_0/t = 2$ (solid line), $\omega_0/t = 1$ (dashed line), $\omega_0/t = 0.5$ (dotted line) and $\omega_0/t = 0.25$ (dash-dotted line). The diamonds in figure (a) indicate the PIMC data for the energy kindly provided by P. E. Kornilovitch at $\omega_0/t = 1$, and the squares on a dash-dotted line in figure (b) denote the ratio $m/m^*$ obtained within the variational approach at $\omega_0/t = 0.25$.

Fig.2 (a) The electron-lattice correlation function $S(R_l)$ at $\omega_0/t = 1$ for different values of the coupling: $\lambda = 0.5$ (circles), $\lambda = 1.25$ (squares), $\lambda = 2.0$ (diamonds), $\lambda = 2.75$ (triangles up), and $\lambda = 3.5$ (triangles down). In the inset the normalized correlation
function $\chi(R_l)$ at $\omega_0/t = 1$ for $\lambda = 0.5$ (circles) and $\lambda = 2.75$ (squares).

(b) The electron-lattice correlation function $S(R_l)$ at $\alpha = 2$ for different values of the adiabatic parameter: $\omega_0/t = 2$ (circles), $\omega_0/t = 1$ (squares), $\omega_0/t = 0.5$ (diamonds), and $\omega_0/t = 0.25$ (triangles up).

Fig. 3 Polaron "phase diagram" for long-range (solid line) and Holstein (dashed line) $el-ph$ interaction. The transition lines correspond in weak coupling to model parameters such that the spectral weight $Z = 0.9$, in strong coupling such that $Z = 0.1$.

Fig. 4 (a) The average kinetic energy $K$ as a function of the constant coupling $\lambda$ at $\omega_0/t = 1$ for long-range (solid line) and local Holstein $el-ph$ interaction (dashed line).

(b) The average kinetic energy $K$ as a function of the adiabaticity ratio $\omega_0/t$ for long-range (solid line) and Holstein (dashed line) $el-ph$ interaction in correspondence of model parameters such that the spectral weight $Z = 0.1$.

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We use the phrase phase diagram between inverted commas to indicate that there is no true phase transition in this one-electron system but a crossover from a quasi-free electron to a carrier strongly coupled to the lattice.

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Crossover

Strong coupling
