Effects of electron-phonon coupling range on the polaron formation

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The polaron features due to electron-phonon interactions with different coupling ranges are investigated by adopting a variational approach. The ground-state energy, the spectral weight, the average kinetic energy, the mean number of phonons, and the electron-lattice correlation function are discussed for the system with coupling to local and nearest neighbor lattice displacements comparing the results with the long range case. For large values of the coupling with nearest neighbor sites, most physical quantities show a strong resemblance with those obtained for the long range electron-phonon interaction. Moreover, for intermediate values of interaction strength, the correlation function between electron and nearest neighbor lattice displacements is characterized by an upturn as function of the electron-phonon coupling constant.
I. INTRODUCTION

In the last years effects due to strong electron-phonon (el – ph) interactions and polaronic signatures have been evidenced in several compounds, such as high-temperature cuprate superconductors\cite{2} collosal magnetoresistance manganites\cite{3,4}, fullerenes\cite{5}, carbon nanotubes\cite{6} and DNA\cite{7}. This amount of experimental data has stimulated the study of different el – ph coupled systems. Among the most studied models there are the Holstein lattice model\cite{8} characterized by a very short-range (SR) el – ph interaction, and the Fröhlich model\cite{9} that takes into account long-range (LR) el – ph couplings in polar compounds treating the dielectric as a continuum medium. Moreover, more realistic lattice interaction models including both SR and LR couplings have been recently introduced\cite{10}.

Within the Holstein model a tight-binding electron locally couples to optical phonon modes. For intermediate el – ph couplings and electron and phonon energy scales not well separated, it has been found by numerical studies\cite{9,11,13} and variational approaches\cite{10,11,13} that the system undergoes a crossover from a weakly dressed electron to a massive localized polaronic quasiparticle, the small Holstein polaron (SHP). A variational approach\cite{10,14} proposed by some of us and based on a linear superposition between the Bloch states characteristic of the weak and strong coupling regime is able to describe all the ground state properties with great accuracy. Moreover this method provides an immediate physical interpretation of the intermediate regime characterized by the polaron crossover.

Recently a discrete version of the Fröhlich model has been introduced in order to understand the role of LR coupling on the formation of the lattice polaron\cite{15}. Due to the LR interaction, the polaron is much lighter than the SHP with the same binding energy in the strong coupling regime\cite{15}. Furthermore the lattice deformation induced by the electron is spread over many lattice sites giving rise to the formation of a large polaron (LP) also in the strong coupling region\cite{16}. Extending the variational approach previously proposed for the study of systems with local el – ph coupling, many properties have been studied by some of us as a function of the model parameters focusing on the adiabatic regime\cite{15}. Indeed 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 due to the LR coupling a strong mixing between electronic and phononic degrees of freedom has been found even for small values of the el – ph coupling constant.

Both the SR Holstein and the LR discrete Fröhlich model can be described by a quite general Hamiltonian $H$

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

(1)

where $f(|\vec{R}_i - \vec{R}_j|)$ is the interacting force between an electron on the site $i$ and an ion displacement on the site $j$. 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 neighbors (nn) 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, and $\alpha$ controls the strength of el – ph coupling. The units are such that $\hbar = 1$. The Hamiltonian (1) reduces to the Holstein model for

$$f(|\vec{R}_i - \vec{R}_j|) = \delta_{\vec{R}_i,\vec{R}_j},$$  

(2)

while in the LR case\cite{15} the interaction force is given by

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

(3)

if the distance $|\vec{R}_i - \vec{R}_j|$ is measured in units of lattice constant.

In addition to the SR and LR case, in this work we analyze the properties of the system where the electron couples with local and nn lattice displacements. In this case the interaction force becomes

$$f(|\vec{R}_i - \vec{R}_j|) = \delta_{\vec{R}_i,\vec{R}_j} + \frac{\alpha_1}{\alpha} \sum_{\delta} \delta_{\vec{R}_i + \delta,\vec{R}_j},$$  

(4)

where $\delta$ indicates the nn sites. For all the couplings of Eqs. (2-4) the el – ph matrix element in the momentum space $M_\mathbf{q}$ is

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

(5)
with $L$ number of lattice sites. Through the matrix element $M_{\mathbf{q}}$ we can define the polaronic shift $E_p$ 

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

(6)

and the coupling constant $\lambda = E_p / z t$, with $z$ lattice coordination number, that represents a natural measure of the strength of the \( el - ph \) coupling for any range of the interaction. Limiting the analysis to the one-dimensional case, the matrix element $M_{\mathbf{q}}$ is reported in Fig. 1 for the $SR$, $LR$, and $nn$ extended range (ER) couplings. In the $SR$ case the coupling is constant as function of the transferred phononic momentum, while in the $LR$ case the vertex is peaked around $q \approx 0$. With increasing the ratio $\alpha_1 / \alpha$, the $ER$ interaction deviates from the constant behavior developing a peak around $q \approx 0$. Actually for the ratio $\alpha_1 / \alpha = 0.3$ the interaction vertex of the $ER$ case is close to the behavior of the $LR$ coupling.

In this paper we adopt the variational approach previously proposed$^{15,16,20}$ for the study of systems with local and $LR$ $el - ph$ interactions in order to study the system with $nn$ $ER$ $el - ph$ coupling. The aim is to investigate the crossover from $SR$ to $LR$ interactions in the $ER$ model. 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 spectral weight giving rise to a polaronic phase diagram. The transition line between the crossover and the strong coupling regime continuously evolves toward that of the $LR$ case by increasing the coupling of the $ER$ system. Finally, for intermediate values of this coupling, the correlation function between electron and $nn$ lattice displacements shows an upturn with increasing the $el - ph$ constant $\lambda$.

In section II the variational approach is reviewed, while in section III the results are discussed.

II. VARIATIONAL WAVE FUNCTION

In this section the variational approach is briefly summarized. Details can be found in previous works.$^{15,16}$

The trial wave functions are translational invariant Bloch states obtained by taking a superposition of localized states centered on different lattice sites

$$|\psi_{\mathbf{k}}^{(i)}> = \frac{1}{\sqrt{L}} \sum_{\mathbf{R}_n} e^{i\mathbf{k} \cdot \mathbf{R}_n} |\psi_{\mathbf{k}}^{(i)}(\mathbf{R}_n)>,$$  

(7)

where

$$|\psi_{\mathbf{k}}^{(i)}(\mathbf{R}_n)> = \sum_{m} \sum_{\mathbf{q}} [\phi_{\mathbf{k}}^{(i)}(\mathbf{q}) e^{i \mathbf{q} \cdot \mathbf{R}_n}] \phi_{\mathbf{m}}^{(i)}(\mathbf{R}_m) e^{i \mathbf{q} \cdot \mathbf{R}_m} |0>.$$  

(8)

In Eq. (7) the apex $i = w, s$ indicates the weak and strong coupling polaron wave function, respectively, $|0>$ denotes the electron and phonon vacuum state, and $\phi_{\mathbf{k}}^{(i)}(\mathbf{R}_m)$ are variational parameters defining the spatial broadening of the electronic wave function. The phonon distribution functions $h_{\mathbf{q}}^{(i)}(\mathbf{k})$ are chosen in order to reproduce polaron features in the two asymptotic limits.$^{15}$

In the intermediate regime the weak and strong coupling wave functions are not orthogonal and the off-diagonal matrix elements of the Hamiltonian are not zero. Therefore the ground state properties are determined by considering as trial state $|\psi_{\mathbf{k}}> = a linear superposition of the weak and strong coupling wave functions

$$|\psi_{\mathbf{k}}>= \frac{A_{\mathbf{k}}|\psi_{\mathbf{k}}^{(w)}> + B_{\mathbf{k}}|\psi_{\mathbf{k}}^{(s)}>}{\sqrt{A_{\mathbf{k}}^2 + B_{\mathbf{k}}^2 + 2A_{\mathbf{k}}B_{\mathbf{k}}S_{\mathbf{k}}}},$$  

(9)

where

$$|\psi_{\mathbf{k}}^{(w)}> = |\psi_{\mathbf{k}}^{(w)}> / \sqrt{<\psi_{\mathbf{k}}^{(w)}|\psi_{\mathbf{k}}^{(w)}>}, \quad |\psi_{\mathbf{k}}^{(s)}> = |\psi_{\mathbf{k}}^{(s)}> / \sqrt{<\psi_{\mathbf{k}}^{(s)}|\psi_{\mathbf{k}}^{(s)}>},$$  

(10)
\[ \frac{S_{\vec{k}}}{2} = \frac{\langle \bar{\psi}_{\vec{k}}^{(w)} | \psi_{\vec{k}}^{(s)} \rangle + h.c.}{\langle \psi_{\vec{k}}^{(w)} | \psi_{\vec{k}}^{(s)} \rangle} \]

is the overlap factor of the two wave functions \( |\psi_{\vec{k}}^{(w)}\rangle \) and \( |\psi_{\vec{k}}^{(s)}\rangle \). 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 for any particular value of \( \vec{k} \). The variational minimization is performed extending the electron wave function up to fifth neighbors.

### III. RESULTS

In this section we discuss ground state properties in the one-dimensional case for the different ranges of \( el - ph \) coupling.

In Fig. 2(a) we report the polaron ground state energy as a function of the \( el - ph \) constant coupling \( \lambda \). The variational method recovers the perturbative results and improves significantly these asymptotic estimates in the intermediate region. In this regime the energy decreases with increasing the range of the \( e - ph \) coupling. Moreover, with increasing the range of the coupling, the crossover between the weak and strong coupling solution becomes less evident. Actually, as shown in Fig. 2(b), there are marked differences in the ratio \( B/A \) that is the weight of the strong coupling solution with respect to the weak coupling one. In the \( SR \) case the strong coupling solution provides all the contribution since the overlap with the weak coupling function is negligible. However, with increasing the range of the interaction, the weight of the weak coupling function increases and the polaronic crossover becomes smooth. Another quantity that gives insight about the properties of the electron state is the average kinetic energy of the interaction, the weight of the weak coupling function increases and the polaronic crossover becomes smooth.

In addition to the quantities discussed in Fig. 2, other properties change remarkably with increasing the ratio \( \alpha_3/\alpha \). An interesting property is the ground state spectral weight \( Z \), that measures the fraction of the bare electron state in the polaronic trial wave function. As plotted in Fig. 3(a), the increase of the \( el - ph \) coupling strength induces a decrease of the spectral weight that is more evident with increasing the range of the \( el - ph \) coupling. In the strong coupling regime the spectral weights calculated for different ranges assume similar small values. While for the local Holstein model \( Z = m/m^* \), as the \( LR \) case is considered, \( Z \) becomes progressively smaller than \( m/m^* \) in analogy with the behavior due to the \( LR \) interaction. We have found that for the ratio \( \alpha_3/\alpha = 0.3 \) there is a region of intermediate values of \( \lambda \) where the ground state is described by a particle with a weakly renormalized mass but a spectral weight \( Z \) much smaller than unity. In Fig. 3(b) we propose a phase diagram based on the values assumed by the spectral weight making a comparison with that obtained in the \( SR \) and \( LR \) case. Analyzing the behavior of \( Z \) it is possible to distinguish different regimes, for example the crossover regime \((0.1 < Z < 0.9)\) characterized by intermediate values of spectral weight and a mass not strongly enhanced for the \( ER \) case, and strong coupling regime \((Z < 0.1)\) where the spectral weight is negligible and the mass is large but not enormous if the range of the coupling increases. With increasing the range of the interactions in the adiabatic case there is strong mixing of electronic and phononic degrees of freedom for values of \( \lambda \) smaller than those characteristic of local Holstein interaction. Furthermore, entering the strong coupling regime, the charge carrier is still mobile and it does not undergo any abrupt localization. Only in the antiadiabatic regime the transition lines separating the crossover from the strong coupling regime tend to superimpose.

Another important quantity associated to the polaron formation is the correlation function \( S(R_t) \)

\[ S(R_t) = S_{k=0}(R_t) = \frac{\sum_n \langle \psi_{k=0} | c_n^\dagger c_{n+1} (a_{n+t} + a_{n+t}^\dagger) | \psi_{k=0} \rangle}{\langle \psi_{k=0} | \psi_{k=0} \rangle}. \]

In Fig. 4(a) we report the correlation function \( S(R_t = 0) \) at \( \omega_0/t = 1 \) for several ranges of the \( el - ph \) interaction. In analogy with the behavior of the average number of phonons discussed in Fig. 2(d), the on-site correlation function is larger with increasing the range of the interaction in the weak coupling regime, but it becomes smaller as function of the coupling constant \( \lambda \) in the strong coupling region indicating the the \( SHP \) is more effective in producing local lattice distortions. Actually in the \( ER \) and \( LR \) case, the lattice deformation is spread over \( nn \) or many lattice sites,
respectively, giving rise to the formation of \( LP \) also in the strong coupling regime. Therefore it is interesting to analyze the behavior of the correlation function at \( nn \) sites. As reported in Fig. 4(b), in the \( SR \) case there is a minimum as function of \( \lambda \) since the particle tends to localize on a single site with increasing the \( el - ph \) coupling. In the \( LR \) case the lattice distortion shows a decreasing behavior with increasing \( \lambda \) indicating that the nearest neighbor contribution is always relevant. However for intermediate values of the ratio \( \alpha_1/\alpha \) in the \( ER \) case, the correlation function shows an upturn as function of the coupling constant \( \lambda \). Actually, for small values of the coupling, this function tends to follow the behavior of the local interaction, but, with increasing the value of \( \lambda \), the coupling to the \( nn \) lattices is able to give deviations from the \( SR \) case. In fact the lattice deformation reaches a maximum, then begins to decrease following the behavior of the \( LR \) interaction. Therefore, as function of \( \lambda \), two different regimes in the correlation function can be evidenced.

IV. DISCUSSION AND CONCLUSION

In this paper we have extended a variational approach in order to study the polaronic ground-state features of a one dimensional \( el - ph \) model with coupling to local and \( nn \) lattice displacements. Many physical quantities such as the ground state energy and spectral weight, the average kinetic energy, the mean number of phonons, and the electron-lattice correlation function have been discussed making a comparison with the results obtained with \( SR \) and \( LR \) interactions. It has been possible to ascertain that most physical quantities are quantitatively equal to those obtained for the \( LR \) interaction as the \( el - ph \) coupling in the \( ER \) case is large. A polaronic phase diagram based on the values assumed by the spectral weight has been proposed. It has been shown that the transition lines between the crossover and the strong coupling regime continuously evolve toward that of the \( LR \) case by increasing the coupling of the \( ER \) system. The deviations of the \( ER \) case from \( LR \) case become evident only in quantities depending on distances larger than the lattice parameter, such as in the electron-lattice correlation function. At neighbor nearest sites for large values of the coupling, the \( ER \) interaction is able to reproduce the correlation function characteristic of the \( LR \), while, at intermediate values of the ratio \( \alpha_1/\alpha \), the lattice deformation shows an upturn as function of the coupling constant \( \lambda \).

Recently, a variational wave function\(^{22} \) has been proposed to study the polaron formation in Su-Schrieffer-Heeger (SSH) model where the electronic transfer integral depends on the relative displacement between \( nn \) sites. Unlike the original SSH model, the non-local electron-lattice coupling has been assumed to be due to the interaction with optical phonon modes. It has been shown that with this type of interaction the tendency towards localization is hindered from the pathological sign change of the effective next-nearest-neighbor hopping. Therefore it is not possible to reach the strong coupling regime where most properties obtained with the \( ER \) density-type \( el - ph \) coupling bear strong resemblance with those in the \( LR \) model. Only the coupling with acoustic phonons is able to provide a solution with localized behavior within the SSH model\(^{22} \).

The variational approach for models with density-type \( el - ph \) coupling can be generalized to high dimensions, where it can still give a good description of ground state features.\(^{15,22} \) However, in order to reproduce with the \( ER \) interaction most physical quantities of the \( LR \) case, with increasing the dimensionality, it is important to include not only coupling terms at \( nn \) sites but also at next nearest neighbors. Actually it is necessary that the expansion of the coupling to near sites gives rise to an \( el - ph \) interaction vertex similar to that obtained in the \( LR \) case. Under these conditions the variational method is able to interpolate between the behavior of the \( SR \) case to the \( LR \) one with increasing the coupling of the interaction with close sites.

Figure captions

Fig.1 The \( el - ph \) matrix element \( M_q \) (in units of \( \alpha \omega_0/\sqrt{L} \)) for different ranges of the interaction as function of the momentum \( q \) (in units of \( \pi \)).

Fig.2 The ground state energy \( E_0 \) in units of \( \omega_0 \) (a), the ratio \( B/A \) at \( k=0 \) (b), the average kinetic energy \( K \) in units of the bare one (c) and the average phonon number \( N \) (d) for \( t = \omega_0 \) as a function of the coupling constant \( \lambda \) for different ranges of the \( el - ph \) interaction: \( SR \) (solid line), \( ER \) with \( \alpha_1/\alpha = 0.05 \) (dash line), \( ER \) with \( \alpha_1/\alpha = 0.1 \) (dot line), \( ER \) with \( \alpha_1/\alpha = 0.2 \) (dash-dot line), \( ER \) with \( \alpha_1/\alpha = 0.3 \) (dash-double dot line), \( LR \) (double dash-dot line).

Fig.3 (a) The ground state spectral weight at \( \omega_0/t = 1 \) as a function of the coupling constant \( \lambda \) for different ranges of interaction: \( SR \) (solid line), \( ER \) with \( \alpha_1/\alpha = 0.05 \) (dash line), \( ER \) with \( \alpha_1/\alpha = 0.1 \) (dot line), \( ER \) with \( \alpha_1/\alpha = 0.2 \) (dash-dot line), \( ER \) with \( \alpha_1/\alpha = 0.3 \) (dash-double dot line), \( LR \) (double dash-dot line).
(b) Polaron phase diagram for $SR$ (solid line), $ER$ with $\alpha_1/\alpha = 0.2$ (dash-dot line), $ER$ with $\alpha_1/\alpha = 0.3$ (dash-double dot line), and $LR$ (double dash-dot line) $e\text{--}p\text{h}$ interaction. The transition lines correspond to model parameters such that the spectral weight $Z = 0.1$.

Fig. 4 The electron-lattice correlation functions $S(R_l = 0)$ (a) and $S(R_l = \delta)$ (b) at $\omega_0/t = 1$ for different ranges of the $e\text{--}p\text{h}$ interaction: $SR$ (solid line), $ER$ with $\alpha_1/\alpha = 0.05$ (dash line), $ER$ with $\alpha_1/\alpha = 0.1$ (dot line), $ER$ with $\alpha_1/\alpha = 0.2$ (dash-dot line), $ER$ with $\alpha_1/\alpha = 0.3$ (dash-double dot line), $LR$ (double dash-dot line).

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Long-Range

Extended $\alpha_1/\alpha = 0.3$

Extended $\alpha_1/\alpha = 0.2$

Extended $\alpha_1/\alpha = 0.1$

Local
