Mobile intersite bipolarons in the discrete Holstein-Hubbard model

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We have explored the properties of a two-fermion system interacting with the phonon field in the framework of the one-dimensional discrete Holstein-Hubbard model. The variational method employed here introduces the correlations between the phonons and the electron wave functions, therefore the composite trial state is not factorized. As a consequence our approach gives reliable results in the whole space of the parameters. We will direct our attention to a new class of solutions found in the intermediate range of values of the nonadiabaticity parameter γ. These solutions are characterized by anomalous (non-Gaussian) fluctuations of the position of the oscillators. An intersite bipolaron with a relatively small effective mass is stable in a wide region of the parameters due to both exchange and nonadiabaticity effects. [S0163-1829(97)01221-6]

I. INTRODUCTION

The pairing of electrons or holes in real space plays an important role in many physical systems. Among these we note transition-metals oxides,[1] superconducting materials,[2] conjugated polimers,[3] and alternating-valence compounds.[4] More recently, the interest in this field has greatly increased due to the possibility that the bipolaron model could give a key to the understanding of high-T_c superconductors.[5]

Many theoretical works just assume the existence of the bipolarons and derive the consequences of this assumption for the behavior of some physical quantities, which characterize the above-mentioned systems. It is worthwhile to mention, for example, that Alexandrov has supposed[6] that in cuprate superconductors the presence of a strong Coulomb repulsion and a strong electron-phonon coupling could induce the stability of intersite bipolarons (e.g., a bound state in which the relative distance between the two polarons is a lattice spacing).

Some other theoretical works take into consideration the problem of the stability of the bound state of an electron pair by using model Hamiltonians. An interesting solution of the Holstein-Hubbard model has been obtained by Aubry[7] in the adiabatic regime (Pekar approximation). In this framework he has been able to show in a certain range of the parameters of the model the stability of bipolarons bounded by a magnetic resonance.

Unfortunately in some of the above-mentioned compounds the realistic values of the parameters are outside the range of validity of some usually used approximations (weak coupling, adiabaticity, etc.). For example in the superconductive Bechgaard salts $(TMTSF)_2ClO_4$, $(TMTTF)_2PF_6$ the nonadiabaticity parameter γ is equal to 0.34–0.37,[8] while in the high-T_c superconductors $\gamma \sim 1$ as can be inferred from the fit of the experimental data by assuming a *single*-band model.[9] For this reason the interest in nonperturbative methods has greatly increased.[10–14] Some authors have obtained exact solutions by numerical diagonalization of the Holstein-Hubbard model with one[10,11] or two particles[11] in a very small cluster (four sites for the two particles system, see Ref. 11). Exact solutions for this model have been studied also in the infinite dimensions limit.[14]

Moreover variational calculations have been used for investigation of electron-phonon Hamiltonians in the continuum limit and have extended the study to the two-particle case. However the calculations performed by using variational wave functions[15,16] are valid only in a restricted range of the parameters which appear in the used Hamiltonian; while the usual approximation for the effective action in the functional approach[17] can be criticized in the case of the Coulomb's repulsion. Furthermore, it has been noticed that the continuum limit approximation is not always adequate.[18,19] The goodness of this approximation depends on the nature of the coupling and on the relative values of the parameters in the Hamiltonians.

In the present work we apply a variational method, previously introduced for a one-particle system in the discrete Holstein model,[19] to the bipolaron problem in a discrete ring ruled by the Holstein-Hubbard model. The approach gives reliable results regardless of the values of the parameters,[19] so that we recover the known solutions in their own limits [the Lee, Low, and Pines (LLP) bipolaron[16] in the weak-coupling limit, the Pekar bipolaron[15] in the strong-coupling adiabatic regime, and the small bipolaron in the far diabatic regime[24]]; and we obtain a reliable solution also when such approximations are not valid. This can be checked by comparing our results with the ones obtained in the case of exact calculations on small clusters.

In the intermediate range of γ, we have found solutions which characterize the ground-state properties by introducing an explicit correlation between the phonons and the electron wave function. In our approach the Franck-Condon factor G shows an explicit dependence on sites n, and we take into account the anomalous (non-Gaussian) fluctuation of the position of the oscillators. These solutions will be studied by looking at the competition between the electron-phonon coupling λ and the on-site Coulomb repulsion U.

One fundamental problem, which we will treat, is how the formation of a bound state depends on these two interactions. Furthermore, the self-trapping of the solution does not present nonanalytical behavior of the ground-state (GS) energy at the self-trapping transition (see also Ref. 19). The self-trapping is strictly related to the question of the bipolaron mobility; however it must be stressed that a localized state does not mean necessarily an immobile state; but only a state which breaks the translational invariance of the model. In fact, as we will show below, the self-trapping transition marks the beginning of a *smooth* transition from mobile to immobile bipolaron.

One limit of our calculation could be the finite size of the system. However the method permits us to study very large systems ($N\sim 50$) by using a standard calculator, while we have verified that the results do not depend on the size of the cluster when $N>20$.[20]

II. THE METHOD

The model Hamiltonian here employed is

$$\hat{H}_{HH}=-J\sum_{\langle m,l\rangle;\sigma} c^{\dagger}_{m,\sigma}c_{l,\sigma}+U\sum_{m}\hat{n}_{m\uparrow}\hat{n}_{m\downarrow}+\hbar\omega\sum_{q} b^{\dagger}_{q}b_{q} + \frac{1}{\sqrt{N}}\chi\sum_{m,\sigma;q} e^{iqma}c^{\dagger}_{m,\sigma}c_{m,\sigma}(b_{q}+b^{\dagger}_{-q}). \tag{1}$$

Here $\hat{n}_{m,\sigma}=c^{\dagger}_{m,\sigma}c_{m,\sigma}$, and the sums on the first term are restricted to the first-neighbor sites. $c^{\dagger}_{m,\sigma}(c_{m,\sigma})$ creates (annihilates) an electron with spin projection σ in the mth site, $b^{\dagger}_{q}$ (b_{q}) creates (annihilates) one phonon for the q *mode*. The model depends on the following parameters: the hopping integral J, the phonons oscillation frequency ω, the *on-site* Coulomb repulsion U, and the electron-phonon coupling parameter χ. The lattice spacing, when $\chi=0$, is labeled by a. In the following we will consider also the adimensional parameters $\widetilde{U}=U/J$, $\gamma=\hbar\omega/J$ and $\lambda=\chi^{2}/2\hbar\omega J$.

Now we will show the main steps of the method. Let us consider the following variational ansatz:

$$|\psi^{(2)}\rangle=\sum_{n,n';\sigma,\sigma'} A_{\sigma,\sigma'}(n,n')c^{\dagger}_{n,\sigma}c^{\dagger}_{n',\sigma'} \times\exp\left\{\frac{1}{\sqrt{N}}\sum_{q}\left[f_{q}(n,n')b^{\dagger}_{q}-f^{*}_{q}(n,n')b_{q}\right]\right\}|0\rangle, \tag{2}$$

where $f_{q}(n,n')=f_{q}(n)+f_{q}(n')$ and apart from the gauge choice $f_{-q}(n)=f^{*}_{q}(n)$ these variational variables are *unrestricted*. We have taken off the spin dependence from the ansatz (2), because there are not *spin-flip* terms in Eq. (1). We will analyze the solutions in the singlet state; however the calculations can be performed analogously for a triplet state. From expression (2) of our variational state the essential features of our approach can be easily understood: (a) the effective two-electron problem of the wave function is exactly treated; (b) the phonons variational variables $f_{q}(n)$ depend on the electron position, i.e., we have introduced an explicit correlation between the phonons and electron states so that $|\psi^{(2)}\rangle$ cannot be factorized in the electron and phonon contributions; (c) the phonon wave function does not necessarily correspond to a collection of displaced oscillators with standard Gaussian fluctuations of the position [such a case can be recovered only if $f_{q}(n)\rightarrow f_{q}\times\exp\{inqa\}$], but a different state can be obtained for the oscillator with anomalous non-Gaussian fluctuations (see Ref. 19, and references therein).

The use of the correlated state, when one deals with the polaron problem, has been introduced in the pioneering papers on the polaron problem.[21] However, apart from the cited discrepancy implied by the use of the continuum limit, the analytical methods involve some other approximations:

(1) to stop the self-consistent procedure at the first step;

(2) the use of some approximate form for the starting wave function (a Gaussian form[21] a sech(x) form[22] or others) the initial form becomes relevant if one does not use a full self-consistent procedure;

(3) the truncation of some series expansion.

With our numerical self-consistent approach we have managed to solve exactly the variational equation therefore we will really discuss with confidence the system properties in the whole region of the parameters. Furthermore we have applied the full correlated state approach to the bipolaron problem, taking into account also the Hubbard interaction.

The extremum equations for the energy functional

$$\mathcal{H}\{f_{n}(q),A(n,n')\}=\langle\psi^{(2)}|\hat{H}_{HH}|\psi^{(2)}\rangle$$

are

$$-J\left[\sum_{n_3\langle n_1\rangle}A(n_2,n_3)e^{-G(n_1,n_3)}+\sum_{n_4\langle n_2\rangle}A(n_1,n_4)e^{-G(n_2,n_4)}\right]+\left[\frac{V(n_1,n_2)+V(n_2,n_1)}{2}+\frac{V(n_1)+V(n_2)}{2}\right]A(n_1,n_2) =E^{(2)}_{S}A(n_1,n_2) \tag{3}$$

and

$$f_{q}(n)=-\frac{\chi}{2}\sum_{\nu}\frac{\sum_{n_1,n_2}A^{*}_{\nu}(n_1,n_2)(e^{-iqn_1a}+e^{-iqn_2a})A_{S}(n_1,n_2)}{E_{\nu}-E^{(2)}_{S}+\hbar\omega}\times\frac{A_{\nu}(n,n)}{A_{S}(n,n)}. \tag{4}$$

Here the symbol $\Sigma_{n'\langle n\rangle}$ indicates the sum over the sites n' nearest to the site n and $E_S^{(2)}$ is the GS energy variational estimate of the two-particle system; while

$$V(n)=\frac{2}{N}\sum_q \hbar\omega|f_q(n)|^2+2\,\mathrm{Re}[\chi e^{iqna}f_q(n)],$$

$$V(n,n_1)=\frac{2}{N}\sum_q \hbar\omega\,\mathrm{Re}[f_q^*(n)f_q(n_1)] +2\,\mathrm{Re}[\chi e^{iqna}f_q(n_1)]+U\delta_{n,n_1},$$

and

$$G(n,n')=\frac{1}{2N}\sum_q |f_q(n)-f_q(n')|^2.$$

The formally explicit expression for the $f_q(n)$ variables (4) has been obtained by using the orthonormal set $\{A_\nu(n_1,n_2)\}$ of the $N\times N$ eigenvectors of Eq. (3).[19]

We note that in the adiabatic limit $f_q(n)\to f_q$ so that $G(n,n+1)\to 0$, $V(n,n_1)\to V(n)$ (Ref. 7) and the electrons see the phonons field as a renormalized mean-field only.[23] Do not assume that this approximation, as in our treatment, is equivalent to introducing correlations between the two particles which are mediated by phonons.

The solutions, always for the discrete case, coincide with the LLP bipolaron if we consider the translational invariance. In fact, in this case the total momentum Q is a good quantum number and we can choose the wave function as

$$A_\nu(n_1,n_2)\to A(r,R)_{\nu',Q}=\frac{1}{\sqrt{N}}A(r)_{\nu'}e^{iQR},$$

where we have considered the following change of the variables:

$$R=\frac{(n_1+n_2)a}{2};\quad r=(n_1-n_2)a$$

and we have substituted the eigenvector label ν, with the pair Q,ν' (for the ground state $Q=0$). In this case expression (4) will take the following form:

$$f_q(n)\to f_q(r)e^{iqR}=-\chi\sum_{\nu'}\frac{\sum_{r'}A^*_{\nu'}(r)\cos\{qr'/2\}A_S(r')}{E_{\nu'q}-E_S+\hbar\omega} \times\frac{A_{\nu'}(0)e^{iqr/2}}{A_S(0)}e^{iqR} \tag{5}$$

and the variational parameters are analogous to those used in Ref. 16. It is worth noting that the continuum LLP bipolaron solution of Ref. 16 is obtained by fixing the functional form $A(r)$, while in our numerical calculations we have not considered further restrictions for the variational parameters.

It is trivial to show that in the far nonadiabatic ($\gamma\gg 1$) limit we will obtain two interacting Lang-Firsov's *small polarons*.[24] In such limit there is not retardation effect [both the Coulomb repulsion and the phonon-mediated attraction have range zero, i.e., $V(n,n_1)\to V\delta_{n,n_1}$] so that model (1) maps on an attractive (repulsive) Hubbard model if $4\lambda>\tilde{U}$ ($4\lambda<\tilde{U}$) and the solutions correspond to an on-site bipolaron (free small polarons).

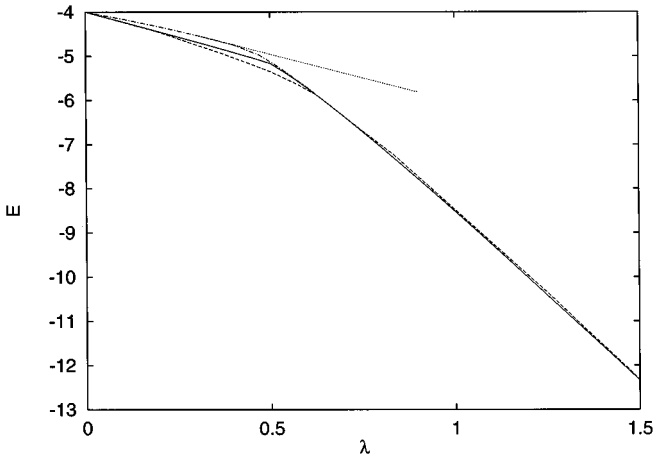

FIG. 1. The comparison between our variational estimate of the ground-state energy $E_S^{(2)}$ (solid line) and the exactly calculated one (dashes) on a four-site cluster. Here we also report $E_S^{(2)}$ calculated on a large chain (30 sites) (points dashes) and the estimate obtained with the LLP discrete delocalized theory (points) on the same chain.

III. THE INTERSITE BIPOLARON

Our attention will be turned now to the solutions in the case of the intermediate value of the adiabaticity ($\gamma\sim 1$), which cannot be explored by means of the usual approximations and which we will call IA (intermediate adiabaticity) solutions. We expect to recover different possibilities for the two-particle solutions (delocalized free state, delocalized bound state, localized free state, and localized bound state) by varying the interaction strengths.

First, we will show the goodness of our method by comparing our (upper bound) variational estimate of the ground-state energy $E_S^{(2)}$ with the exactly calculated one E_{ex} on a four-site cluster.[11] The comparison is reported in Fig. 1 where for consistence our calculation has been performed also on a four-site cluster and the following parameters are considered $\gamma=0.5$ and $\tilde{U}=0$. The general agreement of the two evaluations is manifest but few further comments have to be joined. $E_S^{(2)}$ lies below E_{ex} at strong coupling since a cutoff of the phonon Hilbert space is considered in the exact calculation. The kinklike behavior of the variational estimate at the self-trapping transition is due to finite scale effects; it appears also in the exact calculation[11] but it is exalted by the variational procedure. The kink practically disappears if we consider a larger system (see Fig. 1 again). The calculations on a very small cluster have an unphysical large slope for λ equal to zero which depends on a reduction of the polaronic effect (i.e., the increasing of the effective mass) due to the limited number of allowed phononic modes. More formally such an issue can be seen from the expression for the Franck-Condon factor $G(n+1,n)$ where the sum is only over four q values.

The localized IA ground state, which is stable in a particular region of the parameters (see Fig. 2), has an energy

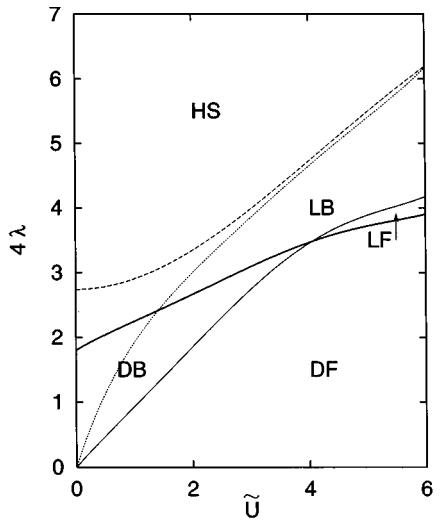

FIG. 2. The ''phase diagram'' in the plane $4\lambda-\tilde{U}$ for $\gamma=0.5$. By increasing λ, the lines mark the following transitions: from a delocalized state to a localized state (heavy full line), from a free state to a bound state (light full line), from an intersite bipolaron to an on-site bipolaron (points), from $(m/m^*)>0.1$ to $(m/m^*)<0.1$ (dashes). We have also labeled the different stability zones. In the region DF we have a delocalized free state, in the region DB a delocalized bound state, in the region LF a localized free state, in the region LB a localized bound state, in the region HS a heavy localized state $(m/m^*<0.1)$.

which lies well below the Pekar-Aubry bipolaron energy in the intermediate region of the electron-phonon coupling. It is characterized by an explicit dependence on the site of the Franck-Condon factor $G(n+1,n)$ and of the on-site potential $V(n)$. Moreover the effective interaction between the particles $V(n,n')$ is affected by the localization, therefore it does not depend only, as in the LLP bipolaron case, on the relative coordinate r. A self-trapped bipolaronic solution is shown in Fig. 3, for some particular values of the parameters. It is worthwhile to note that for these values of the parameters the two-particle wave function $A(n,n')$ picks up for $|\tilde{n}-\tilde{n}'|=1$, i.e., the composite particle is an intersite bipolaron. Such a result can be observed also for a delocalized solution, but in this case the wave function varies more slowly with the relative distance.

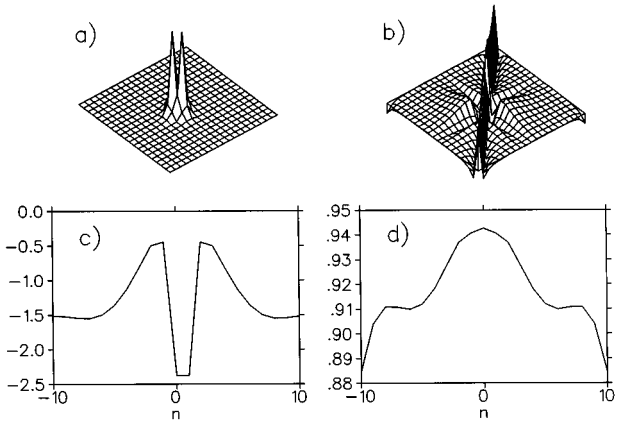

FIG. 3. The localized configuration obtained for the following set of the parameters: $\gamma=0.5$, $\tilde{U}=4.0$, and $\lambda=1.0$. In the four insets we show: (a) the square modulus of the particles wave function $|A(n,n')|^2$, (b) the two-body effective potential $V(n,n')$, (c) the on-site potential $V(n)$, (d) the Franck-Condon factor $G(n,n+1)$. All these quantities are drawn as a function of the site n.

The stability of an intersite bipolaron is due to the retardation of the phonon-mediated interaction for a finite value of γ, which allows the electrons to lower their energies when they lie to a suitable distance one from the other. However for the IA bipolaron solutions the relative position of the two particles never exceeds one lattice spacing. For this reason, this IA state seems to be similar to the intersite bipolaron hypothesized by Alexandrov.[6] Of course the retardation effect causes also the lowering of the critical point for the formation of a IA bound state with respect to value $4\lambda=\tilde{U}$ needed for the formation of a bound state of the type of Lang-Firsov's small on-site bipolaron. This last effect is exalted in the adiabatic limit (for such an issue, see also Ref. 11), but in such a case we recover an intersite bipolaron only in a very narrow zone near the $4\lambda=\tilde{U}$ line.

This complex scenario, in which binding and localization overlap, can be schematized in a phase diagram on the plane $4\lambda-\tilde{U}$ (see Fig. 2, in which we consider $\gamma=0.5$). The two instability lines (heavy full line and light full line in Fig. 2) mark, respectively, the transition between the delocalized and the localized ground state and between the free and the bound state. The localization transition point can be suitably determined, the intersection point between the ground-state energies extracted by means of the delocalized LLP bipolaron theory, and the extrapolation of the curve which joins the points obtained in our numerical calculation (see Fig. 1).

The two instability lines intersect each other at $\tilde{U}=U\simeq 4$ which is a crucial point to define the different regions of stability. For $\tilde{U}<U$ and by increasing λ we have the following sequence of solutions: the free delocalized polarons (DF), the delocalized bipolaron (DB), and the localized bipolaron (LB); while for $\tilde{U}>U$ we obtain the following sequence when λ increases: the DF solution, the localized free polaron (LF) and the LB solution. It is important to note that the critical line for the binding of the two particles has not a constant dependence on the ratio $\lambda/\tilde{U}$ and that for strong coupling it moves far away from the line $4\lambda=\tilde{U}$.

An important problem concerns the mobility of the localized bipolaron. In order to investigate such a problem we have determined the ratio m/m^* between the the free band mass m and the effective mass m^*, in the case of the localized ground state, by means of a method based on the restoring of the translational invariance.[19] It is usually believed that the localization of a polaron is connected with a sharp (discontinuous) increase of the effective mass of the self-trapped quasiparticle. This effect should be even stronger in the case of the bipolaron.

Actually our calculation shows that the bipolaron mass is ever greater than twice the polaron mass. However the transition to a heavy bipolaron state is not so sharp as it is generally believed. This result is reported in Fig. 4, where we have plotted the binding energy $\Delta E=E_S^{(2)}-2E_S^{(1)}$ and the mass ratio m/m^* versus λ for $\tilde{U}=4.0$ and $\gamma=0.5$ (here $E_S^{(1)}$ denotes the free polaron self-energy). This picture

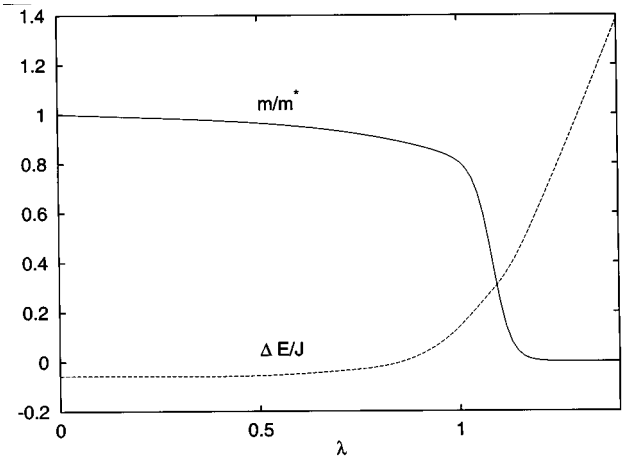

FIG. 4. The mass ratio m/m^* (full line) and the binding energy $\Delta E/J$ (dashes) versus λ for $\gamma=0.5$ and $\tilde{U}=4.0$.

shows a transition from a weakly bound mobile bipolaron to a strongly bound heavy bipolaron. For $0<\lambda<0.86$, both ΔE and m/m^* vary very slowly, while for $0.86<\lambda<1.20$, they vary more rapidly (in such a case, $\lambda=0.86$ is the critical value for the binding of the two polarons). It is important to note that, in this transition zone, the GS is an *intersite bipolaron* and such behavior is favored by a strong Coulomb repulsion and a corresponding strong electron-phonon coupling. The effective mass is never greater than $10m$ if an intersite bipolaron is stable, while it suddenly increases when the GS is an on-site bipolaron (see Fig. 2).

The presence in the intermediate regime of a large region of the parameters where we have not a very great value of m^* is an essential feature of our approach, which is also connected with the presence of the interaction U. For a fixed value of λ by increasing U we increase the region where m^* is small. We have calculated that, for intermediate-coupling strength ($\lambda\sim1$), in the adiabatic regime, regardless of the U values, one gets m^* bigger than $100m$.

IV. CONCLUSION

In summary, we have investigated, by means of a suitable variational scheme, a system of two electrons or holes coupled to the zero range optical phonons, for intermediate values of the nonadiabaticity parameter and in the presence of an on-site Coulomb interaction U.

Our method allows us to treat with confidence the whole range of the parameters of the Holstein-Hubbard model and the reliability of the results can be inferred by looking at the comparison with the exact results taken out on a small cluster. Moreover it improves exact calculations since the size of our cluster is large enough to avoid unphysical finite-size effects.

By means of our approach binding and localization problems can be faced in a single bipolaronic theory, while generally binding has been considered separately from localization in the framework of weak-coupling delocalized or strong-coupling localized bipolaron theory.[16] Such an issue allows us to draw an accurate phase diagram for the ground-state properties.

The bipolarons are bounded not only by exchange effects,[7] which in our scheme are taken into account through the expression of the wave function Eq. (2), but also by the two-body correlations which we have explicitly considered. These IA solutions are particularly important in the transition zone to a heavy strongly bound bipolaron. This zone is characterized by the stability of a mobile intersite bipolaron, if the interactions are strong enough, which resemble the intersite bipolaron hypothesized by Alexandrov.[6]

We believe that the present results give support to the bipolaron theory of the superconductivity if we want to apply it to compounds which present an intermediate adiabaticity like the Bechgaard salts and the high-T_c superconductors. In fact this is the first step in order to elaborate a bipolaronic theory of superconductivity which is reliable in the IA regime, since binding and mobility of the pairs of polarons are the initial requirements to explore the possibility that this composite bosons could manifest condensation. However the extension of our approach to a higher dimensional system and the study of the effect of the overlap between many bipolarons have to be analyzed to get insight into this intriguing subject.

If we consider the many-particle case, we have to include also the correlation between successively emitted virtual phonons, which we have disregarded in this work. Actually, as Zheng[25] and others[26] have shown, this effect is important in the IA regime, but it crucially depends upon the relative number of particles with respect to the number of sites. In the case of two particles in a large cluster (i.e., the low-density limit) this effect is negligible but it will be considered when we will extend our analysis to systems with arbitrary density. Work in this direction is in progress.

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