Formation of bipolarons in the Holstein Hubbard model in one, two and three dimensions

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Abstract. In this paper we have studied the properties of a two-fermion system interacting with the phonon field in the framework of the Holstein Hubbard model in one, two and three dimensions. We have chosen the modified Lang–Firsov variational wave function with on-site and nearest-neighbour lattice distortion for the phonon subsystem to obtain an effective electronic Hamiltonian. This effective electronic Hamiltonian is then solved exactly to obtain the binding energy and effective mass of the bipolaron. We investigated the stability of the bipolaronic phase by comparing the ground-state energy of a bipolaron and two free polarons. We observed a critical repulsive on-site Hubbard interaction U_c below which the bipolaronic phases are stable for a fixed electron–phonon coupling g. In the absence of on-site repulsion, bipolaronic phases are stable over the entire range of electron–phonon coupling for one dimension, whereas there is a critical electron–phonon coupling g_c for formation of a stable bipolaron in two and three dimensions.

1. Introduction

The discovery of high-temperature superconductivity has provided a strong impetus for a renewed effort to study strongly correlated electron systems in the presence of phonons. The many-electron system on a lattice strongly coupled with phonons turns out to be a charged Bose liquid consisting of on-site or inter-site small bipolarons if the Coulomb repulsion is not very strong. This pairing of electrons or holes in real space plays an important role in determining the properties of many-particle systems such as transition metal oxides [1], superconducting materials [2, 3], conjugated polymers [4] and alternating-valence compounds [5]. The model which has most often served as a paradigm for electronic correlation in the presence of electron–phonon interaction is the Holstein Hubbard model (HHM) [6, 7]. There is quite general agreement that an accurate solution to the HHM over the whole region of parameter space will be able to provide an understanding of many physical properties of the above-mentioned materials. However, in spite of the simplicity of the model, a great effort is needed in order to achieve accurate solutions. Recently this electron–phonon problem has been studied through the exact diagonalization of small linear clusters with one [8,9] or two [9] particles and a limited number of phonons and also by quantum Monte Carlo methods [10–12]. Another strategy for studying the electron–phonon problem is by using variational methods [13–17]. La Magna and Pucci [16] have performed a variational study of the one-dimensional bipolaron problem. In their work they provide us with a detailed study of the formation of a bound state in the presence of the on-site Hubbard interaction U in one dimension. To the best of our knowledge, most of the work concerning the bound-state formation in the HHM has been performed for one dimension. However, there remain a large number of strongly correlated systems which

are realized in two or three dimensions. To include those systems in our sphere of investigation, studies on the HHM in higher dimensions are important. In the present work we study the formation of bipolarons in one, two and three dimensions for the discrete Holstein Hubbard model in the non-adiabatic limit. Our model Hamiltonian only takes care of on-site electron–phonon interaction, but due to the retardation effect the lattice deformation can extend beyond the site at which the electron resides. To take this effect into account, we have treated the on-site and the nearest-neighbour-site lattice distortion variationally. This variational scheme is based on Lang–Firsov transformation and is suitable for $\hbar\omega/t \geqslant 1$ [8].

The paper is organized as follows. In section 2 we obtain an effective interacting Hamiltonian from the Holstein Hubbard model. In section 3 we will give an exact solution of this Hamiltonian in the far non-adiabatic limit where the retardation effect is negligible. The effect of retardation and the result of our variational calculation on the formation of bipolarons in one, two and three dimensions are discussed in sections 4 and 5. Finally we present our conclusions in section 6.

2. The effective-electron model

We consider a system of electrons in the framework of the Hubbard model, which is also coupled to a collection of Einstein oscillators. The model Hamiltonian of such an interacting system is

$$H = -t \sum_{\langle ij\rangle,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \hbar\omega \sum_i b_i^\dagger b_i + g \sum_i n_i (b_i^\dagger + b_i) \qquad (1)$$

where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$, $n_i = n_{i\uparrow} + n_{i\downarrow}$ and the symbol $\sum_{\langle ij\rangle}$ denotes the sum of nearest-neighbour sites. The operator $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron with the spin projection σ on the site labelled i, while $b_i^\dagger$ (b_i) creates (annihilates) a quantum of oscillation energy $\hbar\omega$ in the model localized on the site i. The model depends on the nearest-neighbour hopping t, electron–phonon interaction g and an on-site repulsion U between electrons of different spins.

In the presence of strong electron–phonon coupling, the lattice would be deformed around an electron. To take into account the lattice deformation around the electron, we apply the modified Lang–Firsov transformation [14] to the Hamiltonian H:

$$\tilde{H} = \exp(R) H \exp(-R). \qquad (2)$$

That is,

$$H = -t \sum_{\langle ij\rangle,\sigma} \exp(Y_i - Y_j) c_{i\sigma}^\dagger c_{j\sigma} - \epsilon_p \sum_i n_i + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow}$$
$$+ V_1 \sum_{\langle ij\rangle} n_i n_j + V_2 \sum_{i,\delta+\delta'\neq 0} n_{i+\delta} n_{i+\delta'} + \hbar\omega \sum_i b_i^\dagger b_i + V_{pol-ph} \qquad (3)$$

where

$$R = \sum_i \left(\lambda_1' n_i (b_i^\dagger - b_i) + \lambda_2' \sum_\delta (b_{i+\delta}^\dagger - b_{i+\delta}) n_i \right) \qquad (4)$$

$$Y_i = \lambda_1' (b_i^\dagger - b_i) + \lambda_2' \sum_\delta (b_{i+\delta}^\dagger - b_{i+\delta}) \qquad (5)$$

$$\epsilon_p = (2g - \lambda_1)\lambda_1' - z\lambda_2\lambda_2' \qquad (6)$$

$$U_{eff} = U - 2[(2g - \lambda_1)\lambda_1' - z\lambda_2\lambda_2'] \qquad (7)$$

$$V_1 = -2[(g - \lambda_1)\lambda_2'] \qquad (8)$$

$$V_2 = \lambda_2 \lambda_2' \tag{9}$$

$$V_{pol-ph} = \sum_i (g - \lambda_1)(b_i^\dagger + b_i)n_i - \lambda_2 \sum_\delta (b_{i+\delta}^\dagger + b_{i+\delta})n_i. \tag{10}$$

Here ϵ_p is the polaron self-energy, V_1 is the coupling strength of the attractive interaction between nearest-neighbour polarons induced by electron–phonon coupling, V_2 is the strength of the repulsive coupling between next-nearest-neighbour polarons, U_{eff} is the effective on-site interaction and V_{pol-ph} is the polaron–phonon interaction.

$\lambda_1' (=\lambda_1/(\hbar\omega))$ and $\lambda_2' (=\lambda_2/(\hbar\omega))$ are the lattice displacements created around an electron at the same site and the nearest-neighbour sites respectively, which move along with the electron. When $\lambda_1 = g$ and $\lambda_2 = 0$, the transformation is exactly the Lang–Firsov transformation [13]. To obtain an effective polaronic Hamiltonian, we take the average of $\tilde{H}$ over the zero-phonon state ($|0\rangle$) [19]:

$$H_{eff} = \langle 0|H|0\rangle. \tag{11}$$

That is,

$$H_{eff} = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} \exp(-\bar{\lambda}^2) - \epsilon_p \sum_i n_i + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow}$$
$$+ V_1 \sum_{\langle ij \rangle} n_i n_j + V_2 \sum_{i, \delta + \delta' \neq 0} n_{i+\delta} n_{i+\delta'} \tag{12}$$

where

$$\bar{\lambda}^2 = (\lambda_1' - \lambda_2')^2 + (z - 1)\lambda_2'^2. \tag{13}$$

3. Bipolarons in the far non-adiabatic limit ($\hbar\omega/t \gg 1$)

In the far non-adiabatic limit ($\hbar\omega \gg t$) one can neglect the retardation effects. In that case the nearest-neighbour lattice distortion due to on-site electron–phonon interaction vanishes. In this limit, $\lambda_2 = 0$ and $\lambda_1 = g$, and the effective Hamiltonian directly maps onto the Hubbard model:

$$H_{eff} = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} \exp(-g'^2) - \epsilon_p \sum_i n_i + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{14}$$

To study the possibility of the formation of bipolarons, we consider two electrons with spins $\uparrow$ and $\downarrow$ in the lattice. In this case the above effective Hamiltonian can be solved exactly for any dimension. We will write the Hamiltonian in the wave-function representation:

$$|q, m\rangle = \frac{1}{\sqrt{N}} \sum_l \exp(-iql/2) c_{(l+m)/2,\uparrow}^\dagger c_{(l-m)/2,\downarrow}^\dagger |\text{vacuum}\rangle \tag{15}$$

to express the effective Hamiltonian in the form

$$H_{eff} = -2t \exp(-g'^2) \sum_{q,m,\delta} \cos(q/2)|q, m\rangle\langle m + \delta, q| + U_{eff} \sum_q |q, 0\rangle\langle 0, q| - 2\epsilon_p \tag{16}$$

where N is the total number of sites. For a given wave vector q, its form (16) corresponds to a system with a single impurity. When $U_{eff} < 0$, then, depending on the dimensionality, there may exist a bound state with eigenvalues below the band of two polarons. A general solution can be obtained by means of the Green's function [18]. The eigenvalues of the bound state are determined from

$$1 = U_{eff} G_0(E_b, q). \tag{17}$$

The diagonal element of the Green's function ($G_0(E_b, q)$) is given by

$$G_0(E_b, q) = \frac{1}{N} \sum_k \frac{1}{E_b(q) - \epsilon_{k+q/2} - \epsilon_{-k+q/2} + 2\epsilon_p} \tag{18}$$

where $\epsilon_k = 2\tilde{t}\cos(k)$ and $\tilde{t} = t\exp(-g'^2)$.

Now we will discuss the formation of a stable bipolaron in one, two and three dimensions.

3.1. Case I: one dimension

In one dimension,

$$G_0^{1D}(E_b^{1D}, q) = \frac{1}{\sqrt{(E_b^{1D}(q) + 2\epsilon_p)^2 - 16\tilde{t}^2 \cos^2(q/2)}} \tag{19}$$

and the corresponding energy eigenvalues obtained from equation (17) are given by the condition

$$E_b^{1D}(q) = U_{eff}\sqrt{1 + \frac{16\tilde{t}^2 \cos^2(q/2)}{U_{eff}^2}} - 2\epsilon_p. \tag{20}$$

The spectrum represents a bipolaron if $E_{bmin}^{1D}(q)$ is less than the lowest energy ($E_{2p}^{1D} = -2\epsilon_p - 4\tilde{t}$) of two free polarons. So the condition for the formation of 1D bipolarons is

$$E_{2p}^{1D} - E_{bmin}^{1D} > 0 \qquad \text{or} \qquad -U_{eff}\sqrt{1 + \frac{16\tilde{t}^2}{U_{eff}^2}} > 4\tilde{t}. \tag{21}$$

Therefore, for any negative values of U_{eff}, i.e. when $U/(\hbar\omega) < 2g'^2$ one gets a stable bipolaron in 1D. We can also determine the effective mass of the bipolaron from the definition [15]

$$m_{eff}^{1D} = \left(\frac{d^2 E_b^{1D}(q)}{dq^2}\right)^{-1}\Bigg|_{q=0} = \frac{\sqrt{16\tilde{t}^2 + U_{eff}^2}}{4\tilde{t}^2}. \tag{22}$$

3.2. Case II: two dimensions

In two dimensions we assume the density of states to take a simplified form:

$$\rho_{D=2}(\epsilon) = \frac{2}{8\tilde{t}_q}(64\tilde{t}_q^2 - \epsilon^2)^{(D-2)/2} = \frac{2}{8\tilde{t}_q} \tag{23}$$

so as to calculate the two-dimensional Green's function ($G_0^{2D}(E_b^{2D}, q)$):

$$G_0^{2D}(E_b^{2D}, q) = -\frac{1}{16\tilde{t}_q}\log\left(\frac{|E_b^{2D} + 2\epsilon_p| + 8\tilde{t}_q}{|E_b^{2D} + 2\epsilon_p| - 8\tilde{t}_q}\right) \tag{24}$$

in the [1, 1] direction. Here $\tilde{t}_q = \tilde{t}\cos(q/2)$. The corresponding energy dispersion in the [1, 1] direction is given by

$$E_b^{2D} = 8\tilde{t}\cos(q/2)\coth\left(\frac{8\tilde{t}\cos(q/2)}{U_{eff}}\right) - 2\epsilon_p. \tag{25}$$

Here E_b^{2D} represents a stable bipolaron provided that E_{bmin}^{2D} is less than the lowest energy ($E_{2p}^{2D} = -2\epsilon_p - 8\tilde{t}$) of two free polarons in two dimensions, i.e.

$$E_{2p}^{2D} - E_{bmin}^{2D} > 0 \qquad \text{or} \qquad \coth\left(\frac{8\tilde{t}}{U_{eff}}\right) < -1. \tag{26}$$

Therefore, for any $U_{eff} < 0$ (i.e. $U/(\hbar\omega) < g'^2$), bipolaronic phases represent the ground state of the system. From the definition

$$m_{eff}^{2D} = \frac{z}{2}\left(\frac{\mathrm{d}^2 E_b^{2D}}{\mathrm{d}q^2}\right)^{-1}\Bigg|_{q=0} \tag{27}$$

we obtain the effective mass of the 2D bipolaron:

$$m_{eff}^{2D} = 4\Bigg/\left[4\tilde{t}\coth\left(\frac{8\tilde{t}}{|U_{eff}|}\right) - \frac{32\tilde{t}^2}{|U_{eff}|}\operatorname{cosech}^2\left(\frac{8\tilde{t}}{|U_{eff}|}\right)\right]. \tag{28}$$

3.3. Case III: three dimensions

For three dimensions, the eigenvalues have been determined from equation (17) with the Green's function calculated from a simplified density of states:

$$\rho_{D=3} = \frac{2}{144\pi\tilde{t}^2}(144\tilde{t}^2 - \epsilon^2)^{1/2}. \tag{29}$$

Using the above-mentioned DOS, the Green's function ($G_0^{3D}(E_b^{3D}, q)$) and the energy dispersion (E_b^{3D}) in the [1, 1, 1] direction are obtained as

$$G_0^{3D}(E_b^{3D}, q) = \frac{2}{144\tilde{t}_q^2}\left[(E_b^{3D} + 2\epsilon_p) - \sqrt{(E_b^{3D} + 2\epsilon_p)^2 - 144\tilde{t}_q^2}\right] \tag{30}$$

$$E_b^{3D} = U_{eff}\left[\frac{36\tilde{t}^2}{U_{eff}^2}\cos^2(q/2) + 1\right] - 2\epsilon_p. \tag{31}$$

Now $E_b^{3D}(q, q, q)$ represents a stable bipolaron when E_{bmin}^{3D} is less than the lowest energy ($E_{2p}^{3D} = -2\epsilon_p - 12\tilde{t}$) of two free polarons in three dimensions, i.e.

$$E_{2p}^{3D} - E_{bmin}^{3D} > 0 \qquad \text{or} \qquad U_{eff} < -6\tilde{t}. \tag{32}$$

So, for three dimensions there has always been a critical electron–phonon interaction strength g_c required in order to bind two polarons. For $U = 0$ we require a critical value g_c, given by the condition

$$g_c'^2 = 3\frac{t}{\hbar\omega}\exp(-g_c'^2) \tag{33}$$

to form a stable bipolaron. In figure 1 we show the variation of the critical electron–phonon coupling $g_c/(\hbar\omega)$ with respect to $t/(\hbar\omega)$ for $U = 0, 0.5, 1.0, 2.0$ and 4.0. Our calculation shows a finite $g_c/(\hbar\omega)$ even at $U = 0$ for any finite $t/(\hbar\omega)$. Like for 1D and 2D, we can also calculate the effective mass of the bipolaron in three dimensions. The result is

$$m_{eff}^{3D} = \frac{|U_{eff}|}{6\tilde{t}^2}. \tag{34}$$

4. The intermediate range of $\hbar\omega/t$

In this regime of phonon frequency we have to take into account the effect of retardation. We will include the effect of retardation by considering the nearest-neighbour distortion due to the on-site electron–phonon interaction. For the intermediate range of $\hbar\omega/t$ ($\hbar\omega/t \geqslant 1$) the value of λ_2, which is non-zero due to the retardation effect, appears to be small. For simplicity, we neglect the second-nearest-neighbour repulsive term which is of the order of λ_2^2. Moreover, for on-site and nearest-neighbour bipolarons the effect of the second-nearest-neighbour repulsive
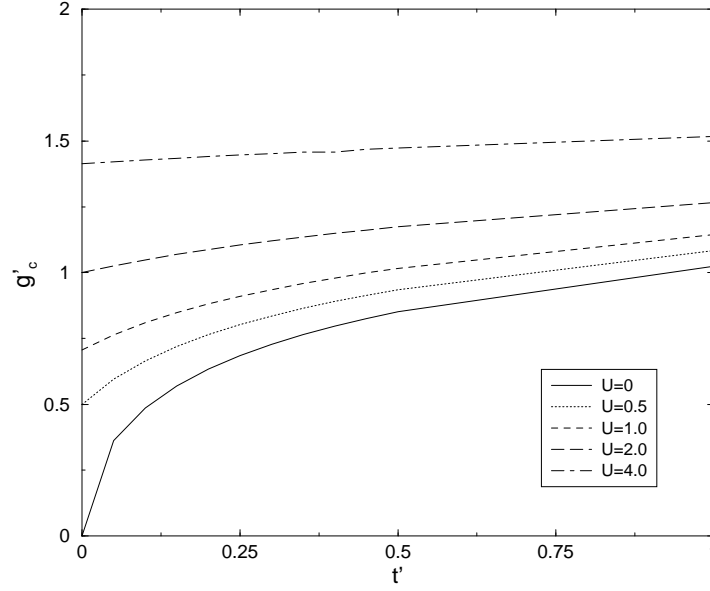
Figure 1. The variation of the critical electron–phonon coupling $g'_c = g_c/(\hbar\omega)$ with respect to $t' = t/(\hbar\omega)$ for $U = 0, 0.5, 1.0, 2.0$ and 4.0 (U is expressed in units of $\hbar\omega$) for the three-dimensional bipolaron in the far non-adiabatic limit.

term is not very significant. So we believe that the inclusion of a second-nearest-neighbour repulsive term will not modify the result significantly. In this approximation, our effective Hamiltonian reduces to

$$H_{eff} = -\tilde{t} \sum_{\langle ij \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} - \epsilon_p \sum_i n_i + U_{eff} \sum_i n_{i\uparrow} n_{i\downarrow} + V_1 \sum_{\langle ij \rangle} n_i n_j \qquad (35)$$

where $\tilde{t} = t \exp(-\bar{\lambda}^2)$. To study the possibility of the formation of bipolarons, we consider two electrons with spin $\uparrow$ and $\downarrow$ in the lattice. We will write the Hamiltonian in the wave-function representation (15) and express the effective Hamiltonian in the form

$$H_{eff} = \sum_q H_q = \sum_q (H^q_0 + H^q_1) \qquad (36)$$

where

$$H^q_0 = -2t \exp(-\bar{\lambda}^2) \sum_{q,m,\delta} \cos(q/2)|q,m\rangle\langle m+\delta, q| - 2\epsilon_p \qquad (37)$$

$$H^q_1 = U_{eff}|q,0\rangle\langle 0,q| + V_1 \sum_\delta |q,0\rangle\langle \delta, q|. \qquad (38)$$

For a given wave vector q, its form (36) corresponds to a system with impurities at site 0 and its nearest neighbour. When U_{eff} or V_1 is negative, then, depending on the dimensionality, there may be a bound state with eigenvalues below the lowest energy of two polarons. A general solution for the bound states of the bipolaron can be obtained from the poles of the Green's function [18]. After some algebra, the eigen-energies for the bound state are given by the condition

$$\det(1 - \langle \alpha^q|G^q_0|\alpha^q\rangle\langle \alpha^q|H^q_1|\alpha^q\rangle) = 0 \qquad (39)$$

where $G_0(E, q)$ is the Green's function for H_0^q and $|\alpha^q\rangle$ represents a $(z+1)$-component vector:

$$[|q, 0\rangle, \ldots, |q, \vec{\delta}\rangle] \tag{40}$$

with $\vec{\delta}$ as the nearest-neighbour position vector. The corresponding solution of the condition (39) is

$$\frac{1}{U_{eff}} = \frac{-(V_1/4z\tilde{t}_q^2)[E_b'(q)G_0(E_b(q), q) - 1] + G_0(E_b(q), q)}{1 - (V_1 E_b'(q)/4z\tilde{t}_q^2)[E_b'(q)G_0(E_b(q), q) - 1]} \tag{41}$$

where $E_b'(q) = E_b(q) - 2\epsilon_p$ and $\tilde{t}_q = \tilde{t}\cos(q/2)$.

The solution of equation (41) will give rise to energy dispersion. These energy eigenvalues are functions of the variational parameters λ_1 and λ_2. We minimize our lowest two-particle energy with respect to λ_1 and λ_2 to obtain λ_1, λ_2 and the ground-state energy. With these values of λ_1 and λ_2, one can readily calculate the effective mass of the bipolaron from the definition

$$\begin{aligned}
m_{eff} &= \frac{z}{2}\left(\frac{\mathrm{d}^2 E_b(q)}{\mathrm{d}q^2}\right)^{-1}\Bigg|_{q=0} \\
&= \frac{z}{2}\left(\frac{2z\tilde{t}^2 + \frac{1}{4}\mathcal{X}(G_0^b + E_b\,\mathrm{d}G_0^b/\mathrm{d}E_b) - 2z\tilde{t}^2 U_{eff}G_0^b}{V_1 + U_{eff}V_1 G_0^b - 2V_1 E_b' G_0^b - (\mathrm{d}G_0^b/\mathrm{d}E_b)\mathcal{X}}\right)^{-1}
\end{aligned} \tag{42}$$

where

$$\mathcal{X} = 4z\tilde{t}^2 U_{eff} - U_{eff}V_1 E_b' + V_1 E_b'^2.$$

Now the energy eigenvalues calculated from condition (41) will represent the spectrum for the bipolaron provided that it has energy less than twice the ground-state energy of a free polaron (E_p). The ground-state energy of a free polaron can be obtained from the minimization of the energy eigenvalue

$$E_p(\lambda_1, \lambda_2) = -z\tilde{t} - \epsilon_p \tag{43}$$

with respect to λ_1 and λ_2.

5. Results and discussion

In this section we will calculate the ground-state energy, the binding energy and the effective mass of one-, two- and three-dimensional bipolarons. For one dimension we use the one-dimensional Green's function ($G_0^{1D}(E_b^{1D}, q)$) given by equation (19), for two dimensions we use the two-dimensional Green's function ($G_0^{2D}(E_b^{2D}, q)$) given by equation (24) and for three dimensions we use the three-dimensional Green's function ($G_0^{3D}(E_b^{3D}, q)$) given by equation (30), with the conditions (41) and (42) for obtaining the corresponding bipolaron ground-state energy and effective mass respectively. The stability of the bipolaronic phase is ensured by requiring that the bipolaron binding energy ($2E_p - E_b$) should be positive in the bipolaronic phase. Our calculation is based on the modified Lang–Firsov transformation which is suitable for $\hbar\omega/t \geqslant 1$ [8]. Therefore, in this work we will confine our investigations to the region where $\hbar\omega/t \geqslant 1$.

In figures 2, 3 and 4 we plot the variations of the ground-state energy of one-, two- and three-dimensional bipolarons with respect to the on-site Hubbard interaction U for different electron–phonon couplings $g/(\hbar\omega)$ when $t/(\hbar\omega) = 1$. In all three cases, we find an almost linear dependence of the ground-state energy on the on-site Hubbard repulsive interaction U. A decrease of the ground-state energy with increase of U confirms the fact that the repulsive Hubbard interaction disfavours the formation of bound states between two polarons. Our
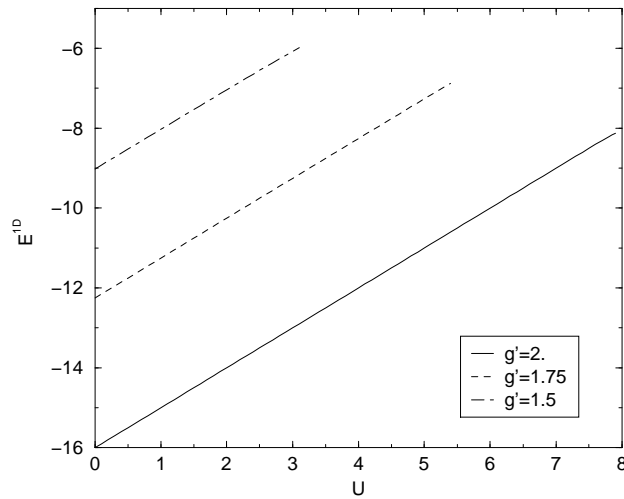
Figure 2. The ground-state energy of the one-dimensional bipolaron E^{1D} versus the on-site Hubbard interaction U for $t/(\hbar\omega) = 1.0$ and $g' = g/(\hbar\omega) = 2.0$, 1.75 and 1.5. (The energies and U are expressed in units of $\hbar\omega$.)
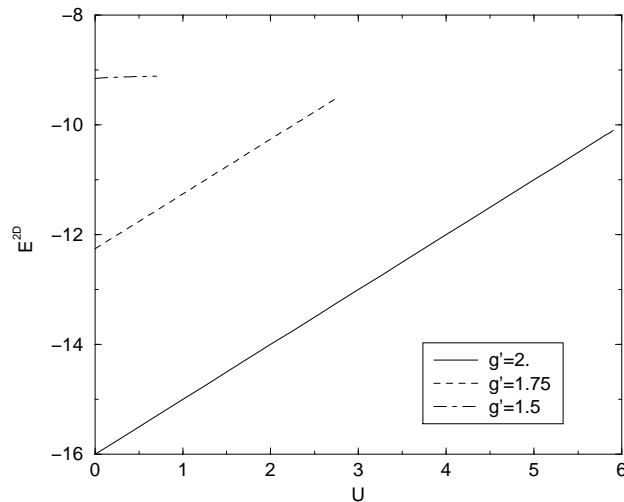

Figure 3. The ground-state energy of the two-dimensional bipolaron E^{2D} versus the on-site Hubbard interaction U for $t/(\hbar\omega) = 1.0$ and $g' = g/(\hbar\omega) = 2.0$, 1.75 and 1.5. (The energies and U are expressed in units of $\hbar\omega$.)

calculation of the ground-state energy for different values of $g/(\hbar\omega)$ shows that the ground-state energy always decreases with increase of the electron–phonon coupling.

In figure 5 we compare the binding energy of one-, two- and three-dimensional bipolarons for $g/(\hbar\omega) = 2$ and $t/(\hbar\omega) = 1$. Here we observe that the binding energy decreases with increase of the on-site Hubbard interaction U, and, beyond a critical value of U, say U_c, the binding energy vanishes. The vanishing of the binding energy implies a transition from a bipolaronic ground state to the polaronic ground state. The transition from the bipolaronic
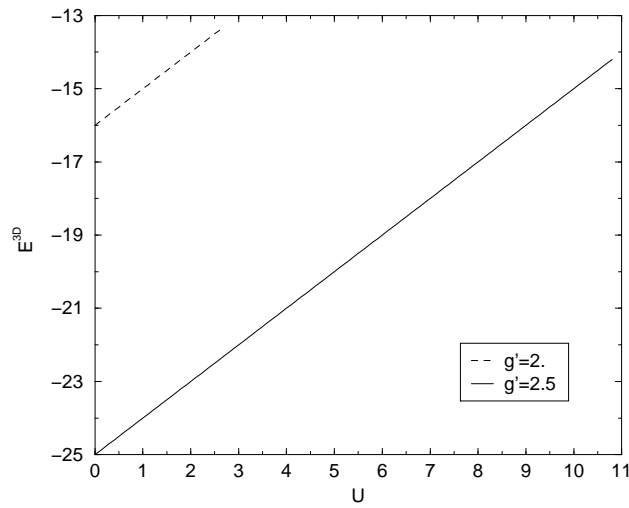
Figure 4. The ground-state energy of the three-dimensional bipolaron E^{3D} versus the on-site Hubbard interaction U for $t/(\hbar\omega) = 1.0$ and $g' = g/(\hbar\omega) = 2.0$ and 2.5. (The energies and U are expressed in units of $\hbar\omega$.)
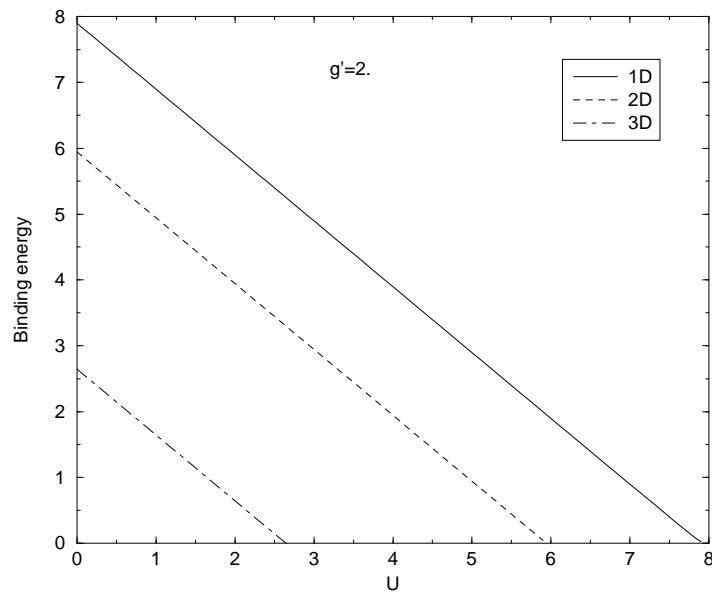

Figure 5. The binding energy of one-, two- and three-dimensional bipolarons versus the on-site Hubbard interaction U for $g' = g/(\hbar\omega) = 2.0$ and $t/(\hbar\omega) = 1.0$. (The energies and U are expressed in units of $\hbar\omega$.)

phase to the polaronic phase occurs at higher values of U as we reduce the dimensionality.

To study the dependence of the binding energy on the electron–phonon coupling $g/(\hbar\omega)$ and the hopping parameter $t/(\hbar\omega)$, we plot the binding energy versus U for $g/(\hbar\omega) = 1.75$ and 1.5 at $t/(\hbar\omega) = 0.5$ in figures 6 and 7.
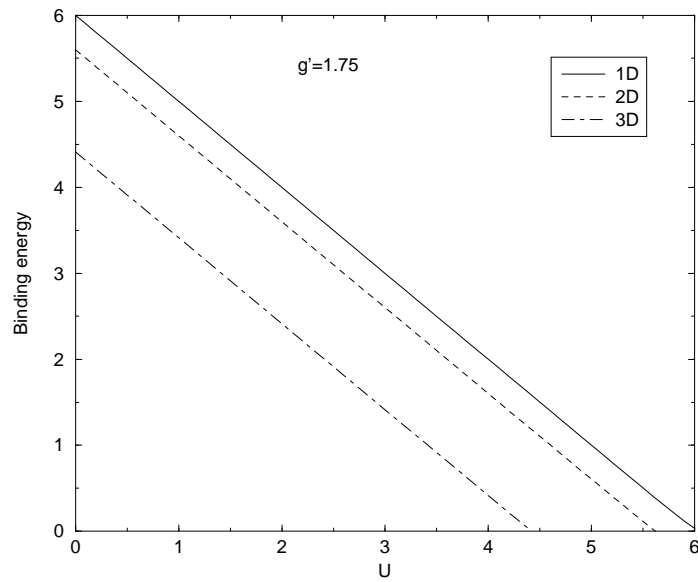
Figure 6. The binding energy of one-, two- and three-dimensional bipolarons versus the on-site Hubbard interaction U for $g' = g/(\hbar\omega) = 1.75$ and $t/(\hbar\omega) = 0.5$. (The energies and U are expressed in units of $\hbar\omega$.)
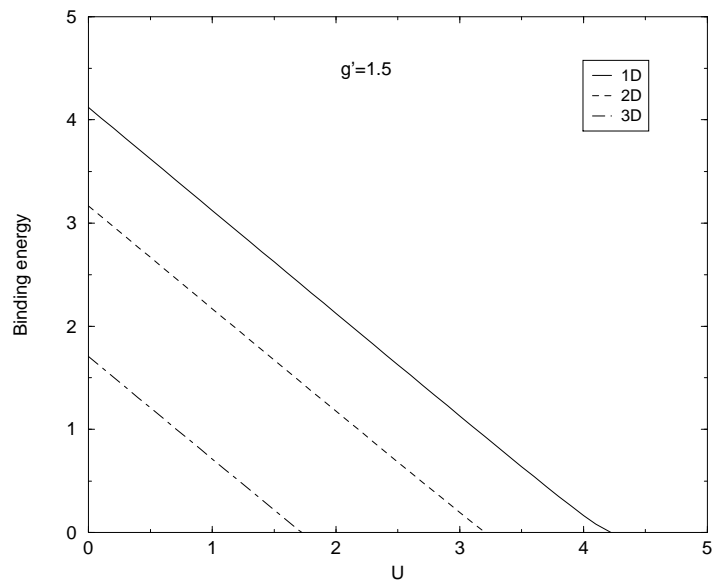

Figure 7. The binding energy of one-, two- and three-dimensional bipolarons versus the on-site Hubbard interaction U for $g' = g/(\hbar\omega) = 1.5$ and $t/(\hbar\omega) = 0.5$. (The energies and U are expressed in units of $\hbar\omega$.)

Since the discovery of high-temperature superconductivity, the mobility of the bipolaron in different dimensions has become an important issue. In order to investigate this problem we

determine the ratio m^*/m between the effective mass m^* of the bipolaron and the free-band mass m. In figure 8 we compare the ratio m^*/m for one-, two- and three-dimensional bipolarons for $g/(\hbar\omega) = 2$ and $t/(\hbar\omega) = 1$. Our calculation shows a decrease of the effective mass with the increase of dimensionality and the increase of the Hubbard on-site interaction U. This result also indicates that the bipolaronic binding is stronger in lower dimensions. To investigate how the electron–phonon coupling $g/(\hbar\omega)$ and the hopping $t/(\hbar\omega)$ affect the effective mass, we studied the variation of the effective mass with respect to U for $g/(\hbar\omega) = 1.75$ and 1.5 at $t/(\hbar\omega) = 0.5$; the results are presented in figures 9 and 10.
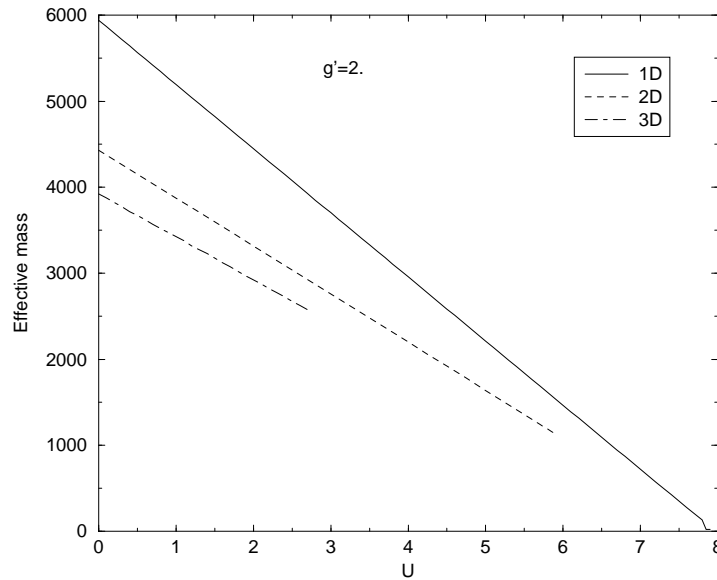

Figure 8. The effective mass of one-, two- and three-dimensional bipolarons versus the on-site Hubbard interaction U (expressed in units of $\hbar\omega$) for $g' = g/(\hbar\omega) = 2.0$ and $t/(\hbar\omega) = 1.0$.

From our earlier discussions, we have found that for any fixed $g/(\hbar\omega)$ there exists a critical on-site interaction $U_c/(\hbar\omega)$ beyond which the polaronic phase becomes stable. Now we will investigate whether there exists a critical electron–phonon coupling $g_c/(\hbar\omega)$ for binding two polarons even when $U = 0$. In figure 11 we plot the variation of $g_c/(\hbar\omega)$ with respect to $t/(\hbar\omega)$ for one-, two- and three-dimensional bipolarons. For one dimension we obtain $g_c/(\hbar\omega) = 0$ for any value of $t/(\hbar\omega)$. This implies that one would get stable bipolarons for any finite electron–phonon coupling when $U = 0$. But the scenario is different in higher dimensions. In two or three dimensions the electron–phonon interaction has to be greater than a critical value to form a stable bipolaron even at $U = 0$. This critical value is higher in higher dimensions for the same value of $t/(\hbar\omega)$. The critical electron–phonon coupling $g_c/(\hbar\omega)$ is an increasing function of $t/(\hbar\omega)$ when the dimension of the electron–phonon system is greater than one.

6. Summary and conclusions

In summary, we have studied a system of two electrons or holes coupled to optical phonons in the non-adiabatic limit and in the presence of an on-site Coulomb repulsion U. We have chosen the modified Lang–Firsov variational wave function with on-site and nearest-neighbour distortion to integrate out the phonon degrees of freedom and obtain an effective interacting
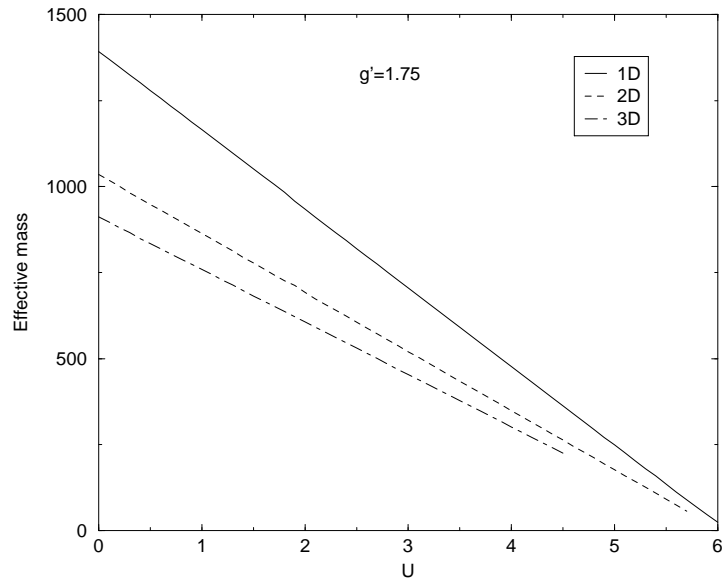
Figure 9. The binding energy of one-, two- and three-dimensional bipolarons versus the on-site Hubbard interaction U (expressed in units of $\hbar\omega$) for $g' = g/(\hbar\omega) = 1.75$ and $t/(\hbar\omega) = 0.5$.
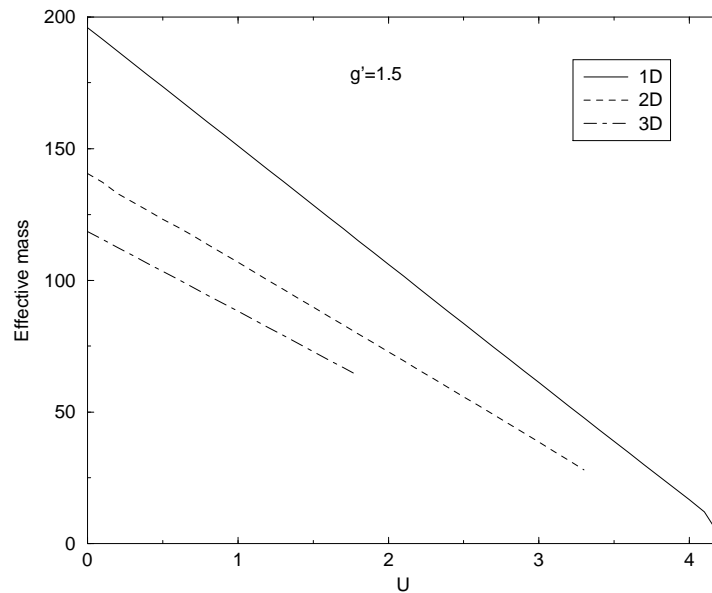

Figure 10. The binding energy of one-, two- and three-dimensional bipolarons versus the on-site Hubbard interaction U (expressed in units of $\hbar\omega$) for $g' = g/(\hbar\omega) = 1.5$ and $t/(\hbar\omega) = 0.5$.

electronic Hamiltonian. This effective electronic Hamiltonian is then solved exactly to obtain the ground-state energy, the binding energy and the effective mass of the one-, two- and three-dimensional bipolarons. While investigating the stability of bipolarons, we observe a critical on-site Hubbard interaction U_c below which the bipolarons are stable. The critical value U_c is
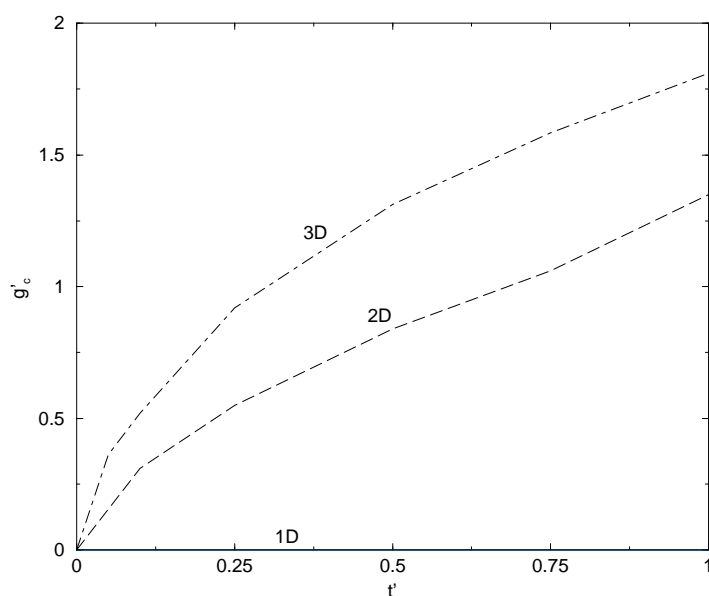
Figure 11. Variation of the critical electron–phonon coupling $g'_c = g_c/(\hbar\omega)$ with respect to $t' = t/(\hbar\omega)$ for one-, two- and three-dimensional bipolarons in the absence of an on-site Hubbard interaction U.

higher in lower dimensions and it increases with increase of the electron–phonon interaction. In the absence of on-site repulsion, the bipolaronic phase is stable for the entire range of electron–phonon interaction for one dimension, but in two or three dimensions the electron–phonon interaction has to be greater than a critical value $g_c/(\hbar\omega)$ for a bound pair of two polarons to form. Since the binding and the mobility of the pair of polarons are the initial requirements for exploring the possibility that these composite bosons could manifest condensation, we believe that the present work will throw some light on the theory of bipolaronic superconductivity.

Acknowledgment

References

[1] Schlenker C 1985 *Physics of Disordered Material* ed D Adler, H Fritzsche and S Ovshinski (New York: Plenum)
[2] Alexandrov A S and Ranninger J 1981 *Phys. Rev.* B **24** 1164
[3] Alexandrov A S and Mott N F 1994 *Rep. Prog. Phys.* **57** 1197
    Mott N F 1987 *Nature* **327** 185
[4] Scott J, Bredas J L, Kaufman J H, Pfluger P, Street S B and Yakushi K 1983 *Mol. Cryst. Liq. Cryst.* **118** 163
[5] Robaszkiewicz S 1984 *Physica* B + C **125** 150
[6] Holstein T 1959 *Ann. Phys., Lpz.* **8** 375
[7] Hubbard J 1963 *Proc. R. Soc.* A **276** 238
[8] Alexandrov A S, Kabanov V V and Ray D K 1994 *Phys. Rev.* B **49** 9915
[9] Marsiglio F 1995 *Physica* C **244** 21
[10] Hirsch J E and Fradkin E 1982 *Phys. Rev. Lett.* **49** 402
    Hirsch J E and Fradkin E 1983 *Phys. Rev.* B **27** 4302

[11] Noack R M and Scalapino D J 1991 *Phys. Rev. Lett.* **66** 778

[12] Marsiglio F 1991 *Electron–Phonon Interaction in Oxide Superconductors* ed R Baquero (Singapore: World Scientific) p 167

[13] Lang I G and Firsov Yu A 1962 *Zh. Eksp. Teor. Fiz.* **43** 1843 (Engl. Transl. 1963 *Sov. Phys.–JETP* **16** 1301)

[14] Das A N and Sil S 1993 *J. Phys.: Condens. Matter* **5** 8265

[15] La Magna A and Pucci R 1996 *Phys. Rev.* B **53** 8449
La Magna A and Pucci R 1997 *Phys. Rev.* B **55** 6296

[16] La Magna A and Pucci R 1997 *Phys. Rev.* B **55** 14 886

[17] Moskalenko V A, Entel P and Digor D F 1999 *Phys. Rev.* B **59** 619

[18] Economou E N 1979 *Green's Functions in Quantum Physics* (Berlin: Springer)

[19] To justify this approximation, let us take the average of $\tilde{H}$ (equation (2)) over the phonon state $|\text{Ph}\rangle = \pi_i(a|0_i\rangle + b|1_i\rangle)$, where $a^2 + b^2 = 1$, instead of the zero-phonon state alone. Now, this modification does not change U_{eff}, V_1 and V_2 directly. Moreover, the contribution of V_{pol-ph} due to our new modified phonon wave function $|\text{Ph}\rangle$ is $-2\sum_{i,\sigma}[(g - \lambda_1) - z\lambda_2]abn_{i,\sigma}$. This is just a site energy and it does not contribute to the binding of two polarons. Therefore, it seems that the modified Lang–Firsov transformation can extract the essential characteristics of the problem of the formation of the bipolaron in the Holstein Hubbard model.