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Roles of phonon-induced potentials for a bipolaron in a superconductor

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Abstract. The bipolaronic system model of an infinite quantum well, in which two electrons or holes are weakly or intermediately coupled with both longitudinal optical (LO) and surface optical (SO) phonons, may be applied to layer-type high-T_c superconductivity. A double unitary transformation of the Hamiltonian is carried out. The numerical results show that when the thickness of the polar slab increases the LO phonon contribution to the binding energy increases but that from the SO phonon decreases. On taking the Coulombic repulsion into account, the binding energy of the bipolaron is found to depend on the distance between the two electrons or holes. It is shown that the potential energy of the effective interaction of the two holes that form the stable bipolaron in a relatively thin polar slab of YBCO has a distinct equilibrium position at its minimum. The magnitude of the binding energy of these two holes becomes larger as the bipolaron size, taken as the equilibrium distance between the holes, becomes smaller.

1. Introduction

With the discovery of the layered oxide cuprate superconductivity [1, 2], it has probably become impossible to explain such a high critical temperature, T_c, within the classical (BCS) theory of superconductivity [3]. A number of novel mechanisms have been developed. In particular, there has been revived interest in the notion of bipolaronic superconductivity [4–9]. The basic idea is that a charged boson-like bipolaron will be formed when the carriers are assumed to bind in pairs within the potential wells produced by the atomic displacements that stabilize the carriers' presence. The bipolaron in a bound state is a real-space pairing of electrons or holes [10], which is different from the $\boldsymbol{k}$-space pairing characteristic of a Cooper pair. The bipolaron carries two negative or two positive charges, depending on the intrinsic properties of the polar crystals.

Adamowski [11] has studied the formation of the Fröhlich bipolaron by calculating the binding energy of a bipolaron as a function of the Fröhlich coupling constant α and the dielectric constant. In [12], Bassani *et al* calculated the energies of bipolaron states variationally in three- and two-dimensional systems, treating the electron–phonon interaction in the Fröhlich approximation. However, their work was focused on the interaction of electrons or holes merely with the bulk longitudinal optical (LO) phonon.

One of us (Gu [13]) has investigated the exciton–phonon system in the two-dimensional case, where the electrons and holes are confined spatially in the same material. By considering the weak and intermediate coupling of electrons and holes with both bulk longitudinal optical phonons and surface optical phonons, the binding energy of the exciton

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and the effect of the exciton on the optical phonon have been studied in great detail [13, 14]. In [15], the exciton–phonon system of the type-II heterostructural quantum well has also been investigated. Since the discovery of high-temperature superconductors in 1986, the bipolaronic theory of high-temperature superconductivity has stimulated a great deal of interest as regards explaining the tremendously high critical temperature of these materials; see [16]. More recently, some researchers have investigated the stability of large bipolarons in three dimensions [17] and in both two and three dimensions [18] for a polar crystal. It was pointed out that the stability region for bipolaron formation is much larger in 2D as compared with 3D [18]. After a careful analysis of the results given in existing references, we note that the Hamiltonian of a bipolaronic system, of either electron type or hole type in the polar crystal, in some sense has a similar form to that of the excitonic system. So, in this paper, we would like to present a formalism for the binding energy of a bipolaronic system, which may be related to the behaviour of a high-T_c superconductor.

In this paper, our task is to consider the interactions of the electrons or holes not only with the bulk longitudinal optical (LO) phonons but also with the surface optical (SO) phonons in the low-temperature limit (at zero temperature) and to investigate the behaviour of the electron- or hole-type bipolaron system in the polar slab by using a double unitary transformation similar to that used in [14, 19], which is particularly applicable for large polarons. We also study how the binding energy of the two electrons or holes in the large bipolaron depends on the distance between them. We consider that the interaction potential $V_I(z_1, z_2, \rho)$ induced by the interaction of the bipolaron is divided into two parts: one, $V_I^0(z_1)(V_I^0(z_2))$, is similar to that given by equation (13) in [14], which depends on z_1 (z_2); the other, $V_I'(z_1, z_2, \rho)$, is the attractive Cooper pair interaction which depends not only on z_1 (z_2) but also on the relative position of the xy projection. On the other hand, the repulsive Coulombic potential is of paramount importance; it reduces the binding energy of the bipolaron when the two electrons or holes are very close. It is less favourable to the formation of the bipolaron.

Note that the results deduced in this paper will be applicable for weakly and intermediately coupled bipolarons in layered polar slabs.

2. Theory

Consider a slab of polar crystal with thickness d, which is surrounded by a vacuum for $[z] > d/2$, and for which the quantum well profiles for the electron- and hole-type bipolaron are as shown in figure 1. We make the generalization that the Hamiltonian of the (either electron- or hole-type) bipolaronic system in the quantum well along the z-direction can be expressed as follows:

$$\begin{aligned}\hat{H}_{bip} = {} & \frac{p_{1z}^2}{2m_1} + \frac{p_{2z}^2}{2m_2} + \frac{P^2}{2M} + \frac{p^2}{2\mu} + \frac{e^2}{\epsilon_\infty[\rho^2 + (z_1 - z_2)^2]^{1/2}} + V_1(z_1) + V_2(z_2) \\ & + \sum_{\boldsymbol{k},m,p} \hbar\omega_{LO}\hat{a}^+_{\boldsymbol{k},m,p}\hat{a}_{\boldsymbol{k},m,p} + \sum_{\boldsymbol{q},p} \hbar\omega_{SOp}\hat{b}^+_{\boldsymbol{q},p}\hat{b}_{\boldsymbol{q},p} \\ & + \sum_{\boldsymbol{k},m}\{B^*[W_{\boldsymbol{k},m,+}(z_1, z_2, \rho)\hat{a}^+_{\boldsymbol{k},m,+} + W_{\boldsymbol{k},m,-}(z_1, z_2, \rho)\hat{a}^+_{\boldsymbol{k},m,-}]e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} + \text{HC}\} \\ & + \sum_{\boldsymbol{q}}\left[\frac{\sinh(qd)}{q}\right]^{1/2} e^{-qd/2}\{C^*[V_{\boldsymbol{q},+}(z_1, z_2, \rho)\hat{b}^+_{\boldsymbol{q},+} \\ & + V_{\boldsymbol{q},-}(z_1, z_2, \rho)\hat{b}^+_{\boldsymbol{q},-}]e^{-i\boldsymbol{q}\cdot\boldsymbol{R}} + \text{HC}\} \end{aligned} \tag{1}$$

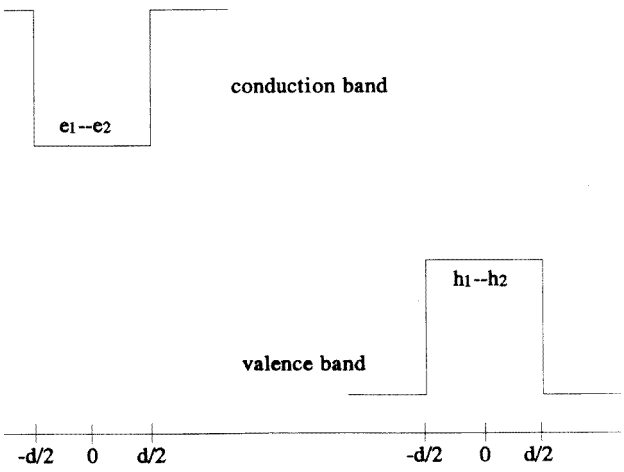

Figure 1. Plots of the quantum well potential profiles along the z-axis for the electron-type bipolaron in the conduction band, and for the hole-type bipolaron in the valence band.

where the infinite quantum wells in which the two electrons or holes trapped are defined as

$$V_1(z_1) = \begin{cases} 0 & |z_1| \leqslant d/2 \\ \infty & |z_1| > d/2 \end{cases} \tag{2}$$

$$V_2(z_2) = \begin{cases} 0 & |z_2| \leqslant d/2 \\ \infty & |z_2| > d/2. \end{cases} \tag{3}$$

In equation (1), except for the Coulombic interaction potential having a different sign, the Hamiltonian of the bipolaronic system is seen to have a similar form to that of the excitonic system [14]. In the bipolaronic system, the Coulombic interaction is repulsive, which takes the positive sign, whereas in the excitonic system, the Coulombic interaction is attractive, and has a negative sign. Furthermore, the above Hamiltonian has been expressed in the coordinate frame of the centre of mass, with $s_1 = m_1/M$, $s_2 = m_2/M$, $M = m_1 + m_2$, $\mu = m_1 m_2/M$. $\boldsymbol{\rho}$ is the difference between the vectors for projection onto the xy-plane of the two electrons or holes which are bounded in the bipolaron, i.e. $\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2$. $\boldsymbol{R}$ is the vector for projection onto the xy-plane of the spatial vector for the centre of mass, i.e. $\boldsymbol{R} = s_1\boldsymbol{\rho}_1 + s_2\boldsymbol{\rho}_2$. ω_{LO} and ω_{SO} are the frequencies of the LO phonons and the SO phonons respectively, which have the following relationships:

$$\omega_{SO\pm}^2 = \omega_{TO}^2 \frac{(\epsilon_0 + 1) \mp (\epsilon_0 - 1)\mathrm{e}^{-qd}}{(\epsilon_\infty + 1) \mp (\epsilon_\infty - 1)\mathrm{e}^{-qd}} \tag{4}$$

$$\omega_{LO}^2 = \omega_{TO}^2 \frac{\epsilon_0}{\epsilon_\infty}. \tag{5}$$

ω_{TO} is the frequency of the bulk transverse optical phonon. ϵ_0 and ϵ_∞ are the static and optical dielectric constants of the polar crystal. $\boldsymbol{k}$ and $\boldsymbol{q}$ are the two-dimensional wavevectors of the LO and SO phonons respectively. m is the quantum number of the z-component of the LO mode, $m = 1, 2, \ldots, N$. $\hat{a}^+_{\boldsymbol{k},m,p}$ ($\hat{a}_{\boldsymbol{k},m,p}$) and $\hat{b}^+_{\boldsymbol{q},p}$ ($\hat{b}_{\boldsymbol{q},p}$) are the creation (annihilation) operators with parity $p = \pm$ for the LO and SO phonons. The other symbols in equation (1)

are defined as follows [20]:

$$W_{\boldsymbol{k},m,+}(z_1,z_2,\rho)=\frac{\cos[m\pi z_1/d]}{[k^2+[m\pi/d]^2]^{1/2}}\mathrm{e}^{-\mathrm{i}s_2\boldsymbol{k}\cdot\boldsymbol{\rho}} +\frac{\cos[m\pi z_2/d]}{[k^2+[m\pi/d]^2]^{1/2}}\mathrm{e}^{\mathrm{i}s_1\boldsymbol{k}\cdot\boldsymbol{\rho}} \qquad m=1,3,5,\ldots \tag{6}$$

$$W_{\boldsymbol{k},m,-}(z_1,z_2,\rho)=\frac{\sin[m\pi z_1/d]}{[k^2+[m\pi/d]^2]^{1/2}}\mathrm{e}^{-\mathrm{i}s_2\boldsymbol{k}\cdot\boldsymbol{\rho}} +\frac{\sin[m\pi z_2/d]}{[k^2+[m\pi/d]^2]^{1/2}}\mathrm{e}^{\mathrm{i}s_1\boldsymbol{k}\cdot\boldsymbol{\rho}} \qquad m=2,4,6,\ldots \tag{7}$$

$$V_{\boldsymbol{q},\pm}(z_1,z_2,\rho)=G_{\pm}(\boldsymbol{q},z_1)\exp(-\mathrm{i}s_2\boldsymbol{q}\cdot\boldsymbol{\rho})+G_{\pm}(\boldsymbol{q},z_2)\exp(\mathrm{i}s_1\boldsymbol{q}\cdot\boldsymbol{\rho}). \tag{8}$$

$$B^*=\mathrm{i}\left[\frac{4\pi e^2}{V}\hbar\omega_{LO}\left[\frac{1}{\epsilon_\infty}-\frac{1}{\epsilon_0}\right]\right]^{1/2} \tag{9}$$

$$C^*=\mathrm{i}\left[\frac{2\pi e^2}{A}\hbar\omega_{TO}(\epsilon_0-\epsilon_\infty)\right]^{1/2} \tag{10}$$

$$G_+(q,z)=\begin{cases}\dfrac{\cosh(qz)/\cosh(qd/2)}{(\epsilon_\infty+1)-(\epsilon_\infty-1)\mathrm{e}^{-qd}}\left[\dfrac{(\epsilon_\infty+1)-(\epsilon_\infty-1)\mathrm{e}^{-qd}}{(\epsilon_0+1)-(\epsilon_0-1)\mathrm{e}^{-qd}}\right]^{1/4} & |z|\leqslant\dfrac{d}{2}\\ \dfrac{\mathrm{e}^{-q|z|}/\mathrm{e}^{-qd}}{(\epsilon_\infty+1)-(\epsilon_\infty-1)\mathrm{e}^{-qd}}\left[\dfrac{(\epsilon_\infty+1)-(\epsilon_\infty-1)\mathrm{e}^{-qd}}{(\epsilon_0+1)-(\epsilon_0-1)\mathrm{e}^{-qd}}\right]^{1/4} & |z|>\dfrac{d}{2}\end{cases} \tag{11}$$

$$G_-(q,z)=\begin{cases}\dfrac{\sinh(qz)/\sinh(qd/2)}{(\epsilon_\infty+1)-(\epsilon_\infty-1)\mathrm{e}^{-qd}}\left[\dfrac{(\epsilon_\infty+1)+(\epsilon_\infty-1)\mathrm{e}^{-q/d}}{(\epsilon_0+1)-(\epsilon_0-1)\mathrm{e}^{-qd}}\right]^{1/4} & |z|\leqslant\dfrac{d}{2}\\ \dfrac{\mathrm{e}^{-q|z|}/\mathrm{e}^{-qd/2}}{(\epsilon_\infty+1)-(\epsilon_\infty-1)\mathrm{e}^{-qd}}\left[\dfrac{(\epsilon_\infty+1)+(\epsilon_\infty-1)\mathrm{e}^{-qd}}{(\epsilon_0+1)-(\epsilon_0-1)\mathrm{e}^{-qd}}\right]^{1/4} & |z|>\dfrac{d}{2}.\end{cases} \tag{12}$$

To solve for the ground-state energy for the bipolaron trapped in the infinite-quantum-well system, which has the Hamiltonian specified in equation (1), is in fact a difficult task. In order to obtain a solution, we need first of all to make a transformation to eliminate the radial vector $\boldsymbol{R}$ by making use of $\hat{U}_1$. Secondly, the transformed Hamiltonian needs to be diagonalized by using the $\hat{U}_2$-operator. Both of these unitary transformation operators are specified below:

$$\hat{U}_1=\exp\left(-\mathrm{i}\sum_{\boldsymbol{k},m,p}\hat{a}^+_{\boldsymbol{k},m,p}\hat{a}_{\boldsymbol{k},m,p}\boldsymbol{k}\cdot\boldsymbol{R}-\mathrm{i}\sum_{\boldsymbol{q},p}\hat{b}^+_{\boldsymbol{q},p}\hat{b}_{\boldsymbol{q},p}\boldsymbol{q}\cdot\boldsymbol{R}\right) \tag{13}$$

and

$$\hat{U}_2=\exp\left(\sum_{\boldsymbol{k},m,p}(\hat{a}^+_{\boldsymbol{k},m,p}f_{\boldsymbol{k},m,p}-\hat{a}_{\boldsymbol{k},m,p}f^*_{\boldsymbol{k},m,p})+\sum_{\boldsymbol{q},p}(\hat{b}^+_{\boldsymbol{q},p}g_{\boldsymbol{q},p}-\hat{b}_{\boldsymbol{q},p}g^*_{\boldsymbol{q},p})\right). \tag{14}$$

By applying a similar transformation to the Hamiltonian given as equation (1) via the double unitary transformation operator, we obtain

$$\hat{\tilde{H}}_{bip}=\hat{U}_2^{-1}\hat{U}_1^{-1}\hat{H}_{bip}\hat{U}_1\hat{U}_2=\hat{H}'_{bip}+\hat{\mathcal{F}}(\hat{a}^+_{\boldsymbol{k},m,p},\hat{a}_{\boldsymbol{k},m,p},\hat{b}^+_{\boldsymbol{q},p},\hat{b}_{\boldsymbol{q},p}) \tag{15}$$

where $\hat{H}'_{bip}$ represents the dominant part of the energy for the bipolaron system, and can be written in the following form:

$$\hat{H}'_{bip}=\hat{H}_{1D}+\hat{H}_{2D}+V_I(z_1,z_2,\rho) \tag{16}$$

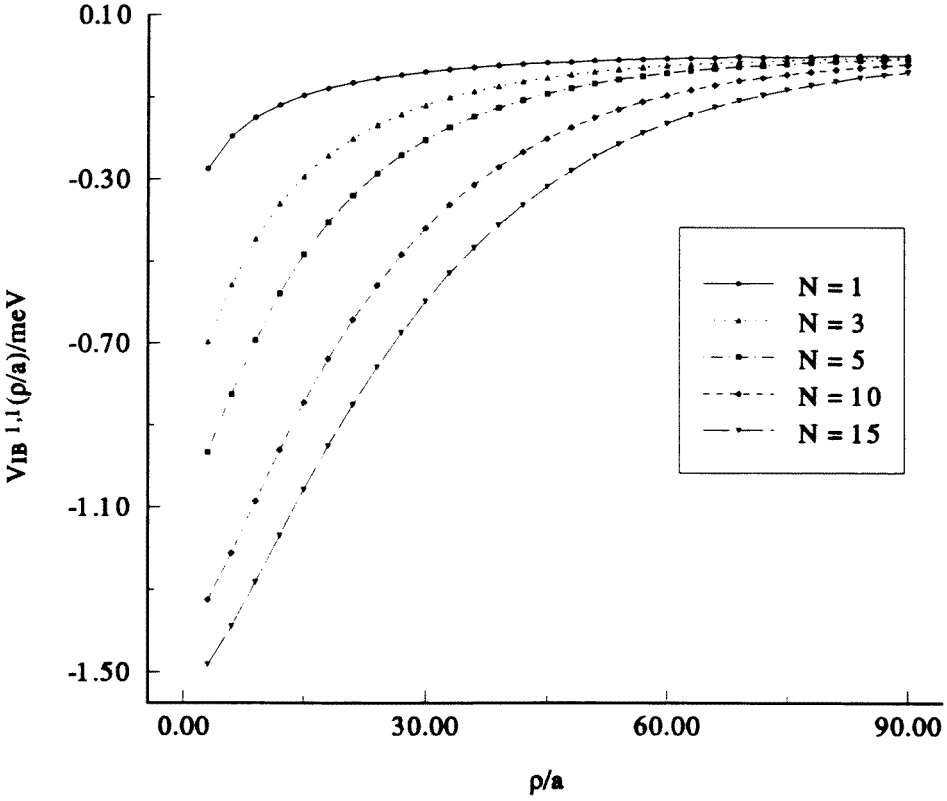

Figure 2. Plots of the bulk-LO-phonon-induced potential $V_{IB}^{1,1}(\rho/a)$, with $l_1 = l_2 = 1$, against the relative position ρ/a of two holes projected onto the xy-plane.

in which

$$\hat{H}_{1D} = -\frac{\hbar^2}{2m_1}\nabla_{z_1}^2 - \frac{\hbar^2}{2m_2}\nabla_{z_2}^2 + V_1(z_1) + V_2(z_2) \tag{17}$$

$$\hat{H}_{2D} = -\frac{\hbar^2}{2\mu}\nabla_{\rho}^2 \tag{18}$$

$$V_I(z_1, z_2, \rho) = V_I^0(z_1) + V_I^0(z_2) + V_I'(z_1, z_2, \rho) + \frac{e^2}{\epsilon_\infty\sqrt{\rho^2 + (z_1 - z_2)^2}}. \tag{19}$$

The function $\hat{\mathcal{F}}(\hat{a}^+_{\boldsymbol{k},m,p}, \hat{a}_{\boldsymbol{k},m,p}, \hat{b}^+_{\boldsymbol{q},p}, \hat{b}_{\boldsymbol{q},p})$, has an extremely complex form. In an approximation, we can neglect the interaction between virtual phonons with different wave vectors emitted by the recoiling bipolaron. The function $\hat{\mathcal{F}}(\hat{a}^+_{\boldsymbol{k},m,p}, \hat{a}_{\boldsymbol{k},m,p}, \hat{b}^+_{\boldsymbol{q},p}, \hat{b}_{\boldsymbol{q},p})$ may have a value of order much less than that of the dominant part stated previously. Recalling the unperturbed Hamiltonian $\hat{H}_{1D}$ on the R.H.S. of equation (16), its eigenvalue is given by $E^{1D}_{l_1 l_2}$ which can be expressed as

$$E^{1D}_{l_1 l_2} = \frac{\pi^2\hbar^2 l_1^2}{2m_1 d^2} + \frac{\pi^2\hbar^2 l_2^2}{2m_2 d^2} \tag{20}$$

where the quantum numbers $l_1, l_2 = 1, 2, \ldots$, and the corresponding wavefunction is [14]

$$\phi_{1D}(z_1, z_2) = \begin{cases} \sqrt{2/d}\sin(l_1(z_1 + 0.5d)\pi/d)\sqrt{2/d}\sin(l_2(z_2 + 0.5d)\pi/d) \\ \qquad \text{when } 0 < |z_1|, |z_2| < d/2 \\ 0 \qquad \text{otherwise.} \end{cases} \tag{21}$$

Note that in the solution of the wavefunction, we have considered the phase difference due to the boundary of the infinite quantum well, namely $\phi = l_i\pi/2$, where $i = 1$ or 2. Furthermore, the orthonormal wavefunction which corresponds to the two-dimensional motion in the xy-plane is assumed to be $\phi_{2D}(\rho)$.

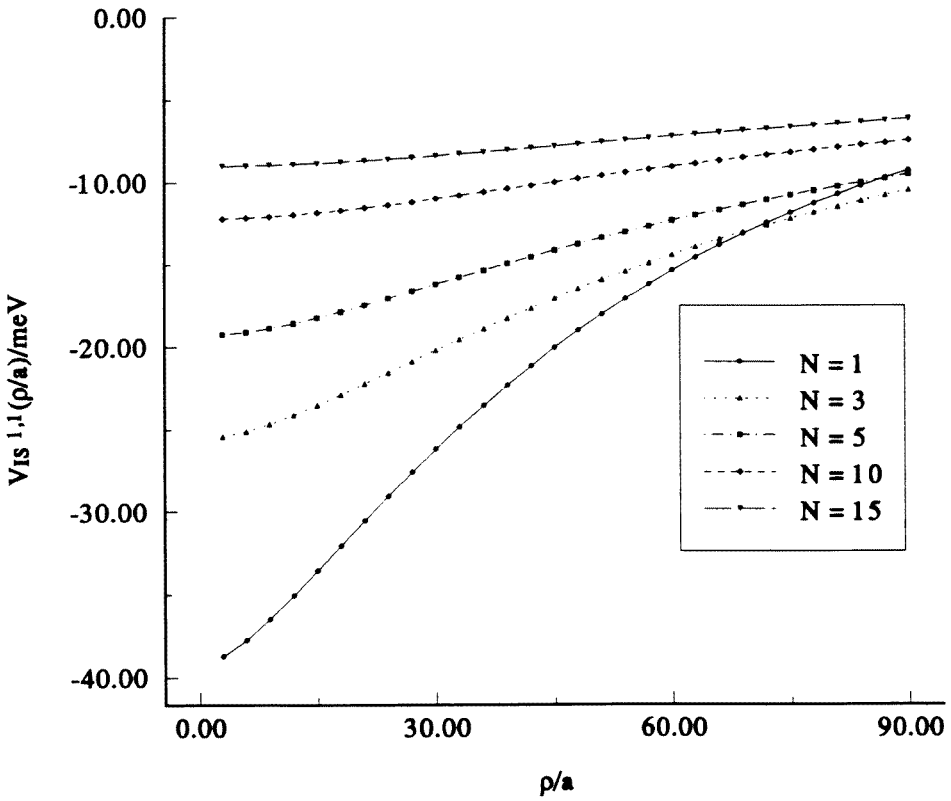

Figure 3. Plots of the SO-phonon-induced potential $V_{IS}^{1,1}(\rho/a)$, with $l_1 = l_2 = 1$, against the relative position ρ/a of two holes projected onto the xy-plane.

The dominant part of the energy for the bipolaron system is determined by equation (16). The first two terms of this energy represent the unperturbed Hamiltonian; they correspond to the kinetic energies due to the one-dimensional (along the z-axis) and the two-dimensional (on the xy-plane) motions of the two free electrons or holes, and also surplus energies due to the potential wells. Overall, equation (17) represents the total energy of the two electrons or holes that move in the potential wells. From equation (19) we note that the interaction potential $V_I(z_1, z_2, \rho)$ is induced by the phonon acting on the bipolaron; it can be divided into three parts. The first part includes $V_I^0(z_1)$ and $V_I^0(z_2)$ which depend on z_1 and z_2 respectively. The second part is $V_I'(z_1, z_2, \rho)$ which depends not only on z_1 and z_2, but also

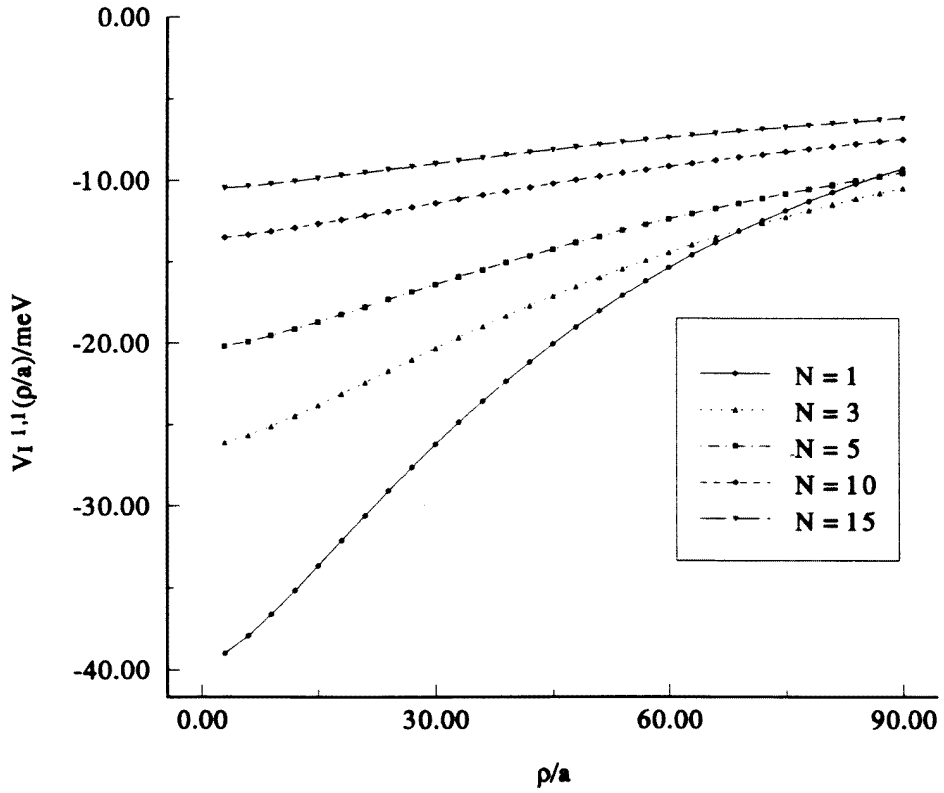

Figure 4. Plots of the total phonon-induced potential $V_I^{1,1}(\rho/a)$, with $l_1 = l_2 = 1$, against the relative position ρ/a of two holes projected onto the xy-plane.

on the coordinate ρ that represents the distance between the two electrons or holes projected onto the xy-plane. This part of interaction is in fact contributed by the bulk longitudinal optical phonon, $V'_{IB}(z_1, z_2, \rho)$, and the surface optical phonon $V'_{IS}(z_1, z_2, \rho)$:

$$V'_I(z_1, z_2, \rho) = V'_{IB}(z_1, z_2, \rho) + V'_{IS}(z_1, z_2, \rho) \tag{22}$$

where

$$V'_{IB}(z_1, z_2, \rho) = -8\frac{\alpha\bar{h}\omega_{LO}u_l}{d}\left[\sum_{m=1,3,\ldots}\cos\left[\frac{m\pi}{d}z_1\right]\cos\left[\frac{m\pi}{d}z_2\right] + \sum_{m=2,4,\ldots}\sin\left[\frac{m\pi}{d}z_1\right]\right.$$
$$\left.\times\sin\left[\frac{m\pi}{d}z_2\right]\right] \times \int_0^\infty \left[1 + \frac{Ms_1s_2k^2}{\mu(k^2+u_l^2)}\right]\frac{kJ_0(\rho k)}{(k^2+u_l^2)[k^2+[m\pi/d]^2}\,\mathrm{d}k \tag{23a}$$

$$V'_{IS}(z_1, z_2, \rho) = -4\alpha\bar{h}\omega_{LO}u_l\epsilon_\infty^{3/2}\epsilon_0^{1/2}\int_0^\infty \sinh(qd)\mathrm{e}^{-qd}q^2J_0(\rho q)$$
$$\times\left[\frac{\cosh(qz_1)\cosh(qz_2)}{\epsilon_1(q)\cosh^2(qd/2)}\left(\frac{1}{q^2(q^2+u_{s+}^2)} + \frac{Ms_1s_2}{\mu(q^2+u_{s+}^2)^2}\right)\right.$$
$$\left.+\frac{\sinh(qz_1)\sinh(qz_2)}{\epsilon_2(q)\sinh^2(qd/2)}\left(\frac{1}{q^2(q^2+u_{s-}^2)} + \frac{Ms_1s_2}{\mu(q^2+u_{s-}^2)^2}\right)\right]\mathrm{d}q \tag{23b}$$

in which $J_0(\rho k)$ and $J_0(\rho q)$ are the zero-order Bessel functions, and

$$\begin{aligned}\epsilon_1(q) &= [\epsilon_\infty + 1 - (\epsilon_\infty - 1)\mathrm{e}^{-qd}]^{3/2}[\epsilon_0 + 1 - (\epsilon_0 - 1)\mathrm{e}^{-qd}]^{1/2} \\ \epsilon_2(q) &= [\epsilon_\infty + 1 + (\epsilon_\infty - 1)\mathrm{e}^{-qd}]^{3/2}[\epsilon_0 + 1 + (\epsilon_0 - 1)\mathrm{e}^{-qd}]^{1/2}.\end{aligned} \tag{24}$$

The last term in equation (19), i.e. $V_{coul}(z_1, z_2, \rho)$, is the Coulombic interaction potential describing the interaction between the two electrons or holes. Summarizing the above results, we can write the eigenfunction for any quantum numbers l_1 and l_2 as a product of $|\phi_{1D}(z_1, z_2, \rho)\rangle$ and $|0\rangle$, i.e.

$$|\bar{\Phi}(z_1, z_2, \rho)\rangle = |\phi_{1D}(z_1, z_2)\phi_{2D}(\rho)\rangle|0\rangle. \tag{25}$$

In this paper, we concentrate on the calculation for the total effective potential energy, which consists of the phonon-induced potential and Coulombic interaction energies, so we mainly give computational results for that effective-potential energy as functions of the relative position of two holes projected onto the xy-plane. This energy represents the contribution for the stability of pairing between holes in the ceramic superconductor when they are attractive. The first-order perturbation of this interaction energy for the system is given by

$$\begin{aligned}E' &= \langle\bar{\Phi}(z_1, z_2, \rho)|V_I'(z_1, z_2, \rho) + V_{coul}(z_1, z_2, \rho)||\bar{\Phi}(z_1, z_2, \rho)\rangle \\ &= \langle\phi_{2D}(\rho)|V_{IB}^{l_1,l_2}(\rho) + V_{IS}^{l_1,l_2}(\rho) + V_{coul}^{l_1,l_2}(\rho)|\phi_{2D}(\rho)\rangle\end{aligned} \tag{26}$$

where

$$\begin{aligned}V_{IB}^{l_1,l_2}(\rho) &= \langle\phi_{1D}(z_1, z_2)|V_{IB}'(z_1, z_2, \rho)|\phi_{1D}(z_1, z_2)\rangle \\ &= -32\frac{\alpha\hbar\omega_{LO}u_l}{d^3}\int_{-d/2}^{d/2}\int_{-d/2}^{d/2}\sin^2\left[\frac{l_1\pi}{d}\left(z_1 + \frac{1}{2}d\right)\right]\sin^2\left[\frac{l_2\pi}{d}\left(z_2 + \frac{1}{2}d\right)\right] \\ &\quad\times\left[\sum_{m=1,3,\ldots}\cos\left[\frac{m\pi}{d}z_1\right]\cos\left[\frac{m\pi}{d}z_2\right] + \sum_{m=2,4,\ldots}\sin\left[\frac{m\pi}{d}z_1\right]\sin\left[\frac{m\pi}{d}z_2\right]\right] \\ &\quad\times\int_0^\infty\left[1 + \frac{Ms_1s_2k^2}{\mu(k^2 + u_l^2)}\right]\frac{kJ_0(\rho k)}{(k^2 + u_l^2)[k^2 + [m\pi/d]^2]}\,\mathrm{d}k\,\mathrm{d}z_1\,\mathrm{d}z_2\end{aligned} \tag{27}$$

$$\begin{aligned}V_{IS}^{l_1,l_2}(\rho) &= \langle\phi_{1D}(z_1, z_2)|V_{IS}'(z_1, z_2, \rho)|\phi_{1D}(z_1, z_2)\rangle \\ &= -16\frac{\alpha\hbar\omega_{LO}u_l\epsilon_\infty^{3/2}\epsilon_0^{1/2}}{d^2} \\ &\quad\times\int_{-d/2}^{d/2}\int_{-d/2}^{d/2}\sin^2\left[\frac{l_1\pi}{d}\left(z_1 + \frac{1}{2}d\right)\right]\sin^2\left[\frac{l_2\pi}{d}\left(z_2 + \frac{1}{2}d\right)\right]\int_0^\infty\sinh(qd) \\ &\quad\times\mathrm{e}^{-qd}q^2J_0(\rho q)\left[\frac{\cosh(qz_1)\cosh(qz_2)}{\epsilon_1(q)\cosh^2(qd/2)}\left(\frac{1}{q^2(q^2 + u_{s+}^2)} + \frac{Ms_1s_2}{\mu(q^2 + u_{s+}^2)^2}\right)\right. \\ &\quad\left.+\frac{\sinh(qz_1)\sinh(qz_2)}{\epsilon_2(q)\sinh^2(qd/2)}\left(\frac{1}{q^2(q^2 + u_{s-}^2)} + \frac{Ms_1s_2}{\mu(q^2 + u_{s-}^2)^2}\right)\right]\mathrm{d}q\,\mathrm{d}z_1\,\mathrm{d}z_2\end{aligned} \tag{28}$$

and the repulsive Coulombic potential is given by

$$\begin{aligned}V_{coul}^{l_1,l_2}(\rho) &= \langle\phi_{1D}(z_1, z_2)|\frac{e^2}{\epsilon_\infty[\rho^2 + (z_1 + z_2)^2]^{1/2}}|\phi_{1D}(z_1, z_2)\rangle \\ &= \frac{4e^2}{d^2\epsilon_\infty}\int_{-d/2}^{d/2}\int_{-d/2}^{d/2}\frac{1}{[\rho^2 + (z_1 - z_2)^2]^{1/2}}\sin^2\left[\frac{l_1\pi}{d}\left(z_1 + \frac{1}{2}d\right)\right] \\ &\quad\times\sin^2\left[\frac{l_2\pi}{d}\left(z_2 + \frac{1}{2}d\right)\right]\mathrm{d}z_1\,\mathrm{d}z_2\end{aligned} \tag{29}$$

where $V_{IB}^{l_1,l_2}(\rho)$ and $V_{IS}^{l_1,l_2}(\rho)$ are the induced attractive potentials for the Cooper pair which is composed of two interacting electrons or holes mediated by the LO phonon and the SO phonon respectively, and $V_{coul}^{l_1,l_2}(\rho)$ is the repulsive Coulombic potential energy, ρ being the average distance between the two electrons or holes. In the following section, we shall briefly discuss and reach conclusions regarding our results based on the equations (27), (28) and (29).

3. Discussion and conclusions

In this section, we take the superconducting material, YBCO, as the subject of our study, and use it to demonstrate the results of our numerical calculations. We regard the two holes as the conducting carriers, having masses of $m_1 = m_2 = m_h$, and make use of the more demanding condition of the ions within the crystal having a sufficiently large displaceability that a large bipolaron will result from two holes that have a certain separation ρ and bind with each other to form a bound state. Note that for this condition we have $\epsilon_0 > 2\epsilon_\infty$ [8]. Furthermore, we set $\epsilon_\infty = 35$ and $\epsilon_0 = 150$. The lattice parameters for YBCO are $a = 3.82$ Å, $b = 3.88$ Å, $c = 11.69$ Å. The parameters used in our calculation are listed in table 1. First of all, on the basis of equations (27) and (28), the bulk LO-phonon- and the SO-phonon-induced potentials with $l_1 = l_2 = 1$ are calculated for various values of ρ/a, where ρ represents the relative position of the two holes projected onto the xy-plane and a is the lattice parameter on the a-axis of the YBCO crystal unit cell, i.e. $a = 3.82$ Å. The option for adopting this lattice parameter a is based on the fact that the bipolaron is formed preferentially along the a-axis (or x-axis), and it will be relatively free to move on the xy-plane throughout the crystal space. The thickness d of the potential well can be taken along the direction of the c-axis of the YBCO crystal. By setting $d = Nc$, with $c = 11.64$ Å for the polar slab, we may plot the functions of $V_{IB}^{1,1}(\rho/a)$ and $V_{IS}^{1,1}(\rho/a)$ against ρ/a with fixed values of N for individual curves (figures 2 and 3). In these figures, it is clearly shown that the induced LO-mode and SO-mode potentials both decrease with increasing relative distance between the holes. These plots are traced out with certain values of N that represent the numbers of unit cells along the c-axis (or z-axis). Furthermore, as can be seen from these figures, the thicker the polar slab, the larger the magnitude of the LO-induced potential. However, for the case of the SO-induced potential, the opposite result is obtained, i.e. the thicker the polar slab, the smaller the magnitude of the SO-induced potential. This can be seen from equation (1): there is a decaying factor, $e^{-qd/2}$, which makes the SO-induced potential drop rapidly. So the hole–SO-phonon coupling is very strong only near the surface of the polar slab. For an extremely thin polar slab, the SO-mode effect is not negligible. The total attractive phonon-induced potential including both the LO mode and the SO mode is plotted in figure 4. It is obvious that when the thickness of the slab decreases, the magnitude of the total phonon-induced potential increases more rapidly for a fixed relative distance between the two holes. Note that the effect for the total induced potential is dominated by the contribution due to the SO mode for our case of a thin polar slab. In figure 5, the repulsive Coulombic potential is plotted against ρ. In general, the Coulombic potential is not dependent on the thickness of the slab, except that the two holes are much closer together, i.e. $\rho/a < 30.00$. We should not neglect the effect of so large a Coulombic repulsion potential.

The sum of the LO-mode- and SO-mode-induced potentials and the Coulombic potential will represent the effective interaction energy of the trapped bipolaron in the infinite quantum well. This effective interaction energy is a measure of the binding energy of the two holes in the bipolaron. One of the most important factors for the stability of large-bipolaron formation

Table 1. Parameters for the polar crystal of YBCO used for our calculations, where m_0 is the free-electron mass.

α	$\hbar\omega_{LO}$ (meV)	ϵ_∞	ϵ_0	m_h/m_0	a (Å)	b (Å)	c (Å)
0.017	79.00	35	150	0.0037	3.82	3.88	11.64

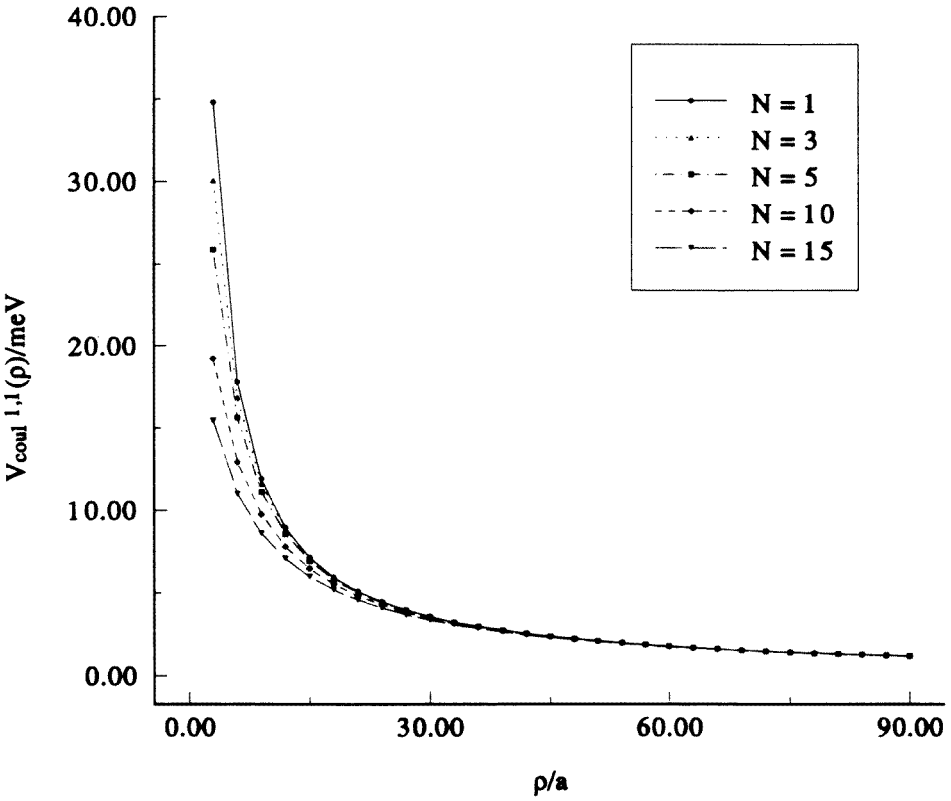

Figure 5. Plots of the repulsive Coulombic potential $V_{coul}^{1,1}(\rho/a)$, with $l_1 = l_2 = 1$, against the relative position ρ/a of two holes projected onto the xy-plane.

is determined by this effective interaction energy. Plots of this effective interaction energy for different thicknesses are shown in figure 6. Since this effective interaction energy involves the attractive phonon-induced potential and the repulsive Coulombic potential, which are functions of ρ, it becomes positive when ρ is extremely small, i.e. $\rho/a < 6$. If the effective potential is positive, the bipolaron will not be stable, since the two holes cannot form a bound state. However, for a relatively thin polar slab, one may obtain a negative effective potential for a bipolaron formation, with the equilibrium distance at the minimum of the effective interaction energy for these two holes. Note that in equation (29) the repulsive Coulombic potential is shielded by the optical dielectric constant, ϵ_∞. The larger the optical dielectric constant, the smaller the Coulombic repulsion. This, in turn, makes the effective potential energy more negative. This may stimulate experimental research into the temperature dependence of the optical dielectric constant, especially at low temperature.

It may also provide a useful clue to how to find the origin of the high critical temperature in ceramic superconductors.

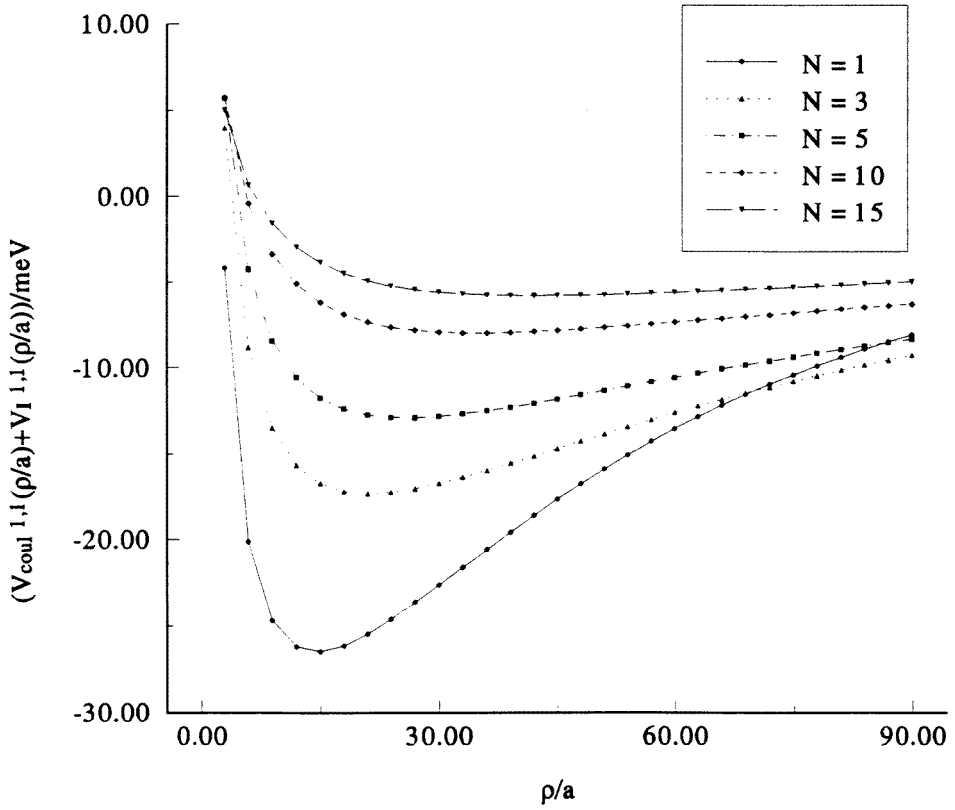

Figure 6. Plots of the total effective potential energy $V_{coul}^{1,1}(\rho/a) + V_I^{1,1}(\rho/a)$, with $l_1 = l_2 = 1$, against the relative position ρ/a of two holes projected onto the xy-plane.

In conclusion, we have investigated the effect of both the LO mode and the SO mode on the binding energy of the bipolaron in a polar slab. It is worth noting that the effect of the SO mode and that of the Coulombic potential are competitive in the process of formation of the bipolaron. There is a size effect due to the thickness of the polar slab, which plays an important role in the formation of a stable bipolaron. The equilibrium distance between the two holes that correspond to the bipolaron can be determined from the effective potential energy. It can be seen from figure 6 that the effective potential energy of the interaction between the two holes in a relatively thin polar slab of YBCO has a distinct equilibrium position at its minimum. The magnitude of the binding energy of these two holes becomes larger as the bipolaron size, taken as the equilibrium distance between the holes becomes smaller. The pairing of such holes will probably make some contribution to the high-temperature superconductivity.

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