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Anharmonic polaronic model and high-T_c superconductivity

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An anharmonic polaronic model is considered. The model consists of the electronic subsystem, described within the extended Hubbard model, coupled to anharmonic local phonons. The canonical-variable-displacement Holstein-Lang-Firsov transformation is used for shifting the phononic coordinate system in order to minimize the energy of the phonons. Then, the effective electronic Hamiltonian is obtained by averaging over the ground state of the phononic subsystem. It is shown that anharmonicity introduces two main additional factors as compared with the harmonic case. First, the band-narrowing factor is a less rapidly decaying function of the electron-phonon interaction strength. Second, anharmonicity introduces further renormalization of the on-site and intersite interaction between fermions. Implications for the application of the polaronic model to the high-T_c systems are twofold. Due to the first factor, higher values of the electron-phonon coupling are allowed without making polarons too heavy as compared with the experimental value of the effective mass in these materials. Second, small anharmonically induced renormalizations may or may not favor superconductivity. Combination of these two effects leads generally to the effective electronic Hamiltonian that yields more favorable conditions for superconductivity to occur than in the harmonic case.

I. INTRODUCTION

After the discovery of high-temperature superconductivity,[1] different microscopic models have been proposed as containing the essential physics of the superconducting oxides. Among others, the one-band Hubbard model,[2] the *t*-*J* model,[3] and the three-band or Emery model[4–6] are those that are based on the assumption that superconductivity in the new materials is basically driven by a purely electronic mechanism with some possible minor modifications due to other excitations like phonons, plasmons, etc. However, taking into account the results of the computer simulation[7,8] and analytic studies,[9] it is controversial whether purely electronic models suffice for explaining the observed phenomena in the oxides. As a consequence, theorists are forced to turn their attention toward models where the electron (hole) subsystem, in which the superconductivity occurs, interacts with one or more subsystems (fields) and where this interaction is responsible for the occurrence of superconductivity.

In previous papers[10,11] we studied superconductivity within the polaronic model in which the hole subsystem, described by the extended Hubbard model, was coupled to the phonons that were assumed to be harmonic and dispersionless. The results of these papers support the idea that the electron-phonon (*e*-ph) interaction may be, at least partly, responsible for high-T_c superconductivity though corrections to the classical BCS treatment seem to be necessary. One of these corrections, that seems to be especially important for the case of the superconducting oxides, is the importance of anharmonic vibrations of the apex oxygen atoms. This fact was pointed out by Müller[12] on the basis of similarities between high-temperature superconductors and high-temperature ferroelectrics. The extended x-ray-absorption fine structure (EXAFS) experiments[13] suggest the existence of anharmonic vibrations of the apex oxygen atoms, the distance of the apex oxygen and the nearest CuO_2 plane was found to be correlated with the transition temperature[14,15] and the results of the x-ray-absorption spectroscopy (XAS) experiments[14,16] had to be fitted to a double well potential of the apex oxygen atoms. The available data on the oxygen isotope effect, as reviewed by Müller,[17] also indicate strong anharmonicity in the oxides.

Much less is done in this respect on the theoretical side. Plakida *et al.*[18] considered a model consisting of coupled nonlinear oscillators, where each oscillator, being modeled by a local two-level system (TLS), represented anharmonic vibrations of an effective mass in a double-well potential. They have shown that anharmonicity enhances the effective *e*-ph coupling constant λ. They have also demonstrated[19] that anharmonicity can greatly change the isotope effect as compared to the harmonic case. De Raedt, Schneider, and Sörensen[20] studied superconductivity in Hubbard models coupled locally to TLS. They showed that such a coupling should lead to a significant enhancement of T_c, even in the case where the repulsive Hubbard-Coulomb interaction U is large. Their approximate analytical results were not confirmed in a quantum Monte Carlo (QMC) simulation study undertaken by Frick *et al.*[21] They found that for local coupling between holes and anharmonic phonons, the repulsive on-site interaction, i.e., Hubbard U, always diminishes the dominant on-site part of the order parameter and only slightly increases long-range contribution. In the next paper,[22] however, the same authors demonstrated that for nonlocal coupling clear evidence for the extended *s*-wave superconductivity was found in the 100-K temperature range for a realistic choice of the parameters. There

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are, however, still some doubts about their results. First, the largest system considered in QMC simulations was 8×8 unit cells and the authors admitted that finite-size fluctuations were relevant in their simulation. Second, the anharmonicity was not well controlled. In other words there was no possibility to switch off the anharmonicity carefully and to see whether superconductivity would or would not be affected. Also we would like to mention here a hypothesis, put forward by Ohta, Tohyama, and Maekawa,[23] which suggests that the energy level of the apex oxygen atoms governs the optimum T_c's for all families of the oxides. Connected with this idea is the suggestion that a double-well potential is responsible for the apex oxygen behavior.[24]

In this paper we try to clarify some of these points. Our main objective is to answer the following question: does the anharmonicity support superconductivity? For this we start from the local harmonic phonons at each site. It is well known that such phonons themselves can induce superconductivity, but with the maximum of the superconducting transition temperature T_c being lower than that found in the oxides. With this starting point we turn on the anharmonic correction to the site's vibration and gradually increase strength of the anharmonicity. By the variable displacement Holstein-Lang-Firsov canonical transformation,[25,26] we minimize the energy of the phononic subsystem and, then, make the average over the phononic ground state. It leaves us with the effective electronic Hamiltonian that may be studied by standard methods. We find that there are two main effects produced by the anharmonic correction to the Hamiltonian. First, the parameters describing the effective on-site and intersite interactions between the fermions are renormalized in a different way than in the harmonic case. Second, due to different form of the phononic ground-state wave function, the effective hopping integrals are different than in the harmonic case. We have found that combination of these two factors may favor superconductivity.

The paper is organized as follows. In Sec. II the model polaronic Hamiltonian is introduced. Section III describes the procedure of obtaining the effective electronic Hamiltonian as a result of eliminating the e-ph interaction and taking average over the ground state of the phononic subsystem. In Sec. IV we investigate numerical effects of the anharmonic corrections on the effective electronic Hamiltonian, especially the question, whether superconductivity is suppressed or enhanced, is addressed there. Finally, Sec. V gives conclusions and final remarks.

II. MODEL POLARONIC HAMILTONIAN

For the electronic Hamiltonian we choose an extended single-band Hubbard model

$$H_e = -\mu \sum_{i,s} n_{i,s} - \sum_{i,j,s} t_{ij} c^\dagger_{i,s} c_{j,s} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \frac{1}{2} \sum_{i,j} V_{ij} n_i n_j, \qquad (2.1)$$

where the summation over i (i,j) runs over all sites (all pairs of sites) of a given lattice. The operator $c^\dagger_{i,s}$ $(c_{i,s})$ creates (destroys) a fermion with a spin s at the site i, $n_{i,s} = c^\dagger_{i,s} c_{i,s}$ is the ith site s-spin fermion number operator with $s = \uparrow$ or $s = \downarrow$, and $n_i = n_{i,\uparrow} + n_{i,\downarrow}$. μ is the chemical potential, U is the Hubbard-Coulomb on-site repulsion, and t_{ij} and V_{ij} are the intersite hopping and Coulomb interaction matrix elements, respectively. We assume the following form of the e-ph interaction

$$H_{e\text{-ph}} = g_1 \sum_i n_i (b_i + b_i^\dagger) + g_2 \sum_{i,\delta} n_i (b_{i+\delta} + b^\dagger_{i+\delta}), \qquad (2.2)$$

where the summation over δ runs over all nearest-neighbor (NN) sites of a given site i and $b_i^\dagger$ (b_i) is the ith site phonon creation (annihilation) operator. From the assumed form of $H_{e\text{-ph}}$ it follows that the fermions interact with on-site and NN intersite local phonons; g_1 and g_2 are the respective strengths of these interactions. The phononic part of the Hamiltonian is

$$H_{\text{ph}} = e_0 \sum_i (b_i^\dagger b_i + \tfrac{1}{2}) + \sum_i V^{(1)}(x_i), \qquad (2.3)$$

where the first term corresponds to local harmonic phonons with frequency $\omega_0 = e_0/\hbar$, $\hbar$ is the Planck constant, and the local potentials $V^{(1)}(x_i)$ $[x_i = (b_i + b_i^\dagger)/\sqrt{2}]$ are introduced in order to describe the anharmonic effects. The total Hamiltonian of the system of interest is the following:

$$H = H_e + H_{e\text{-ph}} + H_{\text{ph}}. \qquad (2.4)$$

At this juncture the following comments are in order. The harmonic part of the phononic Hamiltonian $H^{(0)}_{\text{ph}} = e_0 \sum_i (b_i^\dagger b_i + \frac{1}{2})$ contains the lowest order (i.e., quadratic) nonzero terms of the expansion of potential energy around the equilibrium position of the ions. Because of these quadratic terms, the exact solution of the Schrödinger equation with $H^{(0)}_{\text{ph}}$ may be easily found. Higher-order terms (cubic, quartic, etc.) are incorporated into the anharmonic part of the phononic Hamiltonian $H^{(1)}_{\text{ph}} = \sum_i V^{(1)}(x_i)$, where for most purposes $V^{(1)}(x)$ is assumed to be a fourth-order polynomial. With such a form of $V^{(1)}(x)$, an approximate solution of the Schrödinger equation is then found, mainly by variational techniques.[27] This approach, though the most straightforward one, has some serious disadvantages. First, such anharmonic part $H^{(1)}_{\text{ph}}$ is by no means a perturbation to the zeroth-order harmonic Hamiltonian $H^{(0)}_{\text{ph}}$. In order words, no matter how small the coefficients of $V^{(1)}(x)$ are, for sufficiently large x, $V^{(1)}(x)$ will dominate over the quadratic harmonic potential. This creates some additional mathematical difficulties, since a perturbation theory does not work here. Consequently, it is difficult to study the anharmonic effect in a continuous and systematic way. Second, for modeling a particularly important double-well (DW) potential $V_{\text{DW}}(x)$, which in the simplest case of a power series expansion must be of the form $V_{\text{DW}}(x) = \lambda_2 x^2 + \lambda_4 x^4$, with $\lambda_2 < 0$ and $\lambda_4 > 0$, there is no natural choice of the reference harmonic potential that is, by definition, positive.

To overcome these difficulties, we propose to choose $V^{(1)}(x)$ that is different from zero only in a finite range of x near the origin. This is allowed since, for most cases, the motion of ions is limited to such a region outside which the potential should be only sufficiently large making the wave function there very small. Thus, the purpose of introducing such a form of $V^{(1)}(x)$ is just to model properly the total potential in the region where the ions move around their equilibrium positions. Outside this region we assume that the zeroth-order harmonic potential will make values of the wave function small enough. Namely, we choose

$$V^{(1)}(x) = V_1 \exp\left(-2\gamma x^2\right), \tag{2.5}$$

where V_1 and γ are parameters, which determine the exact shape of the anharmonic deviations of the site potential. The same potential was used by Galbaatar *et al.*[19] in studying the influence of anharmonicity on the isotope effect. It is obvious that the chosen form of $V^{(1)}(x)$, when added to the harmonic potential $V^{(0)}(x) = e_0 x^2/2$, may correctly describe anharmonic deviations in a finite region. Particularly, by a proper choice of the parameters V_1 and γ, the DW potential with desired depth of the well and separation between the minima may be accurately reproduced. By varying continuously V_1 and γ we are able to study the anharmonic effect in a systematic way. Moreover, this form of $V^{(1)}(x)$ makes a mathematical problem of solving the Schrödinger equation with $V^{(0)}(x) + V^{(1)}(x)$ much easier as we will see in the next section.

III. EFFECTIVE ELECTRONIC HAMILTONIAN

To obtain an effective electronic Hamiltonian we proceed in the analogous way as in the case of harmonic phonons.[10,11] First, the phononic coordinate system is shifted by the canonical variable displacement Holstein-Lang-Firsov transformation[25,26]

$$\tilde{H} = \exp(R) H \exp(-R), \tag{3.1}$$

where $R = \sum_i n_i Y_i$,

$$Y_i = \frac{\beta_1}{e_0}(b_i^\dagger - b_i) + \frac{\beta_2}{e_0}\sum_\delta (b_{i+\delta}^\dagger - b_{i+\delta}), \tag{3.2}$$

and β_1 and β_2 are variational parameters. For the harmonic case, i.e., $V_1 = 0$, the transformation (3.1) is usually used with fixed values $\beta_1 = g_1$ and $\beta_2 = g_2$ for they shift the phononic coordinate system to the new equilibrium ionic positions. In this way the energy of the phononic subsystem is minimized. Here, because of anharmonicity, there will be different displacement required to obtain the minimum phononic energy. Therefore, we expect that generally $\beta_1 \neq g_1$ and $\beta_2 \neq g_2$. The transformed Hamiltonian $\tilde{H}$ may be written as

$$\begin{aligned}\tilde{H} = {} & -\sum_{i,s}[\mu + \Delta\tilde{\mu}_i^{(a)}]n_{i,s} - \sum_{i,j,s}\tilde{t}_{ij}c_{i,s}^\dagger c_{j,s} + \sum_i [U + \Delta U^{(a)}]n_{i,\uparrow}n_{i,\downarrow} + \frac{1}{2}\sum_{i,j}[V_{ij} + \Delta V_{ij}^{(a)}]n_i n_j \\ & - \frac{\beta_2^2}{e_0}\sum_{i,\delta}\sum_{\delta'\neq\delta} n_{i,\delta}n_{i+\delta'} + \sum_i \exp(R)V^{(1)}(x_i)\exp(-R),\end{aligned} \tag{3.3}$$

where

$$\begin{aligned}\Delta\mu_i^{(a)} = {} & [\beta_1(2g_1 - \beta_1) + z\beta_2(2g_2 - \beta_2)]/e_0 \\ & + (\beta_1 - g_1)(b_i^\dagger + b_i) \\ & + (\beta_2 - g_2)\sum_\delta (b_{i+\delta}^\dagger + b_{i+\delta}),\end{aligned} \tag{3.4}$$

$$\tilde{t}_{ij} = t_{ij}\exp(Y_i - Y_j), \tag{3.5}$$

$$\Delta U^{(a)} = -2[\beta_1(2g_1 - \beta_1) + z\beta_2(2g_2 - \beta_2)]/e_0, \tag{3.6}$$

$$\Delta V_{ij}^{(a)} = -2[\beta_1(2g_2 - \beta_2) + \beta_2(2g_1 - \beta_1)]/e_0, \tag{3.7}$$

and z is the number of NN of a given site in the lattice. We have neglected the constant term $\sum_i e_0/2$.

Before proceeding further, we would like to make some comments on the form of $\tilde{H}$ given by Eq. (3.3). The e-ph interaction given by Eq. (2.2) renormalizes the chemical potential by the amount of $\Delta\mu_i^{(a)}$ [Eq. (3.4)], makes the effective hopping integrals smaller [Eq. (3.5)], reduces the on-site Coulomb repulsion by the amount of $\Delta U^{(a)}$ [Eq. (3.6)], and reduces the intersite Coulomb interaction by the amount of $\Delta V_{ij}^{(a)}$ [Eq. (3.7)]. The e-ph interaction induces also a second NN attraction between electrons that is proportional to β_2^2 and we neglect this effect for simplicity. Without the last term $\sum_i \exp(R)V^{(1)}(x_i)\exp(-R)$, this form of the Hamiltonian may, in general, result from a system of narrow-band electrons coupled to a bosonic field. The bosonic mode can be phonons, excitons,[28] plasmons,[29] magnons,[30] etc. Here we consider the bosons to be phonons, i.e., the polaronic model. For the case of harmonic phonons, we studied superconductivity within the polaronic model both for small and intermediate $\tilde{U}$,[10] as well as for the large $\tilde{U}$ case.[11] Here small or large $\tilde{U}$ means $\tilde{U} \leq W_p$ or $\tilde{U} \gg W_p$, where W_p is the effective polaronic bandwidth. The bandwidth W_p is much reduced in comparison with the bare electronic bandwidth due to the exponential factors $\exp(Y_i - Y_j)$ in Eq. (3.5).

The transformation $\sum_i \exp(R)V^{(1)}(x_i)\exp(-R)$ is described in details in the Appendix A. Here we just point out the main physical results. The anharmonic potentials $V^{(1)}(x_i)$ renormalize the chemical potential by the amount $\Delta\tilde{\mu}_i^{(b)}$ [Eq. (A7)], the on-site Coulomb repulsion by $\Delta\tilde{U}_i^{(b)}$ [Eq. (A8)], and the intersite Coulomb interaction by $\Delta\tilde{V}_{ij}^{(b)}$ [Eq. (A9)]. They also introduce many higher-order terms with three or more fermion number operators and those terms are neglected for simplicity. We think that this does not change the main conclusions we draw, at least for low density of fermions. Therefore, the transformed Hamiltonian reads

$$\begin{aligned}\tilde{H} = &-\sum_{i,s}[\mu + \Delta\tilde{\mu}_i^{(a)} + \Delta\tilde{\mu}_i^{(b)}]n_{i,s} - \sum_{i,j,s}\tilde{t}_{ij}c_{i,s}^{\dagger}c_{i,s} \\ &+\sum_{i}[U + \Delta U^{(a)} + \Delta\tilde{U}_i^{(b)}]n_{i,\uparrow}n_{i,\downarrow} \\ &+\frac{1}{2}\sum_{i,j}[V_{ij} + \Delta V_{ij}^{(a)} + \Delta\tilde{V}_{ij}^{(b)}]n_i n_j, \end{aligned} \tag{3.8}$$

where the corrections $\Delta\tilde{\mu}_i^{(a)}$, $\Delta\tilde{\mu}_i^{(b)}$, $\Delta\tilde{U}_i^{(b)}$, and $\Delta\tilde{V}_{ij}^{(b)}$ are functions of the phononic coordinates.

At this stage, to obtain an effective electronic Hamiltonian $\hat{H}$, an average with the phonon ground-state wave function $|\Psi_{\text{ph}}\rangle$ is made,[25,31]

$$\hat{H} = \langle\Psi_{\text{ph}}|\tilde{H}|\Psi_{\text{ph}}\rangle, \tag{3.9}$$

and this is reasonable only in the antiadiabatic limit, i.e., when the difference between the ground and the first excited state of the phonons is much larger than the polaronic bandwidth. After this we obtain

$$\begin{aligned}\hat{H} = &-\sum_{i,s}\hat{\mu}_i n_{i,s} - \sum_{i,j,s}\hat{t}_{ij}c_{i,s}^{\dagger}c_{j,s} \\ &+\sum_{i}\hat{U}_i n_{i,\uparrow}n_{i,\downarrow} + \frac{1}{2}\sum_{i,j}\hat{V}_{ij}n_i n_j, \end{aligned} \tag{3.10}$$

where

$$\hat{\mu}_i = \mu + \Delta\mu_i^{(a)} + \Delta\mu_i^{(b)}, \tag{3.11}$$

$$\hat{t}_{ij} = \langle\Psi_{\text{ph}}|\tilde{t}_{ij}|\Psi_{\text{ph}}\rangle, \tag{3.12}$$

$$\hat{U}_i = U + \Delta U_i^{(a)} + \Delta U_i^{(b)}, \tag{3.13}$$

$$\hat{V}_{ij} = V_{ij} + \Delta V_{ij}^{(a)} + \Delta V_{ij}^{(b)}, \tag{3.14}$$

$\Delta\mu_i^{(x)} = \langle\Psi_{\text{ph}}|\Delta\tilde{\mu}_i^{(x)}|\Psi_{\text{ph}}\rangle$ ($x = a$ or $x = b$), $\Delta U_i^{(b)} = \langle\Psi_{\text{ph}}|\Delta\tilde{U}_i^{(b)}|\Psi_{\text{ph}}\rangle$, and $\Delta V_{ij}^{(b)} = \langle\Psi_{\text{ph}}|\Delta\tilde{V}_{ij}^{(b)}|\Psi_{\text{ph}}\rangle$. Because of identical form of all on-site phononic Hamiltonians, $\hat{\mu}_i$ and $\hat{U}_i$ are site independent. The expression for the effective hopping integrals $\hat{t}_{ij}$ may be rewritten in the following way. Using the explicit form of Y_i [Eq. (3.2)] and the real-space representation of the phononic operators b_i and $b_i^{\dagger}$

$$b_i = \frac{1}{\sqrt{2}}\left(x_i - \frac{d}{dx_i}\right), \tag{3.15}$$

$$b_i^{\dagger} = \frac{1}{\sqrt{2}}\left(x_i + \frac{d}{dx_i}\right), \tag{3.16}$$

we can easily derive the following relation:

$$\hat{t}_{ij}/t_{ij} = F(\alpha_{12})F(-\alpha_{12})[F(\alpha_2)F(-\alpha_2)]^{z-1}, \tag{3.17}$$

where $\alpha_{12} = \sqrt{2}(\beta_1 - \beta_2)/e_0$, $\alpha_2 = \sqrt{2}\beta_2/e_0$,

$$F(\alpha) = \int_{-\infty}^{\infty}\psi_i^*(x)\psi_i(x-\alpha)\,dx, \tag{3.18}$$

and $\psi_i(x)$ is the ith-site phononic ground-state wave function. The method of finding $\langle x|\Psi_{\text{ph}}\rangle = \prod_i \psi_i(x)$ for the anharmonic case is given in the Appendix B. After the phononic ground-state wave function $|\Psi_{\text{ph}}\rangle$ is found, the calculation of the parameters that enter the effective electronic Hamiltonian reduces to one-dimensional numerical integrations in Eqs. (3.11)–(3.14).

IV. NUMERICAL RESULTS

To calculate the parameters of the effective electronic Hamiltonian, values of the variables that enter the phononic H_{ph} and the electron-phonon interaction $H_{e\text{-ph}}$ Hamiltonians must be specified. These parameters include the harmonic phonon characteristic energy $e_0 = \hbar\omega_0$, two parameters determining the anharmonic part of the on-site ion potential, i.e., V_1 and γ, and the on-site and intersite e-ph interaction strengths g_1 and g_2, respectively. Out of these parameters, e_0, V_1, and γ define the shape of the on-site ion potential

$$V(x) = e_0 x^2/2 + V_1\exp(-2\gamma x^2). \tag{4.1}$$

In the actual calculations all energy related quantities are measured in units of e_0. The unit of length is given by $d_0 = \hbar/\sqrt{e_0 m_{\text{ion}}}$, where m_{ion} is the mass of an ion in the lattice. Assuming that $e_0 \sim 0.05$ eV and that there are oxygen ions in the lattice, we obtain $d_0 \sim 0.1$ Å. There are many possibilities to vary V_1 and γ and produce DW potentials of desired properties. We have decided to keep constant the separation $\Delta x/d_0 = 3$ between the two minima of the DW potential. Such a value of Δx corresponds to the separation between two minima of the DW potential about 0.3 Å, which is a reasonable value.[32] The analysis has been performed for two values of the interminimum barrier height ΔV, namely, $\Delta V/e_0 = 1$ ("moderate" anharmonicity) and $\Delta V/e_0 = 2$ ("strong" anharmonicity). It is easy to show that there is one-to-one correspondence between two sets of variables $\{V_1, \gamma\}$ and $\{\Delta x, \Delta V\}$. The harmonic potential $V^{(0)}(x)$ corresponds obviously to $V_1 = 0$. In Fig. 1 we plot the

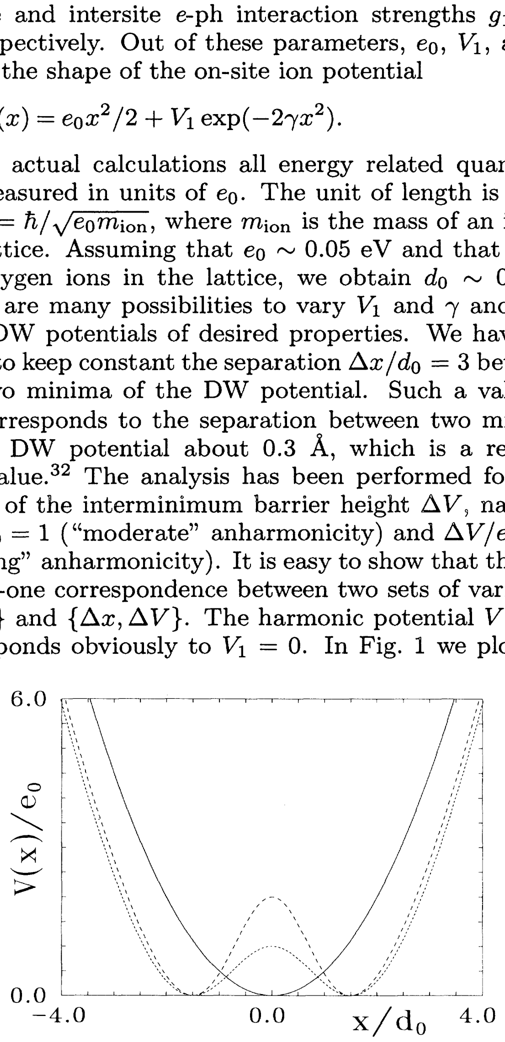

FIG. 1. Variation of the on-site ionic potential $V(x)$, as defined by Eq. (4.1), with the distance x for the harmonic case ($V_1 = 0$; solid line) and for two anharmonic cases: $\Delta V/e_0 = 1$ ($V_1 = 3.09$, $\gamma = 0.26$; short-dashed line) and $\Delta V/e_0 = 2$ ($V_1 = 3.76$, $\gamma = 0.40$; long-dashed line). ΔV is the height of the interminimum potential barrier; d_0 and e_0 are defined in the text.

harmonic potential and two DW potentials as described above. Figure 2 presents the corresponding ground-state wave functions $\psi(x)$. The ground-state energies are 0.5, 0.561, and 0.799, respectively.

Let us start our analysis from the function $F(\alpha)$ as defined by Eq. (3.18). For the harmonic case $F(\alpha) = e^{-\alpha^2/4}$. For the anharmonic case ($V_1 \neq 0$), $F(\alpha)$ has to be calculated with the use of the actual wave function $\psi(x)$. For the chosen potentials $V(x)$, we present values of the function $F(\alpha)$ in Fig. 3. For all cases $F(0) = 1$ and $F(\alpha) \to 0$ for $\alpha \to \infty$. We see that generally $F(\alpha)$ is higher in the anharmonic case, especially for higher values of α. For moderate anharmonicity ($\Delta V/e_0 = 1$), $F(\alpha)$ has similar shape as in the harmonic case but with larger half width. For strong anharmonicity ($\Delta V/e_0 = 2$), however, $F(\alpha)$ is different. Namely, for α between 0 and 1.5, $F(\alpha)$ is close to its harmonic value being smaller than in the $\Delta V/e_0 = 1$ case. Then $F(\alpha)$ is almost constant for $\alpha \in (1.5, 3)$ being higher than in two previous cases. Finally, for $\alpha > 3.0$, $F(\alpha)$ falls to zero slowly.

Before values of the parameters entering the effective Hamiltonian (3.3) may be calculated, values of the variational parameters β_1 and β_2 have to be found. Generally, these values should be determined as a result of the total-energy minimization. In our qualitative considerations we determine β_1 and β_2 by requiring the energy of the phononic subsystem to be minimum, i.e., from the condition

$$\frac{\partial}{\partial \beta_i}\langle \Psi_{\mathrm{ph}}|(\tilde{H}_{\mathrm{ph}} + \tilde{H}_{e\text{-}\mathrm{ph}})|\Psi_{\mathrm{ph}}\rangle = 0. \qquad (4.2)$$

This is justified under the antiadiabatic approximation we have chosen. To simplify determination of β_1 and β_2 we assume, following the harmonic case where $\beta_1/g_1 = \beta_2/g_2 = 1$, that $\beta_1/g_1 = \beta_2/g_2 = \eta$. Generally, since the displacement operator R contains the fermion number operators, η would be density dependent. However, for small average density of fermions per site $\langle n \rangle \leq 0.2$, we have found this dependence to be very weak, and, therefore, we present our results for a fixed value of $\langle n \rangle = 0.1$.

Having determined values of η and the function $F(\alpha)$, the band-narrowing factor given by Eq. (3.17) may be calculated. We present values of $\hat{t}_{ij}/t_{ij}$ versus g_1 and for $g_2/g_1 = 0.1$ in Fig. 4. For the harmonic case ($V_1 = 0$), $\hat{t}_{ij}/t_{ij} = \exp\{-[(g_1 - g_2)^2 + (z-1)g_2^2]/e_0^2\}$ and this formula leads to the well-known effect of the strong band narrowing as the e-ph coupling increases. Strong band narrowing is equivalent to the high effective mass of polarons. On the other side, to obtain high T_c, strong e-ph coupling is necessary to renormalize appropriately the on-site and intersite Coulomb interactions, U and V_{ij}, respectively, making at least one of them negative. Negative effective $\hat{U}$ and $\hat{V}_{ij}$ are necessary if superconductivity is expected to occur. From Fig. 4 we see that in the anharmonic polaronic model much higher values of the e-ph coupling g_1 are allowed without making the polarons too heavy.

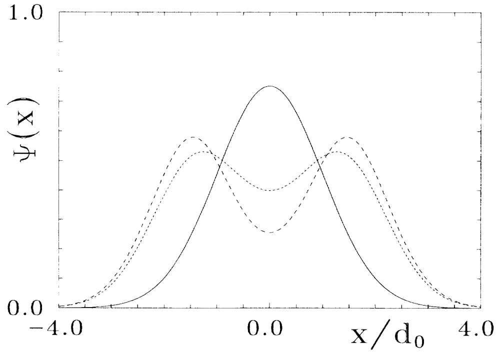

FIG. 2. Ground-state wave function $\psi(x)$ for the potentials shown in Fig. 1. All parameters and labels are the same as in Fig. 1.

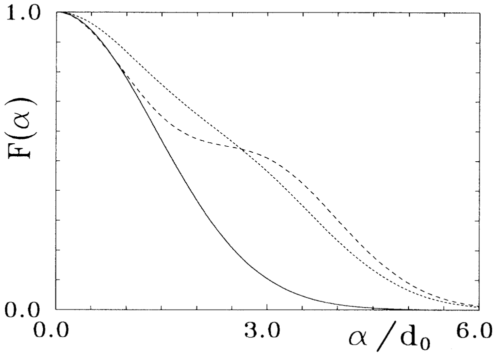

FIG. 3. Function $F(\alpha)$, as defined by Eq. (3.18), for the potentials and wave functions shown in Figs. 1 and 2. All parameters and labels are the same as in Fig. 1.

Figures 5 and 6 present additional anharmonic renormalization of the on-site and the intersite Coulomb interaction, $\Delta U^{(b)}$ ($= \Delta U_i^{(b)}$ for any i) and $\Delta V_{ij}^{(b)}$, respectively. Additional means here that to get the full renormalization, the values plotted in Figs. 5 and 6 should be added to $\Delta U_i^{(a)}$ and $\Delta V_{ij}^{(a)}$, given by Eqs. (3.6) and (3.7), respectively. For the harmonic case $\Delta U^{(b)} = \Delta V_{ij}^{(b)} = 0$. For the two anharmonic cases considered here, the two corrections $\Delta U^{(b)}$ and $\Delta V_{ij}^{(b)}$ are order of magnitude smaller when compared with those corrections given by

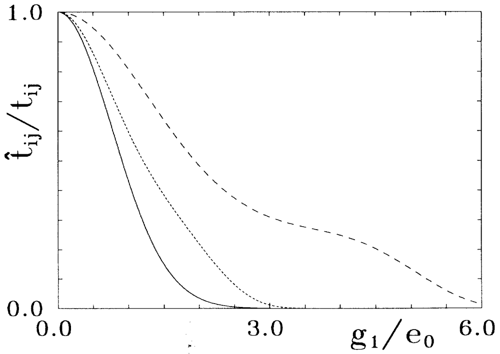

FIG. 4. The band narrowing factor $\hat{t}_{ij}/t_{ij}$, as appearing in Eq. (3.17), as a function of the on-site electron-phonon interaction strength g_1 and for $g_2/g_1 = 0.1$. g_2 is the NN electron-phonon interaction strength [see Eq. (2.2)]. All parameters and labels are the same as in Fig. 1.

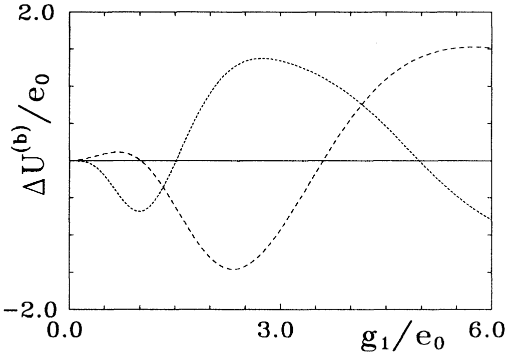

FIG. 5. Additional anharmonic renormalization $\Delta U^{(b)}$ of the on-site Hubbard interaction U as a function of the on-site electron-phonon interaction strength g_1 and for $g_2/g_1 = 0.1$. g_2 is the NN electron-phonon interaction strength [see Eq. (2.2)]. All parameters and labels are the same as in Fig. 1.

Eqs. (3.6) and (3.7), i.e., $\Delta U_i^{(a)}$ and $\Delta V_{ij}^{(a)}$, respectively.

For the high-T_c superconductors, the effective mass m_{eff} of the charge carriers is estimated to be around $10m_e$, i.e., the band-narrowing factor should be close to 0.1. It means that for the harmonic case the e-ph coupling g_1 would be around 1.66 (see Fig. 4). Taking this value of g_1 and the assumed ratio of $g_2/g_1 = 0.1$, as well as the fact that for the harmonic case $\beta_1/g_1 = \beta_2/g_2 = 1$, we can find from the formulas (3.6) and (3.7) that $\Delta U^{(a)} = -5.73e_0$ and $\Delta V_{ij}^{(a)} = -1.10e_0$. With $\Delta U^{(b)} = \Delta V_{ij}^{(b)} = 0$, this yields finally $\hat{U} = U - 5.73e_0$ and $\hat{V}_{ij} = V_{ij} - 1.10e_0$ for the harmonic case. For the moderate anharmonic case ($\Delta V/e_0 = 1$) we find (see Fig. 4) that g_1 would be around 2.42. From the phononic energy minimization we obtain $\eta = 1.15$ and this, with $\beta_1 = \eta g_1$ and $\beta_2 = \eta g_2$ and through formulae (3.6) and (3.7), gives $\Delta U^{(a)} = -11.91e_0$ and $\Delta V_{ij}^{(a)} = -2.29e_0$. For the additional anharmonic corrections (see Figs. 5 and 6) we obtain $\Delta U^{(b)} = 1.30e_0$ and $\Delta V_{ij}^{(a)} = -0.09e_0$. Therefore, for the moderate anharmonicity case we have $\hat{U} = U - 10.61e_0$ and $\hat{V}_{ij} = V_{ij} - 2.38e_0$. Finally, for the strong anharmonicity case, $\hat{t}_{ij}/t_{ij} = 0.1$ gives g_1 around 5.22. With the value of $\eta = 0.57$ we further have $\Delta U^{(a)} = -45.99e_0$, $\Delta V_{ij}^{(a)} = -8.85e_0$, $\Delta U^{(b)} = 1.46e_0$, and $\Delta V_{ij}^{(b)} = -0.21e_0$. Collecting all the contributions together gives $\hat{U} = U - 44.53e_0$ and $\hat{V}_{ij} = V_{ij} - 9.05e_0$.

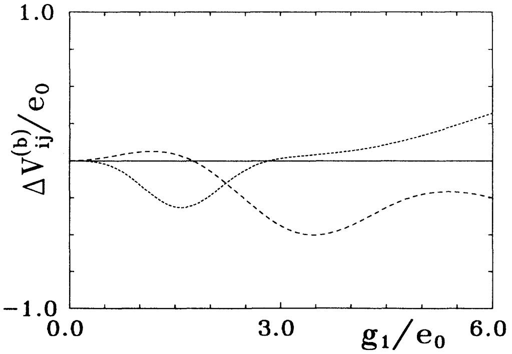

FIG. 6. Additional anharmonic renormalization $\Delta V_{ij}^{(b)}$ of the intersite Coulomb interaction V_{ij} (ij are NN) as a function of the on-site electron-phonon interaction strength g_1 and for $g_2/g_1 = 0.1$. g_2 is the NN electron-phonon interaction strength [see Eq. (2.2)]. All parameters and labels are the same as in Fig. 1.

How can we interpret these numerical estimates? First, it is clear that the bare interactions, U and V_{ij}, are more reduced (negatively renormalized) for more anharmonic on-site ion potentials. The second thing is that higher allowed values of the e-ph interaction, as always leading to higher negative values of $\Delta U^{(a)}$ and $\Delta V_{ij}^{(a)}$, are much more important factor than anharmonically induced renormalizations $\Delta U^{(b)}$ and $\Delta V_{ij}^{(b)}$, which are order of magnitude smaller. Third, values of $\Delta U^{(a)}$ and $\Delta V_{ij}^{(a)}$ are always negative, whereas $\Delta U^{(b)}$ and $\Delta V_{ij}^{(b)}$ may be either positive or negative (see Figs. 5 and 6). For the assumed values of the effective mass, we have $\Delta U^{(b)} < 0$ and $\Delta V_{ij}^{(b)} > 0$. So, in our cases anharmonicity slightly enhances the on-site Hubbard interaction U and reduces the intersite interaction V_{ij}.

The last, but not least, comment is that we measure all quantities in units of e_0. For the harmonic case, each on-site ionic Hamiltonian [Eq. (2.3)] has equidistanced energy levels $e_0/2$, $3e_0/2$, $5e_0/2$, and so on. For the anharmonic cases the energy levels are not equidistanced. However, with our form of the on-site ionic potential [Eq. (4.1)], we do have equidistanced energy levels for sufficiently high energy. Low-energy levels, as is usual for anharmonic potentials, are not equally separated. Particularly, the ground state and the first excited state are separated by less than e_0 ($0.21e_0$ and $0.06e_0$ for $\Delta V/e_0 = 1$ and $\Delta V/e_0 = 2$, respectively). With this in mind we can try to answer the following question: does anharmonic motion of the ions favor superconductivity more than the harmonic motion of these ions does? The answer is yes, but a care is required when giving more quantitative results. Two limiting cases may be distinguished.

(i) Harmonic and anharmonic models are equivalent as regards to the high-energy levels of the ionic Hamiltonians. That is the way we have chosen in this paper.

(ii) We make equal the energy difference between the first excited state and the ground-state energy of the on-site ionic Hamiltonian. It means that $\omega' \overset{\text{def}}{=} \omega_0$ used in the anharmonic Hamiltonian ($V_1 \neq 0$) would be higher than ω_0 used, while considering the harmonic case $V_1 = 0$. For our two cases chosen ($\Delta V/e_0 = 1$ and $\Delta V/e_0 = 2$) and with the energy levels found, we would have $\omega' = 1.67\omega_0$ and $\omega' = 4.76\omega_0$, respectively.

For the high-T_c oxides, the bare on-site Coulomb repulsion on the copper site $U \sim 8$ eV and the intersite copper-oxygen Coulomb interaction $V_{ij} \sim 1$ eV. The energy of the optic phonons is around 0.05 eV.[33] Assuming the first method of comparison between harmonic and anharmonic models, i.e., the equivalence between their high-energy spectra, we obtain $\hat{U} \simeq 7.71$ eV and $V_{ij} \simeq 0.945$ eV for the harmonic case, $\hat{U} \simeq 7.47$ eV and $V_{ij} \simeq 0.881$ eV for the moderate anharmonicity, and $\hat{U} \simeq 5.73$ eV and $V_{ij} \simeq 0.548$ eV for the strong anharmonicity. With the second interpretation, the following values are obtained: $\hat{U} \simeq 7.71$ eV and $V_{ij} \simeq 0.945$ eV for the harmonic case, $\hat{U} \simeq 5.34$ eV and $V_{ij} \simeq 0.469$ eV for the moderate anharmonicity, and $\hat{U} \simeq -29.18$ eV and $V_{ij} \simeq 0.557$ eV for the strong anharmonicity. In either of these situations, the bare interactions between fermions are more reduced when anharmonicity is present. In reality we are closer to the second interpretation, for we normally measure the low-energy excitation spectra for phonons. There may be another possibility for anharmonic phonons to induce pairing interactions. The direct interoxygen hopping is different from zero and the intersite oxygen-oxygen repulsion is smaller than that between copper and oxygen. A smaller value of the bare interaction creates more favorable conditions for phonons to induce negative effective intersite interaction between fermions. Summarizing, anharmonicity creates more favorable conditions for superconductivity to occur.

V. CONCLUDING REMARKS

There is a growing experimental evidence[34] that charge carriers in the new superconducting oxides are associated with lattice deformations, i.e., they are polarons (or bipolarons).[35] In the conventional harmonic polaronic model the e-ph coupling leads to a formation of polarons with an exponentially reduced bandwidth. At the same time the on-site and intersite Coulomb interactions between the polarons are reduced. One of the main objections raised against the polaronic model as applied to the oxides is that the polarons would have been too heavy, as compared with the experimental values of the effective mass, if the e-ph coupling was large enough to induce sufficiently large attractive interaction between the polarons. Such interaction is necessary if high-T_c is expected to occur.

In this paper we have studied the anharmonic polaronic model in which the electronic subsystem, described by the extended Hubbard model, is coupled to the local anharmonic phonons. We have shown that, when going to the effective electronic Hamiltonian, the band narrowing factor is generally a less rapidly decaying function of the e-ph coupling. It allows, at fixed value of the polaronic effective mass, for assuming higher values of the e-ph coupling without making the polarons too heavy. We think that anharmonicity removes one of the main objections raised against the polaronic model as applied to the high-temperature superconductors. To our knowledge this fact has not been pointed out so far. Besides that, anharmonicity introduces additional renormalizations to the on-site and intersite interaction between fermions. For the effective mass corresponding to that of the charge carriers in the high-T_c materials, i.e., for the band narrowing factor around 0.1, these additional renormalizations are much smaller than those following the higher allowed values of the electron-phonon interaction.

The results of this paper give arguments in favor of the polaronic model in application to the high-temperature superconducting oxides. To obtain qualitative implications of the anharmonic polaronic model on the measured properties (phase diagram, thermodynamic, and transport properties), the present model should be generalized with use of the actual geometry and values of the relevant parameters. Such a study is now under way and the results will be published elsewhere.

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APPENDIX A

Here $\sum_i \exp(R) V^{(1)}(x_i) \exp(-R) \overset{\text{def}}{=} \sum_i \tilde{V}^{(1)}(x_i)$ is calculated. $V^{(1)}(x_i)$ is defined by Eq. (2.5) and the operator R (see Sec. III) may be written as $R = \sum_i R_i$, where $R_i = u_i p_i$,

$$u_i = \frac{\beta_1}{e_0} n_i + \frac{\beta_2}{e_0} \sum_\delta n_{i+\delta}, \tag{A1}$$

and $p_i = b_i^\dagger - b_i$. Also the symbol $q_i = b_i^\dagger + b_i$ is introduced; thus $V^{(1)}(x_i) = V^{(1)}(q_i) = V_1 \exp(-\gamma q_i^2)$. First, let us note

$$\begin{aligned} \tilde{V}^{(1)}(q_i) &= \exp\left(\sum_j R_j\right) V^{(1)}(q_i) \exp\left(-\sum_k R_k\right), \\ &= \exp(R_i) V^{(1)}(q_i) \exp(-R_i). \end{aligned} \tag{A2}$$

Then defining the function

$$G(y) = \exp(R_i) \exp(y q_i) \exp(-R_i), \tag{A3}$$

and calculating $d^n G(y)/dy^n$ for $y = 0$ yields

$$\exp(R_i) q_i^n \exp(-R_i) = (q_i - 2u_i)^n\,. \tag{A4}$$

The last relation (A4) with the power series expansion of $V^{(1)}(q_i)$ gives

$$\tilde{V}^{(1)}(q_i) = V_1 \exp\left[-\gamma\,(q_i - 2u_i)^2\right]. \tag{A5}$$

Because of the form of β_i [Eq. (A1)], each ith-site transformed anharmonic potential $\tilde{V}^{(1)}(q_i)$ depends on the ith-site fermion occupation number n_i as well as on the NN fermion number occupations $n_{i+\delta}$. Therefore $\tilde{V}^{(1)}(q_i)$ may be written as

$$\tilde{V}^{(1)}(q_i) = \tilde{V}^{(1)}[q_i; n_i, n_{\text{NN}}(i)], \tag{A6}$$

where $n_{\text{NN}}(i) = \sum_\delta n_{i+\delta}$ is the total number of fermions occupying all NN sites. This gives the following formulas

$$\begin{aligned} \Delta\mu_i^{(b)} &= -[\tilde{V}^{(1)}(q_i; 1, 0) - \tilde{V}^{(1)}(q_i; 0, 0)] \\ &\quad - \sum_\delta [\tilde{V}^{(1)}(q_{i+\delta}; 0, 1) - \tilde{V}^{(1)}(q_{i+\delta}; 0, 0)], \end{aligned} \tag{A7}$$

$$\Delta U_i^{(b)} = [\tilde{V}^{(1)}(q_i;2,0) - 2\tilde{V}^{(1)}(q_i;1,0) + \tilde{V}^{(1)}(q_i;0,0)] + \sum_{\delta}[\tilde{V}^{(1)}(q_{i+\delta};0,2) - 2\tilde{V}^{(1)}(q_{i+\delta};0,1) + \tilde{V}^{(1)}(q_{i+\delta};0,0)], \tag{A8}$$

$$\begin{aligned}\Delta V_{ij}^{(b)} = {} & \tilde{V}^{(1)}(q_i;1,1) - \tilde{V}^{(1)}(q_i;1,0) \\ & -\tilde{V}^{(1)}(q_i;0,1) + \tilde{V}^{(1)}(q_i;0,0) \\ & +\tilde{V}^{(1)}(q_j;1,1) - \tilde{V}^{(1)}(q_j;1,0) \\ & -\tilde{V}^{(1)}(q_j;0,1) + \tilde{V}^{(1)}(q_j;0,0),\end{aligned} \tag{A9}$$

for the anharmonically induced renormalization of the chemical potential, the on-site, and the intersite interaction between fermions, respectively. Here we have neglected terms with more than two fermion operators, and we restrict ourselves only to V_{ij} for ij being the NN.

APPENDIX B

Here a method for finding the phononic ground-state wave function $|\Psi_{\rm ph}\rangle$ is presented. First, we note that, because of Eq. (2.3), $|\Psi_{\rm ph}\rangle = \prod_i |\psi_i\rangle$, with $|\psi_i\rangle$ being the lowest-energy solution of the Schrödinger equation for the ith-site phononic Hamiltonian,

$$\left[H_i^{(0)} + V^{(1)}(x_i)\right]|\psi_i\rangle = \epsilon_i|\psi_i\rangle, \tag{B1}$$

where $H_i^{(0)} = e_0(b_i^\dagger b_i + \frac{1}{2})$ and ϵ_i is the lowest eigenvalue. Since Eq. (B1) has the same form for all i, we drop the subscript i writing $|\psi_i\rangle = |\psi\rangle$, $x_i = x$, $\epsilon_i = \epsilon$, etc., from now on. To find $|\psi\rangle$, we expand it into a series of the eigenfunctions of the harmonic oscillator, i.e.,

$$|\psi\rangle = \sum_{k=0}^{N} c_k|k\rangle, \tag{B2}$$

where

$$H^{(0)}|k\rangle = \epsilon_k|k\rangle, \tag{B3}$$

$$\epsilon_k = \frac{2k+1}{2}e_0, \tag{B4}$$

for $k = 0,1,2,\ldots,N$. With this formulation, the following set of homegeneous linear equations for the coefficients c_k is obtained

$$\sum_{k=0}^{N} c_k(\epsilon_k - \epsilon)\delta_{kl} + \sum_{k=0}^{N} c_k V_{kl}^{(1)} = 0, \tag{B5}$$

for $l = 0,1,\ldots,N$. Here

$$V_{kl}^{(1)} = \int_{-\infty}^{\infty} \psi_k^*(x)V^{(1)}(x)\psi_l(x)\,dx, \tag{B6}$$

is the matrix element of the anharmonic potential $V^{(1)}(x)$ between two ground-state eigenfunctions of the harmonic oscillator; $\psi_k(x) = \langle x|k\rangle$. With the form of $V^{(1)}(x)$ chosen [see Eq. (2.5)], $V_{kl}^{(1)}$ may be calculated analytically, since for the harmonic oscillator $\psi_k(x) = \exp(-x^2/2)H_k(x)$, where $H_k(x)$ is the kth-order Hermite polynomial. This job has to be done only once and the obtained formulas, being the functions of γ and V_1, may then be used in many different applications. We have found the formulas for $V_{kl}^{(1)}$ with the use of a symbolic programming language MATHEMATICA.[36]

To find the ground-state energy ϵ and the corresponding wave function $\psi(x)$, we normally start from a lower number of N, let us say 10. Then we increase N by a small step and monitor carefully evolution of the eigenvalues and eigenfunctions. We have found $N_{\rm min}$ such that for $N > N_{\rm min}$, the lowest eigenvalue of the matrix $M_{kl} = \delta_{kl}\epsilon_k + V_{kl}^{(1)}$ does not change as N increases further. At the same time, the contribution to $\psi(x)$ from higher wavefunctions $\psi_k(x)$ ($k > N_{\rm min}$) is negligible. At this point we conclude that the ground state has been found.

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