Numerical study of the $E \otimes e$ Jahn-Teller polaron and bipolaron

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(March 22, 2022)

The properties of the polaron and bipolaron are explored in the 1D Jahn-Teller model with dynamical quantum phonons. The ground-state properties of the polaron and bipolaron are computed using a recently developed variational method. Dynamical properties of the ground state of a polaron are investigated by calculating the optical conductivity $\sigma(\omega)$. Our numerical results suggest that the Jahn-Teller and Holstein polarons are similar. However, in the strong-coupling regime qualitative differences in $\sigma(\omega)$ between the two models are found and discussed. The influence of the electron-phonon coupling and the electrostatic repulsion on the bipolaron binding energy, bipolaron masses, and correlation functions is investigated.

PACS: 74.20.Mn, 71.38.+i, 74.25.Kc

I. INTRODUCTION

While research on Jahn-Teller (JT) electron phonon coupling spans many decades, a renewed interest in this problem has been sparked by the discovery of colossal magnetoresistance materials (CMR). In CMR’s, it is believed, the colossal magnetoresistance effect is a consequence of the interplay between the double exchange mechanism and the lattice effect [1–4]. Furthermore, recent studies of alkali doped fullerenes $A_{18}C_{60}$ indicate that the Jahn-Teller distortion together with strong Coulomb repulsion could be responsible for unusual electronic properties of these materials [5–9].

Recent advances in computing capabilities have stimulated development of various numerical techniques such as: exact diagonalization techniques (ED) on small clusters [10–12], ED on infinite clusters [13,14], quantum Monte Carlo calculations (QMC) [15,16], variational methods [17], and density matrix renormalization group techniques (DMRG) [18], that have provided valuable results for the Holstein model (HM) in one and more spatial dimensions. The most efficient methods provide energies for the Holstein polaron problem that are accurate up to 21 digits in the thermodynamic limit [14]. In addition to static quantities, dynamic properties such as spectral functions and optical conductivity of the Holstein model have recently been studied on small lattice clusters [19–23]. However, except in the small polaron regime, such calculations are subject to pronounced finite-size effects. In contrast to the HM, there has been much less numerical research devoted to the Jahn-Teller model (JTM), mainly due to the far larger Hilbert space that presents the main obstacle to exact-diagonlazation approaches. Most of the recent numerical calculations of the JTM that take into account the full quantum mechanical nature of the problem consider only one atom [6,7]. A recent path-integral Quantum Monte Carlo approach, developed by Kornilovitch, has proven powerful in computing ground state and spectral properties like the density of states of the Jahn-Teller problem [26]. Calculation of dynamic properties by that method would require analytic continuation from imaginary time, which is very sensitive to statistical noise.

The scope of the present work is to compare the static properties of the JTM and Holstein model (HM) for the case of one and two electrons. In addition, we investigate dynamic properties of the Holstein and Jahn-Teller polaron by calculating the optical conductivity. In this case we devote equal attention to the Holstein and Jahn-Teller models since dynamical properties of the Holstein model calculated using an infinite-lattice variational space have not been published elsewhere. We use a recently developed numerical technique [13,27] to study the JTM for the case of one and two electrons on the 1D infinite lattice. Our main goal is to find the numerically exact solution of the JTM in the thermodynamic limit. The variational method that we use [13,27] is defined on an infinite lattice and is not subject to finite-size effects. A standard Lanczos method is used to find ground and excited states with the selected Hilbert space. The method allows calculation of physical properties at any wavevector $k$. In the intermediate coupling regime where it is most accurate, it provides results that are variational in the thermodynamic limit and gives energies accurate to 21 digits for the Holstein polaron, up to 7 digits for the Holstein bound bipolaron, and 6 digits for the Jahn-Teller polaron. While there are no boundary finite-size effects, there are nevertheless finite-variational-space effects due to a constraint that only a finite separation between the electron and the surrounding phonons is allowed for the polaron, and between two electrons and the polaron cloud for the bipolaron. Nevertheless, results may be fairly accurate even in the two-electron case when electrons are bound into a bipolaron, since then electron-electron correlation functions decrease exponentially for large separations.
II. MODEL

The simplest, so called $E \otimes e$ Jahn-Teller model, consists of two degenerate electron orbitals and two degenerate phonon modes,

$$H = -t \sum_{i,o,s} (c_{i+1,o,s}^+ c_{i,o,s} + \text{H.c.}) + \omega_0 \sum_i (a_i^+ a_i + b_i^+ b_i) +$$

$$+ g \omega_0 \sum_{i,s} \left[ (n_{i,1,s} - n_{i,2,s}) (a_i^+ + a_i) + (c_{i+1,2,s}^+ c_{i,1,s} + c_{i-1,2,s} c_{i,1,s}^+) (b_i^+ + b_i) \right] +$$

$$U_1 \sum_{i,o} n_{i,o,\uparrow} n_{i,o,\downarrow} + U_2 \sum_i (n_{i,1,\uparrow} n_{i,2,\downarrow} + n_{i,2,\uparrow} n_{i,1,\downarrow}), \quad (1)$$

where $c_{i,o,s}^+$ creates an electron on site $i$, orbital $o$ ($o = 1, 2$) and spin $s$, and $a_i^+$ ($b_i^+$) dispersionless phonons of type $a$ ($b$) on site $i$. While the phonon of type $a$ couples to the electron density, the mode $b$ mediates hopping between electronic orbitals that are orthogonal in the absence of phonon $b$. The parameters of the model are the intersite hopping matrix element $t$, dimensionless electron-phonon coupling strength $g$, and optical phonon frequency $\omega_0$. In the bipolaron case we consider electrons with opposite spin. The last two terms in Eq. (1) represent the on-site same-orbital ($U_1$) and different-orbital ($U_2$) Coulomb repulsion. For simplicity we have chosen $U_1 = U_2 = U$.

Most of the calculations will be compared to a simpler Holstein model

$$H = -t \sum_{i,s} (c_{i+1,s}^+ c_{i,s} + \text{H.c.}) + \omega_0 \sum_i a_i^+ a_i +$$

$$+ g \omega_0 \sum_{i,s} n_{i,s} (a_i^+ + a_i) + U \sum_i n_{i,\uparrow} n_{i,\downarrow}. \quad (2)$$

While the basic principles of the method have been explained elsewhere [13,27] we here present only a brief explanation of how the variational space is constructed for the case of two electrons in the JTM. Basis states for the many-body Hilbert space can be written $|\phi\rangle = |j_1, o_1, j_2, o_2; \ldots n_i, n_{i+1}, \ldots m_i, m_{i+1}, \ldots\rangle$, where the $j_1, j_2$ and $o_1, o_2$ are first and second electron site and orbital indices respectively, and there are $n_i$ phonons of type $a$ and $m_i$ phonons of type $b$ on site $i$. A variational subspace is constructed beginning with an initial state where both electrons are on the same site and orbital with no phonons, and operating repeatedly ($N_h$ times) with the off-diagonal pieces ($t$ and $g$) of the Hamiltonian, Eq. (1). The wavefunction is then written in a translation invariant form. To achieve high accuracy in the strong coupling limit where there are many excited phonon quanta, we have constructed towers of $N_{ad}$ ($N_{ad} = 30$ for JTM and $N_{ad} = 200$ for HM) additional phonon excitations (for the JT case: one tower for each phonon type) that were located on the electron site and on the first neighbor site to the left or to the right of the electron position. Such towers play a crucial role in achieving convergence in the small polaron regime.

III. JAHN-TELLER POLARON

A. Static correlation functions

We start by presenting results of the JT polaron (JTP). To investigate the shape of the JTP, we have computed various static correlation functions. We first present the correlation function for the distribution of the number of excited phonons in the vicinity of the electron

$$\gamma(i-j) = \langle \psi_k | n_i (a_{i,j}^+ a_{i,j}) | \psi_k \rangle, \quad (3)$$

where $n_i = n_{i,1} + n_{i,2}$ and $|\psi_k\rangle$ is the polaron wavefunction at momentum $k$. Numerical results presented in Fig. (1) show $\gamma(i-j)$ calculated at various coupling strengths and different wavenumbers. When comparing results at different $k$ it becomes evident that the size of the polaron at $k = \pi$ is larger than that at $k = 0$. As the coupling strength increases, $\gamma(0)$ increases while $\gamma(i-j \neq 0)$ does not change substantially at $k = 0$ while for larger values of $k$, $\gamma(i-j \neq 0)$ slightly decreases. We should stress that due to the the symmetry of the pseudospin rotation [30], $\langle \psi_k | n_i a_{i,j}^+ a_{i,j} | \psi_k \rangle = \langle \psi_k | n_i b_{i,j}^+ b_{i,j} | \psi_k \rangle$.

In Fig. (1) we also compare JTP with the Holstein polaron (HP), where $\gamma$ is calculated at $g = 1.2$. While differences at small $k$ are very subtle, they become more pronounced at larger $k$ where $\gamma(0)$ of the HP is larger than that of the JTP.

![FIG. 1. $\gamma(i-j)$ vs. $(i-j)$ for the JTP calculated at three different coupling strengths and $\omega_0 = t = 1$ (open symbols). Results of the HP are presented as black diamonds.](image)
Next we present the phonon-phonon correlation function of the JTP

$$\varepsilon(i - j) = \langle \psi_k | a_i^+ a_j b_j^+ b_i | \psi_k \rangle ,$$

(4)

shown in Fig. 2. As expected, phonons of two different types are only weakly correlated. At small values of $k$ the electron mediated phonon-phonon interaction is always attractive (it has a maximum at $(i - j) = 0$), however, at larger values of $k$ and in the weak to intermediate coupling regime it becomes repulsive ($\varepsilon(i - j)$ peaks at $(i - j) = \pm 1$). In contrast, the expectation for the same phonon type, $\langle \psi_k | a_i^+ a_j^+ a_j a_i | \psi_k \rangle$, always peaks at $(i - j) = 0$ (not shown).

![Fig. 2. $\varepsilon(i - j)$ vs. $(i - j)$ calculated at three different coupling strengths and $\omega_0 = t = 1$. Note that vertical scales are different for $k = 0, \pi/4$ and $k = \pi/2, \pi$.](image)

The static correlation function between the electron position and the oscillator displacement is defined as

$$\chi(i - j) = \langle \psi_k | n_i (a_i^+ + a_j) | \psi_k \rangle .$$

(5)

We should stress that when using properly symmetrized ground-state wavefunction in the pseudo-spin space, we numerically obtain the following equality: $\langle \psi_k | n_i (b_i^+ + b_j) | \psi_k \rangle = \langle \psi_k | n_i (a_i^+ + a_j) | \psi_k \rangle$. In Fig. (3) we present $\chi(i - j)$ in the intermediate coupling regime, i.e. $g = 1$. At $k = 0$, where the group velocity is zero, the deformation around the electron position is limited to only a few lattice sites, $\chi(i - j)$ is always positive and seems to be exponentially decaying. At finite but small $k = \pi/4$, the local deformation around the electron increases in amplitude. We also notice a ringing effect (oscillating deformation) as a consequence of a finite velocity at $k \neq 0$. At $k = \pi/2$ the ringing effect is strongly enhanced while the spatial extent of the deformation increases in comparison to $k = 0$. The range of deformation reaches its maximum at $k = \pi$ while at the same time the lattice displacement on the electron site decreases in comparison to smaller values of $k$. In comparison with HP (also presented in Fig. (3)), the main difference is in $\gamma(0)$ which in the case of the JTP diminishes strongly with increasing $k$.

![Fig. 3. $\chi(i - j)$ vs. $(i - j)$ for JTP and HP, $t = 1$.](image)

An important advantage of defining the Hilbert space on an infinite lattice is in the ability to calculate the energy of the system $E$ at arbitrary value of $k$. This makes our method extremely efficient for computing the effective mass of the polaron

$$m^{*-1} = \frac{\partial^2 E(k)}{\partial k^2} |_{k=0} .$$

(6)

The second derivative is evaluated by finite differences in the neighborhood of $k = 0 + dk$. Comparison between the JTP and HP effective mass is presented in Fig. (4). In accordance with the Kornilovitch results [26], the effective mass of the HP polaron is smaller than the JTP in the weak to intermediate coupling regime. With increasing coupling the JTP becomes lighter than the HP. From Fig. (4) it seems as if the effective mass of the JTP and HP displays similar behavior in the strong coupling limit.
The evolution of a polaron state with changing $k$ can be inspected by calculating the quasiparticle weight
and the mean phonon number $N_{k}^{ph}$:

$$Z_{k} = |\langle \psi_{k}|c_{k}^{\dagger}|0\rangle|^{2},$$

(7)

$$N_{k}^{ph} = \sum_{i}\langle \psi_{k}|a_{i}^{\dagger}a_{i} + b_{i}^{\dagger}b_{i}|\psi_{k}\rangle,$$

(8)

where $c_{k}^{\dagger}|0\rangle$ represents a state with an electron and no excited phonons and $|\psi_{k}\rangle$ is the solution of the model at finite $k$. Note that the difference between $Z_{k=0}$ and the inverse effective mass Eq. (6) comes from $k-$ dependence of the polaron self-energy $\Sigma(k,\omega)$ [14]. At finite $k$, $Z_{k}$ measures the electronic character of the polaronic wavefunction. In Fig. (5) we present $Z_{k}$ and $N_{k}^{ph}$ for the HP and JTP calculated at two different coupling strengths $g = 0.7$ and $g = 2.0$. Consistent with results for the effective mass in Fig. (4), $Z_{k}$ of the JTP is slightly larger than the HP at $k = 0$, $g = 2.0$. With increasing $k$ we observe a smooth crossover from the predominantly electronic character (large $Z_{k}$) towards the phononic character (small $Z_{k}$) of a polaron. This crossover is sharper in the HP case as $Z_{k}$ of the JTP intersects $Z_{k}$ of the HP close to $k = 0.3\pi$ ($g = 0.7$). This intersection is also reflected in $N_{k}^{ph}$ even though $N_{k}^{ph}$ does not differ substantially between the two models. In the case of large coupling, $g = 2.0$, $Z_{k}$ for the JTP is larger than $Z_{k}$ of HP which is consistent with the behavior of the effective mass in the strong coupling regime. Moreover, $N_{k}^{ph}$ of the JTP is substantially smaller than $N_{k}^{ph}$ of HP.

### B. Optical conductivity

Applying standard linear-response theory, the real part of the conductivity takes the form (in the limit $T = 0$),

$$\Re\sigma(\omega) = D\delta(\omega) + \sigma^{reg}(\omega > 0),$$

(9)

where $D$ is the Drude weight at $\omega = 0$ and $\sigma^{reg}$ is the finite-frequency response given by

$$\sigma^{reg}(\omega) = \pi e^{2} \sum_{n} \frac{|\langle \psi_{0}|J|\psi_{n}\rangle|^{2}}{E_{n} - E_{0}} \delta(\omega + E_{0} - E_{n}),$$

(10)

where all states $|\psi_{n}\rangle$ for $n = 1, 2, \ldots$ belong to $k = 0$ space. It is important to stress that in Eq. (10), the current operator $J$ has the same form in the Jahn-Teller and Holstein model,

$$J = -i\epsilon t \sum_{i,o} (c_{i+1,o}^{\dagger}c_{i,o} - H.c.).$$

(11)

Therefore we should expect a similar behavior of $\sigma^{reg}(\omega)$ in both models. We next introduce the $\omega$-integrated spectral weight

$$S^{reg}(\omega) = \int_{0}^{\omega} \sigma^{reg}(\omega)d\omega$$

(12)

and arrive at the sum rule

$$S^{tot} = \frac{\pi\epsilon^{2}}{2} (-H_{kin}) = S^{reg} + \pi\epsilon^{2} tm^{-1},$$

(13)

where $S^{reg} = S^{reg}(\infty)$. The sum rule may be used to test the numerics by calculating the effective mass by first
using Eq. (6) and second, Eq. (13). In all cases presented the numerical sum rules are satisfied to at least 6 digits.

While our numerical method, defined on the infinite lattice, enables us to keep the numerical precision in the thermodynamic limit of static correlation functions including \( m^*, S^{\text{tot}} \) and \( S^{eig} \) within a linewidth, there are finite-size effects when presenting finite-frequency quantities. The reason is that the obtained spectrum is discrete and we are thus forced to use a small \( \epsilon \sim 0.05 \) to smooth the continued-fraction form of Eq. 10. On the other hand, the integrated spectral weight \( S^{eig}(\omega) \) does not depend on \( \epsilon \) and is thus more reliable.

We first present \( \sigma^{eig}(\omega) \) and its integral \( S^{eig}(\omega) \) in Fig. (6) for the JT and HM in the weak to intermediate coupling regime. The precision of our results in the thermodynamic limit can be tested in the weak coupling regime. The optical conductivity threshold is known to be at \( \omega = \omega_0 \). In this case, other methods, defined on finite systems, show pronounced finite-size effects due to discreteness in the \( k - \) space which are reflected in the threshold, larger than \( \omega_0 \) in the weak-coupling limit [19–21], and rather well separated peaks corresponding to scattering of the initial \( k = 0 \) electron state into finite-\( k \) states. The main signatures of \( \sigma^{eig}(\omega) \) at \( g = 1.0 \) of both models (JT and HM) are: the spectra are strongly asymmetric in frequency, which is a characteristic of large polarons [24]. Both spectra seem to share the same threshold frequency \( \omega_0 \) [25]. The first two broad peaks are due to one and two phonon emission processes. Peaks are more pronounced in the JT than in the HM case. With increasing coupling \( g \), \( \sigma^{eig}(\omega) \) of both models shifts towards higher frequencies and remains similar. The threshold frequency does not change significantly.

We feel obliged to discuss the constraint of the finite Hilbert space effects on presented spectra in more detail. In the inset of Fig. (6) we present \( \sigma^{eig}(\omega) \) for the JTP calculated for three different sizes of the Hilbert space. We can clearly see that broad features (two broad peaks in \( \sigma^{eig}(\omega) \) converge rather well, however, the number and position of small peaks that compose broad peaks change slightly with increasing \( N_h \). Excited states that contribute to \( \sigma^{eig}(\omega) \) in the total \( k = 0 \) sector can be represented as a polaron with the wavevector \( k_p \) and excited phonon or phonons with the total wavevector \( k_{ph} = -k_p \). Small peaks therefore represent scattering of the polaron into different \( k_p \) states with one or multiple phonon emissions. Since in our variational space phonons are allowed only \( N_h \) steps away from the electron, there are only discrete \( k_p \)'s allowed for such scattering. In the inset of Fig. (6) we present also the integrated conductivity \( S^{eig}(\omega) \) for the same sizes of the Hilbert space. The convergence in this case is excellent.

For small hopping \( t \), one can readily calculate optical conductivity \( \sigma^{eig}(\omega) \) using strong-coupling perturbation theory, i.e., the Lang-Firsov transformation. For a two-site Holstein model [31], we have

\[
\sigma^{eig}(\omega) = \sum_{n=1}^{\infty} \sigma_n \delta(\omega - n\omega_0)
\]

\[
= \pi e^2 t^2 e^{-2g^2} \sum_{n=1}^{\infty} \frac{(2g^2)^n}{n!} \omega_0^n \delta(\omega - n\omega_0) + O(t^4). \tag{14}
\]

We note that \( \sigma^{eig}(\omega) \) is not quite Poisson distributed. It is composed of a series of Dirac \( \delta \)-functions centered at the frequencies \( \omega = n\omega_0 + O(t) \). Their weights, \( \sigma_n \), are second-order in \( t \). For \( g \gg 1 \), the largest \( \sigma_n \) in Eq. 14 occurs when \( n = 2\omega_0(g^2 - 1) \sim 2E_p \), which is consistent with previous numerical studies [22]. Figure 7a shows good agreement between perturbation theory and the numerical result.

In contrast, applying perturbation theory to the JTP is much more difficult because the single-site problem does not have an exact solution. Reasonably accurate trial wave functions for the low-lying levels have been proposed [32,33]. However, obtaining the analytic wave functions for the whole spectrum remains an arduous task. In the following, we evaluate the second-order perturbation based on the numerically exact solutions of the single-site problem. It is known that the eigenfunctions \( \phi_{n,j} \) of a JTP site are characterized by the radial quantum number \( n \) and the angular quantum number \( j \). Each state is doubly degenerate and \( n = 0, j = \pm 1/2 \) for ground states. Thus, for a two-site JTP we chose the ground state to be

\[
|\psi_0\rangle = \frac{1}{\sqrt{2}} \left[ c_1^0 |\phi_{n,1/2}(0,0)\rangle + c_2^0 |\phi_{n,1/2}(0,0)\rangle \right] \tag{15}
\]

where \( |0,0\rangle \) is the phonon state on the site without the electron. We have

\[
\sigma^{eig}(\omega) = \pi e^2 t^2 \sum_{n,m_1,m_2=0}^{\infty} \frac{|\langle \phi_n |0,0\rangle |\langle m_1,m_2 |\phi_0\rangle|^2}{E_n - E_0 + (m_1 + m_2)\omega_0} \times \delta[\omega - E_n - E_0 - (m_1 + m_2)\omega_0] + O(t^4). \tag{16}
\]

where \( E_n \) is the eigenvalue of \( \phi_n \) and \( n + m_1 + m_2 > 0 \). The quantum number \( j \) is left out because it is conserved by current operator. All the nonzero matrix elements exist only between states with \( j = 1/2 \). In addition, the radial excitation of the JTP is anharmonic due to its Mexican-hat potential surface. Therefore, the \( \delta \) -function peaks are not necessarily located near \( n\omega_0 \). We illustrate the distinct feature in Fig. 7b in which the anharmonicity manifests itself clearly when the excited states come near the cone of the Mexican-hat potential. (The height of the cone is \( g^2\omega_0 \) measured from the bottom of the potential surface.) There are actually two peaks near \( \omega_0 \) and three peaks near \( 2\omega_0 \) because the excited phonon quanta can either be harmonic or anharmonic. An excellent agreement between perturbation theory Eq. 16 and Lanczos diagonalization is found in Fig. 7c. Although the total weight of the JTP and HP are approximately equal, in the low-frequency regime, we note that \( S^{eig}_{JTP}(\omega) \gg S^{eig}_{HP}(\omega) \) as a
result of the fact that the JTP has a larger quasiparticle weight than the HP [30,33].

FIG. 6. $\sigma^{reg}(\omega)$ and $S^{reg}(\omega)$ vs. $\omega$ for $g = 1$ (top) and $g = 1.5$ (bottom) for JTP (full lines) and HP (dashed lines). Inset (top) shows $\sigma^{reg}(\omega)$ and $S^{reg}(\omega)$ for the JTP calculated at three sizes of the Hilbert space with $N_h = 12, 13, \text{and } 14$. Convergence of $S^{reg}(\omega)$ is within the linewidth.

Turning to the sum rules presented in Fig. (8), we notice a monotonic decrease of the total sum rule $S^{tot}$, which indicates a suppression of the electronic kinetic energy in the strong coupling regime. The drop in $S^{tot}$ is accompanied by a decrease in the Drude weight $D$, which is a measure of the coherent transport properties of a polaron. Although the decrease is less steep in the JTP case, the two models show strong similarities. The dependence of the regular part $S^{reg}$ of the optical conductivity, which measures the dissipative part of $\sigma(\omega)$, is not monotonic in the electron phonon coupling $g$. It first increases with increasing $g$, reaches the peak near the crossover from large to small polaron regimes and then decreases with further increase of $g$. Such an enhancement of $S^{reg}$ in the intermediate coupling regime has already been observed in the Holstein case [19]. In the strong coupling limit $S^{tot}$ of both models approach the asymptotic value $S^{tot} \sim t^2/\omega_0 g^2$ (see Fig. (8)), which can be obtained by integrating Eq. (14) and summing over all phonon excitations in the limit $g \gg \omega_0$. It is rather surprising that even though the strong coupling expansion is in principle not valid for the JT case, $S^{tot}$ for the JT model seems to approach the same asymptotic behavior. All quantities in Fig. (8) have an error less than a linewidth.

FIG. 7. Optical conductivity: second-order perturbation theory is compared with the numerical result. The height of the peaks represents the weight of the $\delta$-functions. The numerical calculations are performed on the 2-site Holstein or Jahn-Teller models with $t = 0.05$ and $\omega_0 = 1$. The electron-phonon coupling is $g = \sqrt{5}$ for all panels.

FIG. 8. Partial and total sum rules for $\omega_0 = 0.5$ (top) and $\omega_0 = 1.0$ (bottom) as a function of coupling $g$, $t = 1$. Thicker lines represent JTP results, thinner lines HP. The thin dotted line is a strong coupling result.
IV. BIPOLARON

The following section does not apply to manganites, since the strong Hund’s rule coupling renders JT bipolarons unbound. It does, however, apply to other transition metal oxides with filled $t_{2g}$ shells, such as Ni or Co. As we will see in this section, similarities between the JT and Holstein models persist in the case of two electrons. We start by comparing electron-electron correlation function

$$C(i - j) = \langle \psi_k | n_{i} n_{j} | \psi_k \rangle,$$

(17)

where $n_i = n_{i,1} + n_{i,2}$ and $|\psi_k\rangle$ is the bipolaron wave function at momentum $k$. In Fig. (9a) and Fig. (9b) we present $C(i - j)$ for $k = 0$ and different values of the electron-phonon and Coulomb interactions. For $U = 0$ the JT bipolaron (JTB) and Holstein bipolaron (HB) show very small differences. At smaller coupling $g = 1$, Fig. (9a), the effect of increased $U$ on the JTB and HB is similar. The main effect of finite $U$ is to enlarge the size of the bipolaron, caused by the electrons trying to avoid double occupancy. At slightly larger coupling $g = 1.3$, Fig. (9b), the effect of finite $U$ is slightly more pronounced in the case of JTB than HB. We can conclude that the JTB in the intermediate to strong coupling regime has a slightly larger radius at finite $U$ than the HB.

![Graph 1](image1)

**FIG. 9.** $C(i - j)$ vs. $i - j$. We have used $N_{h} = 18$ for HB and $N_{h} = 11$ for JTB.

A larger radius of the bipolaron should imply a larger mobility of the bipolaron. It is known that in the HB, with increasing $U$ the on-site bipolaron transforms into an intra-site bipolaron with a reduced effective mass [27–29]. We may therefore expect the JTB to have a smaller effective mass than the HB due to a larger radius observed in Fig. (9b). This indeed turns out to be the case as seen in Fig. (10) where we show the bipolaron effective mass vs. $U$ in units of the polaron mass for two different coupling strengths. We see that JTB effective mass is smaller than HB effective mass by up to a factor 2 for all $U$ and for both coupling strengths. As shown in the inset of Fig. (10), the JTB at $g = 1.3$ has a smaller binding energy than the HB, corresponding to its larger radius and smaller mass. The binding energy is defined as $\Delta = E_{bi} - 2E_{po}$, where $E_{bi}$ and $E_{po}$ are bipolaron and polaron ground state energies respectively.

![Graph 2](image2)

**FIG. 10.** Effective mass of JTB and HB vs. $U$ for $\omega_0 = 1.0$. Inset: JTB and HB binding energies vs. $U$. Finite-Hilbert space scaling was used for better accuracy.

We conclude our numerical investigation of the JTB with the phase diagram presented in Fig. (11) for the transition from unbound polarons to bound bipolarons. We have obtained the phase diagram using the condition $\Delta(U, g) = 0$. It is important to stress that a bound bipolaron exists in both models at $U = 0$ and at any finite $g$. In the weak coupling limit, i.e. $g \ll 1$, the phase boundary is given by $U_c = 2\omega g^2$, represented by the dashed line in Fig. (11). This result can be derived in the classical limit and it is identical for both the JT and H models. With increasing $g$, the JT phase boundary deviates slightly downwards from the given analytical estimate, while for the HB it deviates upwards. Approaching the strong coupling regime, $U_c(g)$ for the JTB seemingly approaches phase boundary of the HB which in the strong coupling regime follows $U_c = 4\omega g^2$ [27]. Due to the large Hilbert space of the JTB we were unable to investigate the strong coupling regime of the JTB more precisely in order to determine weather the two phase boundaries merge with increasing $g$. 

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Strong similarities between HM and JTM persist also in the case of two bound polarons. Similar to the one polaron case, the Jahn-Teller bipolaron has a smaller effective mass than Hubbard bipolaron in intermediate coupling independent of the strength of $U$. This is mostly a consequence of smaller binding energy.

J.B. gratefully acknowledges the support of Los Alamos National Laboratory where part of this work has been performed, the financial support by the Slovene Ministry of Science, Education and Sport. This work was supported in part by the US DOE and by LANL LDRD.

V. CONCLUSIONS

We have performed a detailed numerical analysis of the JTM in one spatial dimension. The main conclusion is that the simple $E \otimes e$ JTM is, despite extra orbital and phonon degrees of freedom, very similar to the Holstein model (although the former has a doubly degenerate ground state and the latter does not). This result agrees with recent quantum Monte Carlo calculations [26] and analytical comparison of both models [30]. Closer examination reveals that the effective mass of the JTM is larger than HP effective mass in the weak coupling regime and smaller by roughly a factor of $g$ in the strong coupling regime, where the effective masses of JTP and HP share the same exponent.

Turning to spectral properties, our numerical method gives extremely reliable results for $\sigma^{reg}(\omega)$, which can be seen in weak to intermediate coupling by observing the threshold frequency (the gap in the spectra). This agrees with the weak-coupling prediction, i.e. $\omega_{tr} = \omega_0$. We also support this claim by providing $\sigma^{reg}(\omega)$ for systems with different numbers of variational states. $\sigma^{reg}(\omega)$ at $g = 1.0$ clearly shows two broad peaks corresponding to one- and two-phonon emission. These peaks are much more pronounced in the JTM than in the HM. In the strong-coupling regime, we find excellent agreement of $\sigma^{reg}(\omega)$ for the Holstein model with a simple Lang-Firsov strong coupling analytical expression. However, the spectrum of the Jahn-Teller polaron is qualitatively different. Due to the anharmonicity of its radial phonon excitation, the peaks of $\sigma^{reg}(\omega)$ are not necessarily located near the multiples of $\omega_0$. For both models, the sum rule in this regime is given by $S^{tot} \sim t^2/\omega_0 g^2$.  

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