

Exact solutions of the Holstein model with different site energies

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Abstract. The two-site Holstein model with different site energies, the simplest model to mimic disorder, is analytically studied by a diagonalization method of coherent states. The solutions obtained in our work are exact, and agree well with those derived by a modified Lang-Firsov (MLF) method in the weak- and strong-coupling regimes. The deviation from the MLF solution in the intermediate-coupling regime implies that our solution, including the higher order correlation terms overlooked in the MLF treatment, gives a more accurate description. To check the validity of our approach, we have also calculated the case with the same site energies, which shows that our exact solution could be consistent with a previous treatment of the Holstein model using the coherent expansion method [Phys. Rev. B **65**, 174303 (2002)]. The method and the results in the present work would be useful for testing various approximate methods for the Holstein model, and are applicable to more complicated situations.

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1 Introduction

The Holstein model [1] has been widely employed for studying the interaction between narrow band electrons and the local phonons in crystals. In the case of weak electron-phonon (e-ph) coupling, the Holstein model can be solved under the Migdal approximation [2], which involves renormalized phonons and electrons with effective mass. However, this approximate approach cannot work well for strong e-ph coupling with small polarons produced by self-trapped electrons. As strong e-ph coupling is important to current studies for various new materials such as Tc cuprates [3], manganites [4], organic polymer conductors [5], and for charge transport in DNA [6], we had to use instead the Lang-Firsov transformation [7]. We found that although it could improve on the Migdal approximation in several aspects [8–10], the Lang-Firsov transformation is still unable to yield quantitatively accurate results. That is why a modified Lang-Firsov transformation, referred to as the MLF method, was recently proposed [11, 12] and widely adopted. In addition, the Holstein model has also been investigated numerically [13–16].

In this paper, we focus on the few-site Holstein model, which is not only simple enough to lead to accurate and analytical results, but also gives similar features to that of

the many-site Holstein model under strong e-ph and short-range interactions. Due to the localization of the polarons, i.e., the effective distribution over only a few sites, the few-site Holstein model involves the essential characteristics of the many-site one. The two-site Holstein model is the simplest few-site model [17–19], for which exact solutions have been derived analytically using continued fractions [18] and in [20] by using coherent-state expansion method [21, 22]. However once disorder is introduced in the Holstein model, the above models no longer work and we have to resort to a more complicated model, for example, the Holstein model with different site energies.

We note that a MLF method, using a fifth-order perturbative expansion, was used to investigate a two-site Holstein model involving disorder [23]. Nevertheless, since the essential characteristics of the Holstein model, e.g., the correlation function, is very sensitive to the high-order correlation terms, it is natural for us to ask if we could have a more accurate description of the disordered situation by involving expansion terms higher than the fifth-order. In the present paper, we will exactly solve a two-site Holstein model with different site energies, the simplest model for mimicking disorder. Our method, basically analytical, is based on diagonalization in two Fock-state subspaces after some transformations. The favorable features of this approach are that: (1) it could apply to a wider range of parameters than in [20], e.g., for both the same and different

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site energies; (2) it could present a complete and exact eigenenergy spectrum; (3) it can be directly extended to a Holstein model involving more than two sites. In what follows, we will first present our analytical solutions, and then compare to results by numerical computation and by comparison with [20] and [23].

2 The model and our solution

The two-site Holstein model under consideration is

$$H = \epsilon_1 |1\rangle \langle 1| + \epsilon_2 |2\rangle \langle 2| - t(|1\rangle \langle 2| + |2\rangle \langle 1|) + \omega(b_1^\dagger b_1 + b_2^\dagger b_2) + g_1 |1\rangle \langle 1| (b_1 + b_1^\dagger) + g_1 |2\rangle \langle 2| (b_2 + b_2^\dagger), \quad (1)$$

where the first two terms are for electrons in different sites with different energies ϵ_1 and ϵ_2 , t is the hopping integral, and ω is the frequency of the local phonon. b_i, b_i^\dagger ($i = 1, 2$) are annihilation and creation operators of the local phonons at the i th site, respectively. g_1 accounts for the on-site coupling between the electron and the phonons. With the different on-site energies introduced, the two-fold degeneracy in the ordered Holstein model disappears in the absence of the hopping. So such a model makes it possible to investigate the competition between the inter-site electronic hopping and the localization of the polaron. After a transformation, $a = (b_1 + b_2)/\sqrt{2}$, $d = (b_1 - b_2)/\sqrt{2}$ in equation (1), we have

$$H = H_a + H_d, \quad (2)$$

where

$$H_a = (a^\dagger + g)(a + g) - g^2, \quad (3)$$

$$H_d = \epsilon_1 |1\rangle \langle 1| + \epsilon_2 |2\rangle \langle 2| - t(|1\rangle \langle 2| + |2\rangle \langle 1|) + d^\dagger d + g(d + d^\dagger)(|1\rangle \langle 1| - |2\rangle \langle 2|), \quad (4)$$

with $g = g_1/\sqrt{2}$. We have assumed $\omega = 1$ for simplicity. As H_a represents a collective vibration, which is nothing to do with the e-ph interaction, our investigation below will be made only in equation (4), for which we assume a static solution to be

$$| \rangle = |\varphi_1\rangle |1\rangle + |\varphi_2\rangle |2\rangle, \quad (5)$$

with $|\varphi_i\rangle$ the wavefunction of the phonon at the i th site. Putting equation (5) into the Schrödinger equation of equation (4), we have,

$$\begin{aligned} & \epsilon_1 |\varphi_1\rangle |1\rangle + \epsilon_2 |\varphi_2\rangle |2\rangle - t(|\varphi_2\rangle |1\rangle + |\varphi_1\rangle |2\rangle) \\ & + d^\dagger d (|\varphi_1\rangle |1\rangle + |\varphi_2\rangle |2\rangle) + g(d^\dagger + d) (|\varphi_1\rangle |1\rangle - |\varphi_2\rangle |2\rangle) = \\ & E (|\varphi_1\rangle |1\rangle + |\varphi_2\rangle |2\rangle). \quad (6) \end{aligned}$$

Due to the orthogonality between $|1\rangle$ and $|2\rangle$, equation (6) is divided into two parts:

$$\epsilon_1 |\varphi_1\rangle + d^\dagger d |\varphi_1\rangle + g(d^\dagger + d) |\varphi_1\rangle - t |\varphi_2\rangle = E |\varphi_1\rangle, \quad (7)$$

$$\epsilon_2 |\varphi_2\rangle + d^\dagger d |\varphi_2\rangle - g(d^\dagger + d) |\varphi_2\rangle - t |\varphi_1\rangle = E |\varphi_2\rangle. \quad (8)$$

By introducing new bosonic operators, $A = d + g$, $A^\dagger = d^\dagger + g$, $B = d - g$, and $B^\dagger = d^\dagger - g$, we reduce the above equations to

$$(A^\dagger A - g^2 + \epsilon_1) |\varphi_1\rangle - t |\varphi_2\rangle = E |\varphi_1\rangle, \quad (9)$$

$$(B^\dagger B - g^2 + \epsilon_2) |\varphi_2\rangle - t |\varphi_1\rangle = E |\varphi_2\rangle. \quad (10)$$

To solve equations (9) and (10), we may expand $|\varphi_1\rangle$ and $|\varphi_2\rangle$ in complete bases $\{|n\rangle_A\}$ and $\{|n\rangle_B\}$, respectively, i.e., $|\varphi_1\rangle = \sum_{n=0}^N c_n |n\rangle_A$ and $|\varphi_2\rangle = \sum_{n=0}^N d_n |n\rangle_B$, where $|n\rangle_A$ and $|n\rangle_B$ are Fock states, respectively, in the subspaces regarding operators A and B . They can be denoted in the subspaces regarding operator d (d^\dagger) as,

$$|n\rangle_A = \frac{1}{\sqrt{n!}} (d^\dagger + g)^n e^{-gd^\dagger - \frac{g^2}{2}} |0\rangle, \quad (11)$$

$$|n\rangle_B = \frac{1}{\sqrt{n!}} (d^\dagger - g)^n e^{gd^\dagger - \frac{g^2}{2}} |0\rangle. \quad (12)$$

Therefore, equations (9) and (10) become

$$(A^\dagger A - g^2 + \epsilon_1) \sum_{n=0}^N c_n |n\rangle_A - t \sum_{n=0}^N d_n |n\rangle_B = E \sum_{n=0}^N c_n |n\rangle_A, \quad (13)$$

$$(B^\dagger B - g^2 + \epsilon_2) \sum_{n=0}^N d_n |n\rangle_B - t \sum_{n=0}^N c_n |n\rangle_A = E \sum_{n=0}^N d_n |n\rangle_B. \quad (14)$$

Then we multiply ${}_A \langle m|$ and ${}_B \langle m|$ in equations (13) and (14), respectively, which yield,

$$(m + \epsilon_1) c_m - t \sum_{n=0}^N d_n {}_A \langle m | n \rangle_B = (E + g^2) c_m, \quad (15)$$

$$(m + \epsilon_2) d_m - t \sum_{n=0}^N c_n {}_B \langle m | n \rangle_A = (E + g^2) d_m. \quad (16)$$

Equations (15) and (16) are algebraic equations for coefficients $\{c_m\}$ and $\{d_m\}$. Direct deduction gives

$${}_A \langle m | n \rangle_B = \frac{1}{\sqrt{m!n!}} \sum_{i,j} C_m^i C_n^j g^{m-i} (-g)^{n-j} \Phi_{ij}^{(1)}(g)$$

with

$$\Phi_{ij}^{(1)}(g) = e^{-2g^2} \sum_{l=0}^i \frac{i!}{(i-l)!l!} \left[\prod_{k=0}^{l-1} (j-k) \right] (-g)^{j-l} g^{i-l},$$

and

$${}_B \langle m | n \rangle_A = \frac{1}{\sqrt{m!n!}} \sum_{i,j} C_m^i C_n^j (-g)^{m-i} g^{n-j} \Phi_{ij}^{(2)}(g)$$

with

$$\Phi_{ij}^{(2)}(g) = e^{-2g^2} \sum_{l=0}^i \frac{i!}{(i-l)!l!} \left[\prod_{k=0}^{l-1} (j-k) \right] g^{j-l} (-g)^{i-l},$$

where

$$C_m^i = \frac{m!}{(m-i)!i!} \quad \text{and} \quad C_n^j = \frac{n!}{(n-j)!j!}.$$

3 Numerical results and discussion

Before studying the physics involved in the Holstein model, we have to first make sure of the convergence of our solution. As shown in Figures 1 and 2, we have tried to find a suitably big number N in our numerical solution of equations (15) and (16), which guarantees only negligible terms beyond the subspace under consideration. In the calculation below we set $N = 75$ so that high-order terms are negligible, i.e., $c_{n>75} < 10^{-23}$ and $d_{n>75} < 10^{-23}$. Due to the big subspace and the good convergence of the expansion in $\{|n\rangle_A\}$ and $\{|n\rangle_B\}$, we can exactly obtain an eigenenergy spectrum $\{E^{(l)}\}$ and the coefficients $\{c_n^{(l)}\}$ and $\{d_n^{(l)}\}$.

To check the validity of our approach, we first consider the case of $\varepsilon_1 = \varepsilon_2$. Figures 3 and 4 give such a comparison between the present calculation and the results in [20]. Following the convention in [23], we define $\varepsilon_d = \varepsilon_2 - \varepsilon_1$ to be the disorder strength. In the absence of site disorder, our present solution agrees well with that in [20]. Both the solutions demonstrate that the ground state energies decrease with the coupling g and finally approach constant values, while the energy variation in excited states is complicated: the energy spacing becomes small and big repeatedly with the coupling g , and the higher the energy, the more frequent the variation.

From now on we consider the situation with different site energies. For convenience of our description and comparison, we will demonstrate in the figures the results by both our approach and the MLF. We first investigate the local polaronic character of the electrons, denoted by the static correlation functions $\langle n_1 u_1 \rangle_0$ and $\langle n_1 u_2 \rangle_0$ with,

$$\langle n_1 u_1 \rangle / \langle n_1 \rangle = \frac{1}{2} \left[\sum_{i=0}^N \sqrt{i+1} c_{i+1}^* c_i + \sum_{i=0}^N \sqrt{i} c_{i-1}^* c_i \right] / \sum_{i=0}^N c_i^* c_i - 2g, \quad (17)$$

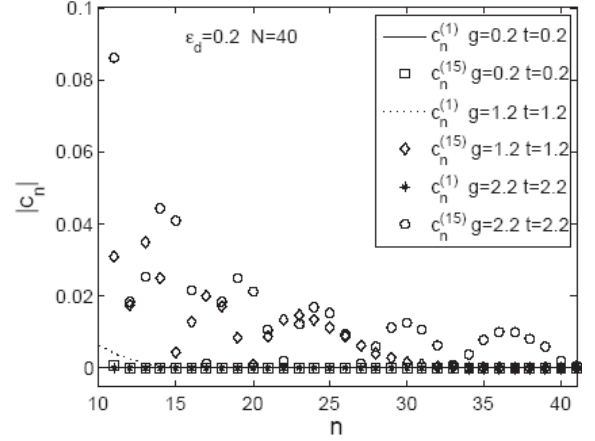


Fig. 1. Distribution of coefficient c_n with n (the phonon number) in the subspace regarding the operator A . For clarity we only demonstrate the coefficients regarding the ground state and the fourteenth excited state denoted by $\{c_n^{(1)}, c_n^{(15)}\}$. To understand the physical meaning of the parameters, see text.

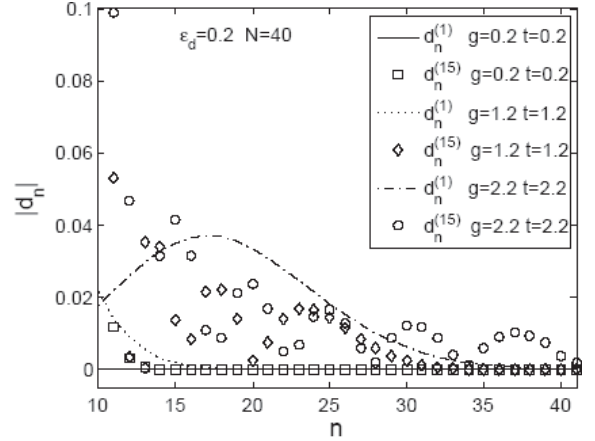


Fig. 2. Coefficient d_n distribution with n (the phonon number) in the subspace regarding the operator B , where for clarity we only demonstrate the coefficients regarding the ground state and the fourteenth excited state denoted by $\{d_n^{(1)}, d_n^{(15)}\}$.

$$\langle n_1 u_2 \rangle / \langle n_1 \rangle = -\frac{1}{2} \left[\sum_{i=0}^N \sqrt{i+1} c_{i+1}^* c_i + \sum_{i=0}^N \sqrt{i} c_{i-1}^* c_i \right] / \sum_{i=0}^N c_i^* c_i, \quad (18)$$

where n_i is the number operator of the electron at i th site, u_i is the deformation of the i th site of the crystal, and $\langle \rangle$ is the expectation value with respect to the ground state wavefunction (we omit the subscript $\{0\}$ for brevity and the detailed deduction of equations (17) and (18) can be found in Appendix). As the summation of equations (17) and (18) is $-2g$, we may only calculate one of them, e.g., equation (18), as shown in Figure 5. It demonstrates clearly that the agreement between our exact solution and that by MLF in [23] occurs in the regimes of small coupling (i.e., $g < 0.5$) and strong coupling (i.e., $g > 1.5$). For the intermediate coupling strength, our solution deviates upwards from that of the MLF. Since the

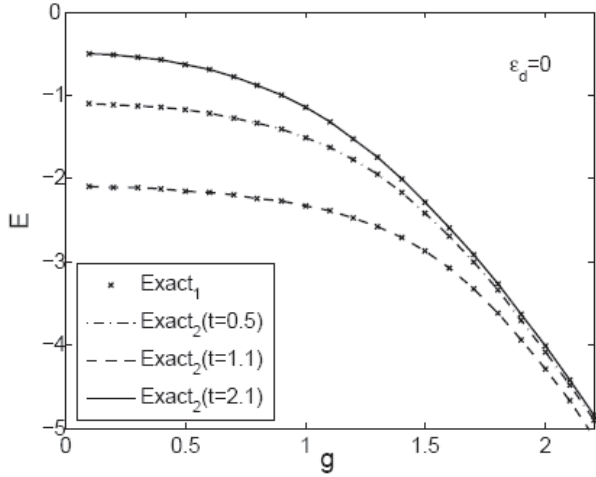


Fig. 3. Ground state energy versus coupling g in the absence of disorder, where Exact1 and Exact2 are solutions in [20] and in the present work, respectively.

correlation function shows the retardation which is independent from the effect of disorder in the weak and strong coupling limits [23], we should pay attention only to the intermediate coupling regime. The discrepancy in Figure 5 physically implies that the retardation is actually stronger than the prediction by the MLF. The reason is that the MLF does not converge well when the e-ph coupling is intermediate. It reminds us that, although it has much improved the solution by the Lang-Firsov transformation from a description of only the weak coupling regime to a description of both the weak and the strong coupling regimes, the MLF is unable to work well in the intermediate coupling case. In contrast, our treatment has good convergence throughout the parametric subspace, which leads to a solution involving the higher-order correlation terms overlooked in the MLF. Moreover, as a byproduct, we have also considered the case of $\varepsilon_d = 0$, and compared with the method in [20] which is only applicable to the ordered case. The comparison confirms that our approach could also work well in the ordered case.

The relative correlation function $\chi = \langle n_1(u_1 - u_2) \rangle / 2g \langle n_1 \rangle$ could examine the behavior of the large-to-small polaron crossover. Small χ corresponds to a big polaron with an obvious associated retardation effect, but when χ approaches 1, this retardation effect becomes negligible, corresponding to a small polaron. Our interest is in the crossover regime, as shown in Figure 6 where the continuous change, in the case of different site energies, from a big polaron to a small polaron with the increase of g , should be less sharp, according to our calculation, than the prediction by MLF in [23]. But in the case of the same site energies, no difference could be found between our solution and that by MLF. This comparison shows again that the higher order correlation terms play visible roles only in the disordered Holstein model.

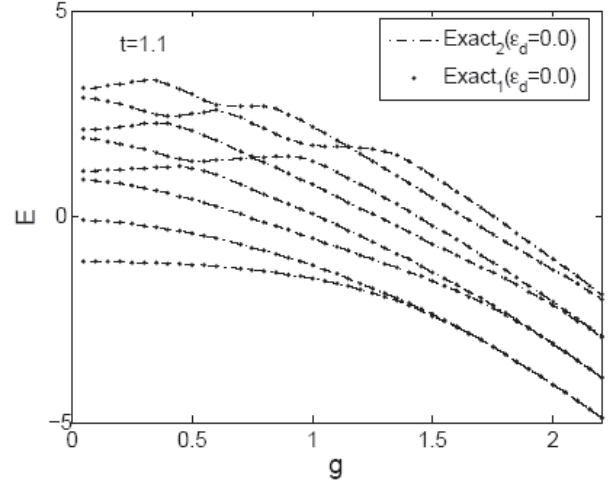


Fig. 4. Excited energies versus the coupling g in the absence of disorder, where Exact1 and Exact2 are solutions in [20] and in the present work, respectively. We have assumed $t = 1.1$ in the calculation.

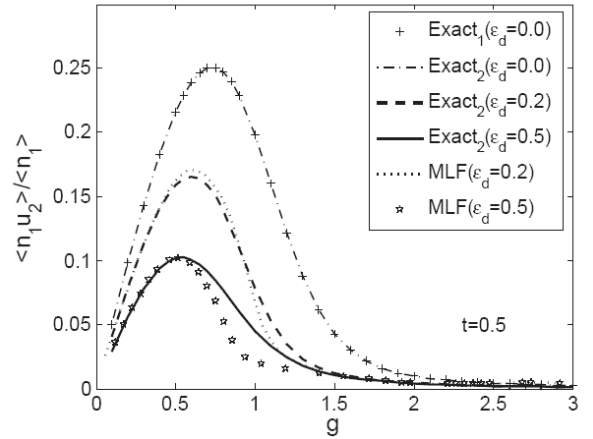


Fig. 5. Correlation function versus the coupling g , where Exact1 and Exact2 are solutions in [20] and in the present work, respectively. (\cdot , \star) are for MLF results from [23]. $t = 0.5$ is assumed in our calculation.

We have also calculated the occupation number of the polaron for the ground state at $k = 0$ and $k = \pi$, respectively, using

$$n(k=0) = \frac{1}{2} \left\{ 1 - \frac{E + g^2}{t} + \frac{1}{t} \sum_{i=0}^N [|c_i|^2 (i + \varepsilon_1) + |d_i|^2 (i + \varepsilon_2)] \right\}, \quad (19)$$

$$n(k=\pi) = \frac{1}{2} \left\{ 1 + \frac{E + g^2}{t} - \frac{1}{t} \sum_{i=0}^N [|c_i|^2 (i + \varepsilon_1) + |d_i|^2 (i + \varepsilon_2)] \right\}, \quad (20)$$

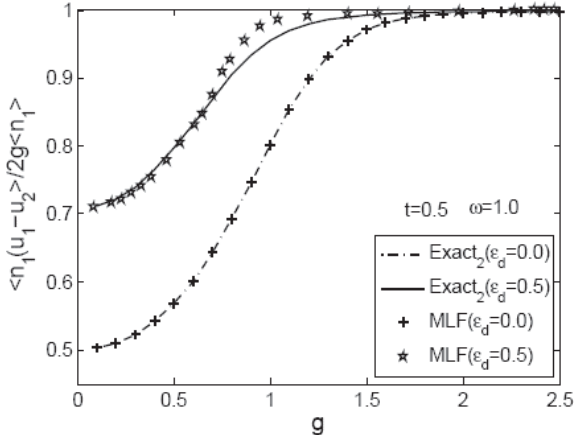


Fig. 6. Relative correlation function versus the coupling g , where $(\star, +)$ are results from MLF [23], and Exact2 correspond to the present solution. We have used $t = 0.5$ and $\omega = 1.0$.

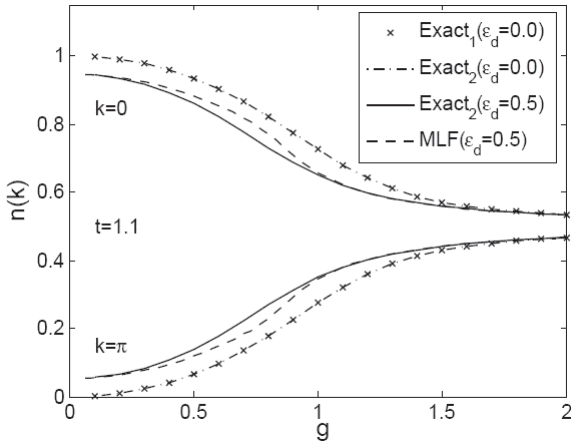


Fig. 7. Occupation numbers versus the coupling g , where Exact1 and Exact2 are solutions in [20] and in the present work, respectively. The dashed curve is for MLF in [23]. $t = 0.5$ is assumed in our calculation.

whose derivation can be found in Appendix. The difference of above occupation numbers is strongly related to the localization of the polaron. Consider that the system remains in the ground state, e.g., $n(k=0)$ much larger than $n(k=\pi)$ in the case of a small g , under a certain hopping strength, $n(k=\pi)$ will become almost the same as $n(k=0)$ with the increase of g . Since the disordered effect suppresses the kinetic energy of the polaron, the difference of the occupation numbers decreases with respect to the ordered case. We may find the discrepancy of our present solution from that in [23] in the regime of $0.2 < g < 1$ in Figure 7, which indicates again that our solution could give more accurate results in the intermediate coupling regime in the disordered case due to the convergent treatment of the higher order correlation terms.

It is evident from the above results that the approximate solutions such as the MLF results in [23], are good enough for the Holstein model in the ordered case, and are also good in the disordered case for the weak and strong e-ph couplings. But they cannot work well in the

intermediate coupling regime of the disordered Holstein model. So the discrepancy of our solution from the MLF results in [23] in the regime of the intermediate coupling indicates the complicated physics never discovered previously. As mentioned in [23], the more disordered effect leads to a weaker retardation between the electron and the associated deformation, and also results in more polaron crossover. Our solution with the deviation downwards from the MLF one shows that there are actually a slightly stronger retardation and a less intensive polaron crossover in the disordered situation than the prediction by [23]. The discrepancy comes from the missing of the higher order perturbative expansion in [23], because both the correlation function and the occupation numbers in the intermediate coupling case are very sensitive to the higher order correlation terms. We note that the MLF perturbation could have very fast convergence in both regimes of weak and strong couplings due to very small higher-order terms with alternate signs [20]. But in the intermediate coupling regime, convergence gets worse and worse in the MLF treatment. As a result, our treatment, involving all the higher terms, could provide a complete and accurate description for the Holstein model.

As an efficient method, our treatment could be applied to a more general situation and be used to study different characteristics of the Holstein model. As an example, we investigate the variation of the entropy with respect to the temperature T and the coupling g_1 . The entropy is defined as

$$S_{\epsilon_1, \epsilon_2} = k \left(\ln Z - \beta \frac{\partial}{\partial \beta} \ln Z \right), \quad (21)$$

where $Z = \sum_{n=1}^N e^{-\beta E_n}$, and $\beta = 1/(kT)$, with k the Boltzmann constant and T the temperature. Figure 8 shows that the more different the on-site energies, the smaller the entropy for g_1 and the small T . It implies that the entropy becomes sensitive to the large e-ph coupling at low temperature. Since the larger difference of the on-site energies would lead to more ordered electronic tunneling, the entropy reduces with the disordered strength ϵ_d . So it is interesting physically that the system with larger disorder actually has smaller entropy with respect to the variation of the e-ph coupling.

4 Conclusion

In summary, we have exactly solved the Holstein model involving different site energies, which corresponds to the simplest treatment of disorder. We have compared with previous work in different cases and shown that our exact solutions agree well with the results in [20] in the ordered case, and are also consistent with the MLF solutions in [23] in the weak and strong e-ph coupling regimes in the presence of disorder. Our interest is in the intermediate coupling regime, in which the discrepancy is evident between our solution and that of the MLF. We think our solution is exact, which could work well throughout the parametric

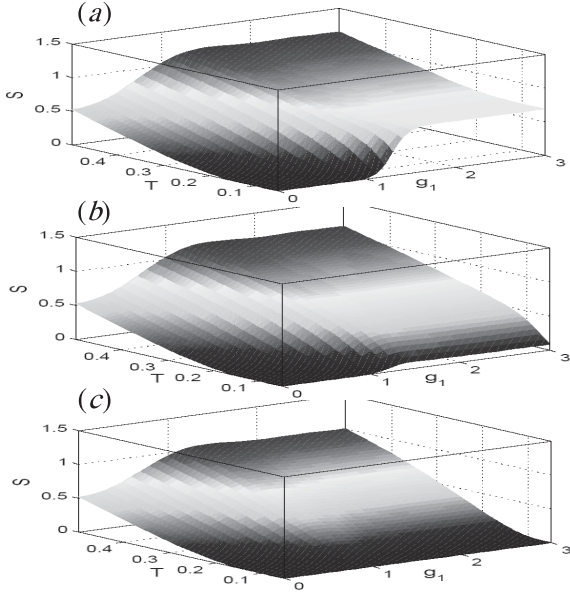


Fig. 8. The variation of the entropy with respect to T and g_1 in units of k , where $t = 1.1$, and (a) $\varepsilon_d = 0$, (b) $\varepsilon_d = 0.2$, (c) $\varepsilon_d = 0.6$.

subspace for the two-site Holstein model involving disorder. Moreover, comparing with purely numerical methods, our analytical treatment could present more useful information for understanding the physics hidden in the Holstein model.

We argue that our method would be very helpful for testing various approximate solutions, and applicable to more complicated situations of the Holstein model, e.g., with more sites and more complex disordered effects. For example, the case of more sites corresponds to a multi-level model. From the viewpoint of mathematics, it could be transformed to be a series of solvable equations regarding two-level models like equation (4). Physically speaking, we could not simply denote the disordered effect in such a case by difference of site energies, but by an average over different site energies. As a result, the treatment would be more complicated. Nevertheless, it is available with the framework of our approach.

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Appendix

Here we give the detailed deduction for correlation functions equations (17) and (18). By using $n_1 = |1\rangle\langle 1|$, $n_2 = |2\rangle\langle 2|$, $n = |1\rangle\langle 1| + |2\rangle\langle 2|$, $n_1 \cdot n = n_1$, $n_2 \cdot n = n_2$, and

$$\langle n_1 u_{1,2} \rangle = {}_0\langle n_1 [\pm (d + d^+) - 2gn] / 2 \rangle_0, \quad (\text{A.1})$$

where n_1 and n_2 are number operators with respect to the first and second sites, respectively, n is the total number

operator, and u_1 and u_2 are deviations from the balanced positions regarding the first and the second sites, respectively, we have, with respect to the ground state wavefunction,

$$\begin{aligned} \langle n_1 u_1 \rangle / \langle n_1 \rangle &= {}_0\langle \{ n_1 \cdot [(d + d^+) - 2gn] / 2 \} \rangle_0 / {}_0\langle n_1 \rangle_0 \\ &= {}_0\langle \{ n_1 \cdot [(d + d^+) - 2g] / 2 \} \rangle_0 / {}_0\langle n_1 \rangle_0 \\ &= \frac{1}{2} (\langle \varphi_2 | \langle 2 | + \langle \varphi_1 | \langle 1 | \} \{ |1\rangle\langle 1| [A^+ \\ &\quad + A - 4g] \} (|\varphi_1\rangle |1\rangle + |\varphi_2\rangle |2\rangle) / \langle \varphi_1 / \varphi_1 \rangle \\ &= \frac{1}{2} \langle \varphi_1 | \{ [A^+ + A - 4g] \} | \varphi_1 \rangle / \langle \varphi_1 / \varphi_1 \rangle \\ &= \frac{1}{2} \left[\sum_{i=0}^N \sqrt{i+1} c_{i+1}^* c_i + \sum_{i=0}^N \sqrt{i} c_{i-1}^* c_i - 4g \sum_{i=0}^N c_i^* c_i \right] / \sum_{i=0}^N c_i^* c_i \\ &= \frac{1}{2} \left[\sum_{i=0}^N \sqrt{i+1} c_{i+1}^* c_i + \sum_{i=0}^N \sqrt{i} c_{i-1}^* c_i \right] / \sum_{i=0}^N c_i^* c_i - 2g, \end{aligned} \quad (\text{A.2})$$

$$\begin{aligned} \langle n_1 u_2 \rangle / \langle n_1 \rangle &= \\ &{}_0\langle \{ n_1 \cdot [-(d + d^+) - 2gn] / 2 \} \rangle_0 / {}_0\langle n_1 \rangle_0 \\ &= {}_0\langle \{ n_1 \cdot [-(d + d^+) - 2g] / 2 \} \rangle_0 / {}_0\langle n_1 \rangle_0 \\ &= \frac{1}{2} (\langle \varphi_2 | \langle 2 | + \langle \varphi_1 | \langle 1 | \} \{ |1\rangle\langle 1| [-A^+ - A] \} \\ &\quad \times (|\varphi_1\rangle |1\rangle + |\varphi_2\rangle |2\rangle) / \langle \varphi_1 / \varphi_1 \rangle \\ &= \frac{1}{2} \langle \varphi_1 | \{ [-A^+ - A] \} | \varphi_1 \rangle / \langle \varphi_1 / \varphi_1 \rangle \\ &= \frac{1}{2} \left[- \sum_{i=0}^N \sqrt{i+1} c_{i-1}^* c_i - \sum_{i=0}^N \sqrt{i} c_{i+1}^* c_i \right] / \sum_{i=0}^N c_i^* c_i \\ &= -\frac{1}{2} \left[\sum_{i=0}^N \sqrt{i+1} c_{i+1}^* c_i + \sum_{i=0}^N \sqrt{i} c_{i-1}^* c_i \right] / \sum_{i=0}^N c_i^* c_i, \end{aligned} \quad (\text{A.3})$$

where we have made the above analytical deduction using equation (5).

Now, let us turn to the deduction of the occupation numbers equations (19) and (20),

$$\begin{aligned} n_{0,\pi} &= \frac{1}{2} (|1\rangle\langle 1| \pm |1\rangle\langle 2| \pm |2\rangle\langle 1| + |2\rangle\langle 2|), \quad (\text{A.4}) \\ n(k=0) &= \frac{1}{2} \langle (|1\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 2|) \rangle \\ &= \frac{1}{2} (\langle \varphi_1 | \varphi_1 \rangle + \langle \varphi_2 | \varphi_2 \rangle + \langle \varphi_1 | \varphi_2 \rangle + \langle \varphi_2 | \varphi_1 \rangle) \\ &= \frac{1}{2} \left\{ \sum_{i=0}^N |c_i|^2 + \sum_{i=0}^N |d_i|^2 + \sum_{ij=0}^N c_i^* d_j A \langle i | j \rangle_B \right. \\ &\quad \left. + \sum_{ij=0}^N d_i^* c_j B \langle i | j \rangle_A \right\}. \end{aligned} \quad (\text{A.5})$$

From equations (15) and (16), we have,

$$\sum_{j=0}^N d_{jA} \langle i | j \rangle_B = (i + \epsilon_1 - E - g^2) c_i / t, \quad (\text{A.6})$$

$$\sum_{j=0}^N c_{jB} \langle i | j \rangle_A = (i + \epsilon_2 - E - g^2) d_i / t. \quad (\text{A.7})$$

So we can simplify (A.5) to be,

$$\begin{aligned} n(k=0) &= \frac{1}{2} \left\{ \sum_{i=0}^N |c_i|^2 + \sum_{i=0}^N |d_i|^2 + \sum_{i=0}^N c_i^* \sum_{j=0}^N d_{jA} \langle i | j \rangle_B \right. \\ &\quad \left. + \sum_{ij=0}^N d_i^* \sum_{j=0}^N c_{jB} \langle i | j \rangle_A \right\} \\ &= \frac{1}{2} \left\{ \sum_{i=0}^N |c_i|^2 + \sum_{i=0}^N |d_i|^2 \right. \\ &\quad \left. + \sum_{i=0}^N |c_i|^2 (i + \epsilon_1 - E - g^2) / t \right. \\ &\quad \left. + \sum_{i=0}^N |d_i|^2 (i + \epsilon_2 - E - g^2) / t \right\} \\ &= \frac{1}{2} \left\{ \sum_{i=0}^N \left[|c_i|^2 \left(1 + \frac{i + \epsilon_1 - E - g^2}{t} \right) \right. \right. \\ &\quad \left. \left. + |d_i|^2 \left(1 + \frac{i + \epsilon_2 - E - g^2}{t} \right) \right] \right\}. \quad (\text{A.8}) \end{aligned}$$

Similarly, we have

$$\begin{aligned} n(k=\pi) &= \frac{1}{2} \left\{ \sum_{i=0}^N \left[|c_i|^2 \left(1 - \frac{i + \epsilon_1 - E - g^2}{t} \right) \right. \right. \\ &\quad \left. \left. + |d_i|^2 \left(1 - \frac{i + \epsilon_2 - E - g^2}{t} \right) \right] \right\}, \quad (\text{A.9}) \end{aligned}$$

$$\begin{aligned} n(k=0) &= \frac{1}{2} \left\{ 1 - \frac{E + g^2}{t} + \frac{1}{t} \sum_{i=0}^N [|c_i|^2 (i + \epsilon_1) \right. \\ &\quad \left. + |d_i|^2 (i + \epsilon_2)] \right\}, \quad (\text{A.10}) \end{aligned}$$

$$\begin{aligned} n(k=\pi) &= \frac{1}{2} \left\{ 1 + \frac{E + g^2}{t} - \frac{1}{t} \sum_{i=0}^N [|c_i|^2 (i + \epsilon_1) \right. \\ &\quad \left. + |d_i|^2 (i + \epsilon_2)] \right\}. \quad (\text{A.11}) \end{aligned}$$

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