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Exact solutions for the two-site Holstein model

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The two-site Holstein model is studied by the analytical method of the coherent-state expansion. We obtain the recursive relationship among the expansion coefficients, which leads to the exact solutions of the eigenstate properties. The exact ground-state results in the whole coupling strength region and from antiadiabatic to adiabatic limits are in perfect agreement with that available by the exact numerical diagonalization technique. Comparison with the best perturbation results shows the success and shortcoming of the perturbative method. The coherent-state expansion method is a promising approach in studying electron-phonon (e-ph) coupling systems.

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The polaron problem presents a highly nonlinear dynamical system in which the charge and lattice deformations are intricately coupled together.[1,2] The complexity of the system challenges analytical methods. In the weak electron-phonon (e-ph) coupling adiabatic regime, the system can be described well by the Migdal approximation,[3] with renormalized phonon frequencies and electron effective mass. When the coupling of the electron to the atomic displacements is strong, the electron is self-trapped and produces a small polaron. Small polarons are believed to play an essential role in some new materials with exceptional properties such as the high-T_c cuprates, the nickelates, and manganites.[4–6] As one of the fundamental models describing interactions of conduction electrons with local lattice deformations, the two-site Holstein model[7] is not only instructive for studying features of small polarons on the basis of small units, but also applies to true physically relevant situations.

The property of the small polaron has been extensively studied,[8–10] generally based on the Lang-Firsov (LF) transformation,[11] followed by approximations treating the fully localized polaron state as the starting point and introducing the hopping of the electrons by perturbative means. It is shown, however, that neither the Migdal approximation nor the LF approximation provides satisfactory quantitative results for intermediate coupling strength. Recently, Das and co-workers developed a perturbation expansion up to the sixth order using the LF, modified LF (MLF), and MLF with squeezing transformations.[12,13] Much improved results are obtained and the sixth-order perturbative MLF is the best analytical method known to date. Nevertheless, the most reliable results have to rely upon the numerical diagonalization technique.[14–18] In this paper, we report an analytical method describing the ground state of the Holstein model exactly for the entire range of the coupling strength.

The two-site single-polaron Holstein model describes an electron hopping between two adjacent sites (diatomic molecules), each of which exhibits an optical mode with frequency ω_0. The Hamiltonian can be separated into two terms.[18] One describes a shifted oscillator that does not couple to the electronic degree of freedom. The other describes the effective e-ph system where phonons couple directly with the electronic degrees of freedom and is defined by the Hamiltonian[12,18]

$$H=\sum_i \epsilon n_i - t(c_1^\dagger c_2 + c_2^\dagger c_1) + \omega_0 g(n_1-n_2)(d+d^\dagger) + \omega_0 d^\dagger d, \tag{1}$$

where $i=1$ or 2 denotes the site. $c_i(c_i^\dagger)$ is the annihilation (creation) operator for the electron at site i, $n_i(=c_i^\dagger c_i)$ is the corresponding number operator, g denotes the on-site e-ph coupling strength, t is the usual hopping integral, $d(d^\dagger)$ is the annihilation (creation) operator for the oscillator, and ϵ is the bare site energy of electron. In the following we set $\omega_0=1$.

From the Hamiltonian $\hat{H}$, we can see that the electron couples linearly to the oscillator and the number of phonons is nonconservative due to $[d^\dagger d,\hat{H}]\neq 0$. Therefore it is particularly appropriate to write the wave function of the two-site system in the coherent-state space.[19] The coherent states span the whole Fock space. Their overcompleteness enables any vector of the Fock space to be represented exactly. The eigenstate of the Hamiltonian $\hat{H}$ then could be supposed to have the form

$$|\rangle=\left[\sum_{i=0}^{\infty}\rho_{1,i}(d^\dagger)^i\right]|A_1\rangle|1\rangle+\left[\sum_{i=0}^{\infty}\rho_{2,i}(d^\dagger)^i\right]|A_2\rangle|2\rangle, \tag{2}$$

where $\rho_{1,0}=1$, $\rho_{2,0}=f$. f and $\rho_{1,i},\rho_{2,i}$ are parameters to be determined, $|1\rangle$ and $|2\rangle$ are wave functions for the electron in site 1 and 2, respectively. $|A_i\rangle$, $i=1,2$ is the coherent state of the phonon at site i with the form

$$|A_i\rangle=\exp(\alpha_i d^\dagger)|0\rangle, \quad i=1,2, \tag{3}$$

where $|0\rangle$ denotes the vacuum state of the phonon mode, α_i is the eigenvalue of the operator d with $d|A_i\rangle=\alpha_i|A_i\rangle$, $i=1,2$. It is not difficult to find that $|A_1\rangle$ and $|A_2\rangle$ have relations

$$|A_1\rangle=\exp[(\alpha_1-\alpha_2)d^\dagger]|A_2\rangle, \tag{4}$$

$$|A_2\rangle = \exp[(\alpha_2-\alpha_1)d^\dagger]|A_1\rangle. \tag{5}$$

Substituting Eq. (2) into the Schrödinger equation $\hat{H}|\rangle = E|\rangle$ and utilizing Eqs. (4), (5), and the commutation relation $[d,d^\dagger]=1$, we get

$$\begin{aligned}E'\left[\sum_{i=0}^{\infty}\rho_{1,i}(d^\dagger)^i|A_1\rangle|1\rangle+\sum_{i=0}^{\infty}\rho_{2,i}(d^\dagger)^i|A_2\rangle|2\rangle\right]\\ =-t\left[\sum_{i,j=0}^{\infty}\rho_{1,i}\frac{(\alpha_1-\alpha_2)^j}{j!}(d^\dagger)^{i+j}|A_2\rangle|2\rangle\right.\\ \left.+\sum_{i,j=0}^{\infty}\rho_{2,i}\frac{(\alpha_2-\alpha_1)^j}{j!}(d^\dagger)^{i+j}|A_1\rangle|1\rangle\right]\\ +g\left\{\sum_{i=0}^{\infty}\rho_{1,i}[(d^\dagger)^{i+1}+i(d^\dagger)^{i-1}+\alpha_1(d^\dagger)^i]|A_1\rangle|1\rangle\right.\\ \left.-\sum_{i=0}^{\infty}\rho_{2,i}[(d^\dagger)^{i+1}+i(d^\dagger)^{i-1}+\alpha_2(d^\dagger)^i]|A_2\rangle|2\rangle\right\}\\ +\sum_{i=0}^{\infty}\rho_{1,i}[i(d^\dagger)+\alpha_1(d^\dagger)^{i+1}]|A_1\rangle|1\rangle\\ +\sum_{i=0}^{\infty}\rho_{2,i}[i(d^\dagger)+\alpha_2(d^\dagger)^{i+1}]|A_1\rangle|1\rangle,\end{aligned}\tag{6}$$

where $E'=E-\epsilon$. From Eq. (1), it can be seen that the Hamiltonian is invariant under the transformation $c_1^\dagger(c_1)\leftrightarrow c_2^\dagger(c_2)$ and $d^\dagger(d)\leftrightarrow -d^\dagger(-d)$. This means that $(E',\ f,\ \alpha_1,\ \alpha_2,\ \rho_{1,i},\ \rho_{2,i})$ and $(E',\ 1/f,\ -\alpha_2,\ -\alpha_1,\ (-1)^i\rho_{2,i}/f,\ (-1)^i\rho_{1,i}/f)$ are both the solutions for the system. Generally, this leads to the double degeneration, which is caused by the symmetric nature of the two-site system. However, the two solutions are identical when $f=1/f$, leading to the singlet states of the system with $\alpha_1=-\alpha_2$ and $\rho_{1,i}=(-1)^i\rho_{2,i}/f$. The ground state is expected to be a bonding singlet with $f=1$.[18] Equating the coefficients of nth level correlation effect $(d^\dagger)^n|A_i\rangle|i\rangle$ $(n=1,2,\dots)$, we have a set of nonlinear equations, which determine the parameters of the system, leading to the recurrence equation for $\rho_{1,n}$

$$\rho_{1,n}=\frac{1}{ng}\left\{(-tf-n+1)\rho_{1,n-1}-(g+\alpha_1)\rho_{1,n-2}+(-1)^{n-1}tf\sum_{\substack{i,j=0\\ i+j=n-1}}^{\infty}\frac{(2\alpha_1)^j}{j!}\rho_{1,i}\right\},\quad n=2,\dots,\infty \tag{7}$$

and

$$E'=g\alpha_1-tf, \tag{8}$$

$$\rho_{1,1}=\rho_{2,1}=0. \tag{9}$$

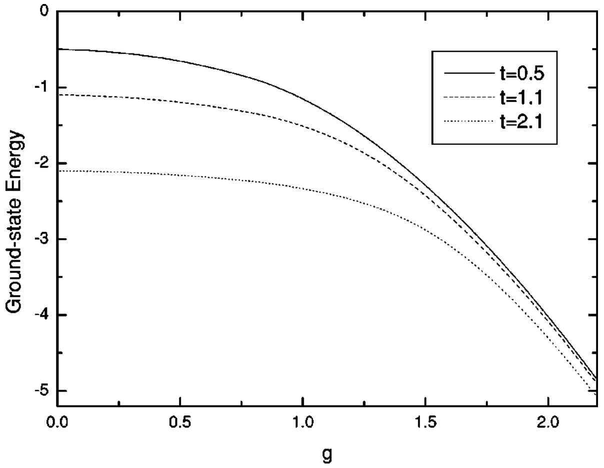

FIG. 1. Ground-state energy versus g for $t/\omega_0=0.5$, 1.1, and 2.1.

Considering the fact that the high-order correlation effect contributes relatively little to the system, we could approach the real system with the omission of high-level correlation effects, for example, omitting the terms $(d^\dagger)^n|A_i\rangle$ with $n>n_t$, where n_t is the truncation order. The truncation of the (n_t+1)th-order recurrence equation gives

$$\rho_{1,n_t}=\frac{-1}{tf+n_t+(-1)^{n_t+1}tf}\left\{(g+\alpha_1)\rho_{1,n_t-1}+(-1)^{n_t+1}tf\sum_{\substack{i=0,j=1\\ i+j=n_t}}^{\infty}\frac{(2\alpha_1)^j}{j!}\rho_{1,i}\right\}. \tag{10}$$

For a given α_1, all correlation coefficients $\rho_{1,i}$, $i=0,\dots,n_t$ can be obtained from Eq. (7) . Substituting $\rho_{1,i}$ to the truncated equation (10) provides a nonlinear equation for determining α_1. This equation can be easily solved by the bisection method,[20] yielding a set of solutions corresponding to the ground and excited states of the system. All physical properties are then available with the resulting wave functions.

Obviously, one can include in the above calculation arbitrarily high order phonon correlations by taking the corresponding truncation order n_t, and the results with arbitrarily high precision can be obtained. The calculation needs less than 1 CPU sec of a PIII 833 PC computer to obtain the result with the 50th order correlation effects, which is much more than necessary to achieve the machine accuracy for all the cases tested. Therefore, the analytical coherent-state expansion (CE) described above provides a simple method to get the exact solutions for the two-site system.

The exact ground-state energies for systems with $t/\omega_0=0.5$, 1.1, and 2.1 are shown in Fig. 1. These values of t cover the crossover region from the antiadiabatic limit to the adiabatic limit. Our ground-state energies show very good convergence with the truncation order. It is noticed, however, that when the coupling strength g increases, the correlation effects become strong and higher-order correlation effects

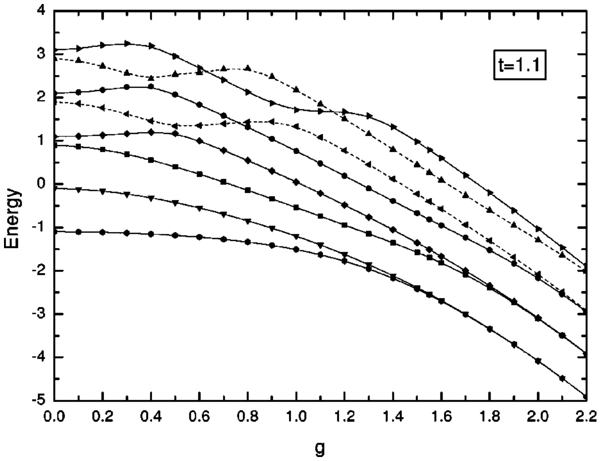

FIG. 2. Eight lowest-energy levels for the $t/\omega_0 = 1.1$ system as a function of the coupling strength g.

have to be included in order to obtain results with similar precisions. The results by the exact numerical diagonalization technique for $t/\omega_0 = 1.1$ (Ref. 18) are indistinguishable from our results in the whole coupling region, confirming the validity of our approach. The sixth-order perturbation MLF method also provides excellent results, with energies almost identical to ours for $t/\omega_0 = 0.5$ and $t/\omega_0 = 1.1$.[12] With our method, we could also conveniently obtain excited states. As an example, Fig. 2 shows the eight lowest energies for the $t/\omega_0 = 1.1$ system. All curves show very good agreement with the results of the numerical diagonalization method.

The polaronic character of the electrons are usually studied by the static correlation functions $\langle n_1 u_1\rangle$ and $\langle n_1 u_2\rangle$, which indicate, respectively, the strength of polaron induced lattice deformations and their ranges, where u_1 and u_2 are the lattice deformations at site 1 and 2, respectively, produced by an electron at site 1. The ground-state correlation functions could be written as[12]

$$\langle n_1 u_{1,2}\rangle = \langle n_1/2\,[\pm(d+d^{\dagger}) - 2gn]\rangle, \tag{11}$$

where n_1 is the number operator for the electron at site 1 and $n = 1$ is the total electron number. The positive and negative sign correspond to $\langle n_1 u_1\rangle$ and $\langle n_1 u_2\rangle$, respectively. The functions $\langle n_1 u_1\rangle$ and $\langle n_1 u_2\rangle$ versus g for the ground state of $t/\omega_0 = 0.5$, 1.1, and 2.1 systems are plotted in Figs. 3(a) and 3(b). For small g, i.e., in the weak e-ph coupling region, $-\langle n_1 u_1\rangle$ and $-\langle n_1 u_2\rangle$ increase linearly with g, as expected. In the strong e-ph coupling region, $-\langle n_1 u_1\rangle$ increases monotonically whereas $-\langle n_1 u_2\rangle$ gradually decreases to zero with increasing g. This indicates that the deformation is large and tends to be localized at site 1, a clear sign of a self-trapped small polaron. Notice that for a given e-ph coupling strength g, the larger hopping parameter (t) increases the amplitude of off-site deformation ($\langle n_1 u_2\rangle$) while it reduces that of the on-site correlation ($\langle n_1 u_1\rangle$). The transition from a large polaron (quasifree electron) to a small polaron (self-trapped electron) is thus driven by a competition between the kinetic and potential energy of the electron. Our static correlation functions for $t/\omega_0 = 1.1$ agree very well with that by the exact numerical diagonalization technique in the whole coupling range.[18]

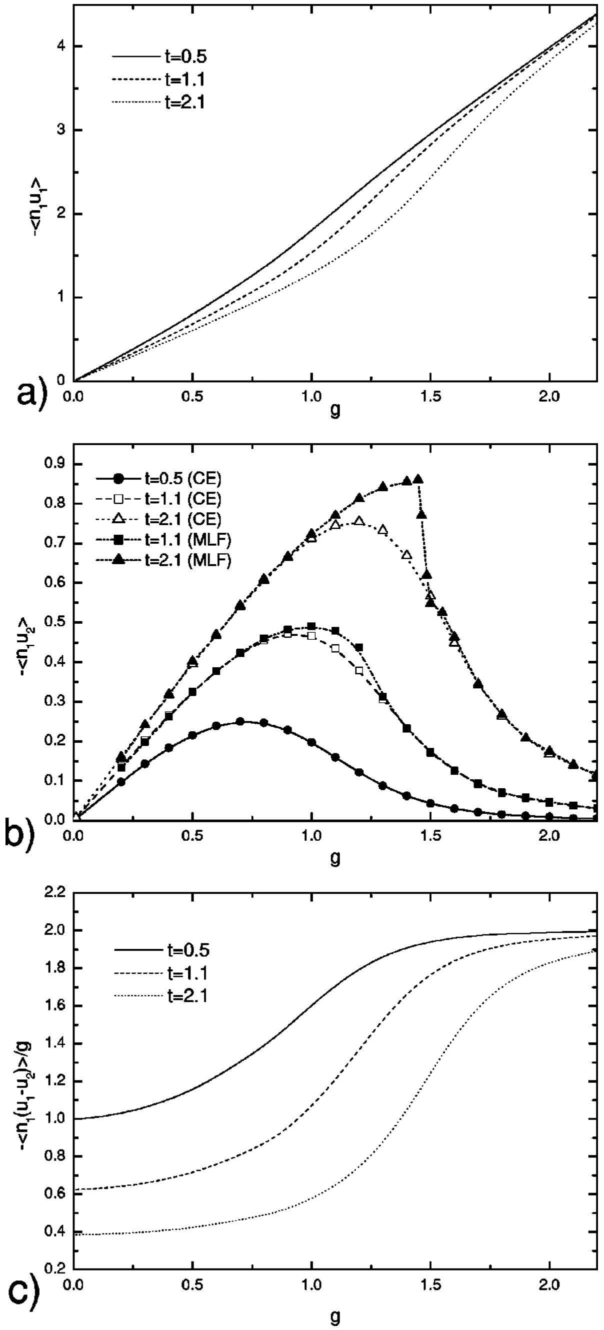

FIG. 3. Correlation functions versus g for the systems with $t/\omega_0 = 0.5$, 1.1, and 2.1. (a) $-\langle n_1 u_1\rangle$, (b) $-\langle n_1 u_2\rangle$; (c) $-\langle n_1(u_1 - u_2)\rangle/g$.

The nature of the crossover from a delocalized (large) to a localized (small) polaron can also be studied by the correlation function $\langle n_1(u_1 - u_2)\rangle/g$. The exact results against g for $t/\omega_0 = 0.5$, 1.1, and 2.1 systems are plotted in Fig. 3(c). No abrupt crossover from a large to small polaron is seen. This is consistent with Lowen's conclusion that there cannot be any abrupt crossover in the ground state of an e-ph system for a finite phonon frequency.[21] The plot, however, does

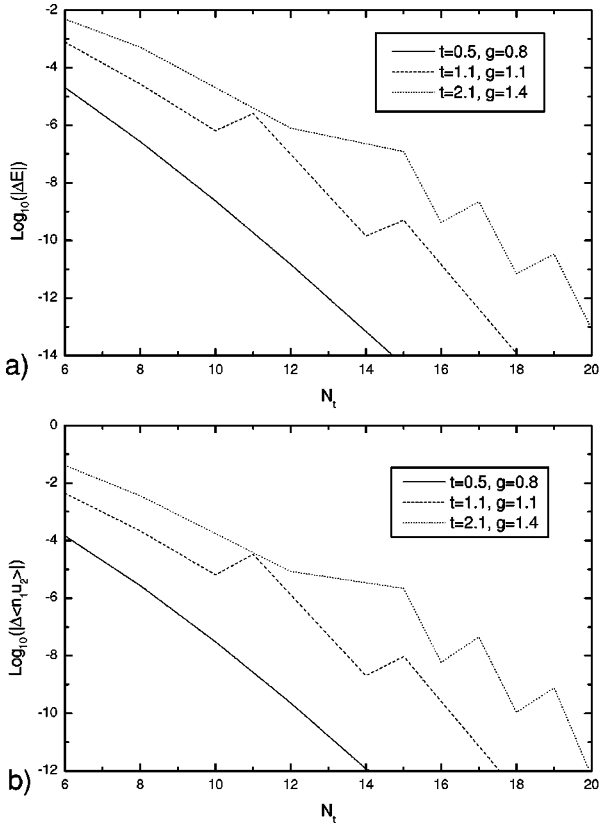

FIG. 4. Logarithmic error versus truncation order for the ground state with $(t/\omega_0=0.5,\ g=0.8)$, $(t/\omega_0=1.1,\ g=1.1)$, and $(t/\omega_0=2.1,\ g=1.4)$. (a) Logarithmic error for energy $\ln(|\Delta E|)$, (b) logarithmic error for the correlation function $\ln(|\Delta\langle n_1u_2\rangle|)$.

show a more abrupt crossover in the adiabatic region (larger t), though the coupling strength for the crossover is larger than that for smaller t. All polarons are localized with sufficiently strong e-ph coupling. There is no unique quantitative criterion for the crossover from a delocalized to localized polaron. A plausible criteria is with the coupling strength g_0, at which $\langle n_1(u_1-u_2)\rangle/g_0$ reaches half of its maximum value. That is, $-\langle n_1(u_1-u_2)\rangle/g_0=1$. In this sense, all polarons in the antiadiabatic limit, with $t/\omega_0\leqslant 0.5$, are localized ones for any e-ph coupling strength. The crossover coupling strength is about 0.9 and 1.4 for $t/\omega_0=1.1$ and $t/\omega_0=2.1$, respectively.

It is worth noting that the correlation functions are sensitive to the high-order correlation effects. Though it is not difficult for our CE method to provide accurate results for any combination of t and g, they are not easy to calculate accurately by other analytical approximation methods, especially when t is large. For comparison, the fifth-order perturbation MLF results are also plotted in Fig. 3(b).[12] For $t/\omega_0=0.5$, the results by the fifth-order perturbation MLF method are virtually the same as ours in the whole coupling range. For $t/\omega_0=1.1$ and 2.1, the fifth-order perturbation MLF also gives very accurate results in both strong- and weak-coupling regions. However, in the intermediate-coupling region, the fifth-order perturbation MLF results deviate from the accurate ones. The deviation is most significant for $t/\omega_0=2.1$ in the vicinity of the crossover from a delocalized to a localized polaron. The good energy results by the perturbation MLF are due to the fact that higher-order corrections are successively smaller in magnitude and are of alternate signs, resulting in a fast converging perturbation series. However, this is not the case for the correlation functions in the intermediate-coupling region. Therefore, a convergent energy does not necessarily mean convergent correlation functions. In the CE method, however, the wave function (expansion coefficients) is determined accurately, resulting in accurate correlation functions. Figure 4 shows the logarithmic errors of the ground-state energy $\ln(|\Delta E|)$ and the correlation function $\ln(|\Delta(\langle n_1u_2\rangle)|)$ calculated by different truncation orders n_t for $(t/\omega_0=0.5,\ g=0.8)$, $(t/\omega_0=1.1,\ g=1.1)$, and $(t/\omega_0=2.1,\ g=1.4)$, which are representative $(t,\ g)$ combinations of the slowest convergency in the perturbation MLF method. Clearly, all the CE energies and correlation functions converge very rapidly, and the machine accuracy for $(t/\omega_0=0.5,\ g=0.8)$ can be achieved easily.

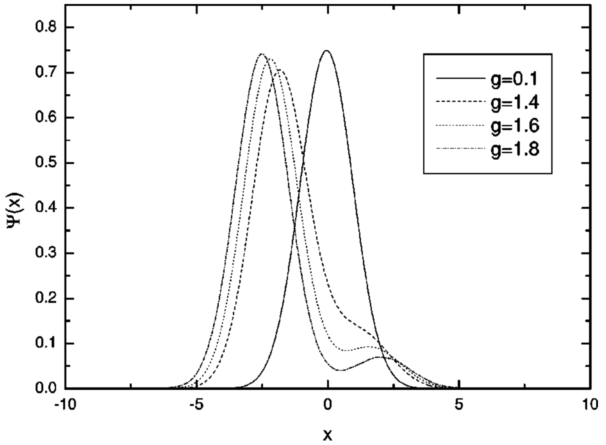

FIG. 5. Ground-state wave function for $t/\omega_0=1.1$ system with $g=0.1$, 1.4, 1.6, and 1.8.

The ground-state wave functions for the d oscillator as a function of $x=(u_1-u_2)/\sqrt{2}$ for different values of the e-ph coupling strength when the electron is located at site 1 are plotted in Fig. 5 for $t/\omega_0=1.1$. For a weak e-ph coupling $(g=0.1)$, the electron rapidly hops between the two molecular sites without inducing a local deformation. The ground-state wave function shows a Gaussian-like behavior centered near $x=0$. As g increases, the center position of the wave function shifts towards $x<0$ gradually, and a shoulder at $x>0$ develops and becomes apparent at around $g=1.3$–1.4. This indicates that a significant polaronic effect sets in and the correlations between the position of the electron and the deformation on the sites become strong. The growth of the shoulder as g increases also illustrates the enhancement of the retardation effects between the motion of the electron and the molecular deformation created by the electron. The results agree completely with the known fact.[12,18]

To summarize, we have demonstrated that an analytical method, i.e., the coherent-state expansion method, can provide the exact solutions for the two-site Holstein model. Although the achievement is so far limited to a two-site system, we hope it would facilitate better progress for analytical studies of many-site systems. It is worth noting that the CE method with truncations up to the third order has been successfully used to find solutions of some e-ph coupling problems.[22–24] We expect that the CE method with a suitable order of correlation effects can be applied to a variety of e-ph coupling systems, and it provides a promising alternative to the variational and perturbation methods.

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