A comparison of perturbative expansions using different phonon basis for two-site Holstein model

Jayita Chatterjee and A. N. Das

Saha Institute of Nuclear Physics
1/AF Bidhannagar, Calcutta 700064, India

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Abstract

The two-site single-polaron problem is studied within the perturbative expansions using different standard phonon basis obtained through the Lang Firsov (LF), modified LF (MLF) and modified LF transformation with squeezed phonon states (MLFS). The role of these convergent expansions using the above prescriptions in lowering the energy and in determining the correlation functions are compared for different values of coupling strength. The single-electron energy, oscillator wave functions and correlation functions are calculated for the same system. The applicability of different phonon basis in different regimes of the coupling strength as well as in different regimes of hopping are also discussed.

* e-mail: moon@cmp.saha.ernet.in
† e-mail: atin@cmp.saha.ernet.in
1. Introduction

The Holstein model [1] is one of the fundamental models describing the interactions of conduction electrons with lattice vibrations. The model in the simplest form consists of one electron hopping term, dispersionless phonons and an interaction term which couples the electron density and ionic displacements at a given site. The interaction term favours localization of the electron. When the interaction is strong, the gain in the localization energy outweighs the kinetic energy of the electron and a self-trapping of the electron (or a hole as the case may be) occurs with the creation of lattice deformation in the immediate vicinity of the charge carrier. The motion of the electron is then accompanied by the lattice deformation which results in a reduced effective hopping of the dressed electron (polaron). In the antiadiabatic limit, where the phonon frequency ($\omega_0$) is greater than the electronic hopping integral ($t$), the confinement of the lattice deformation around the charge carrier is very local for large electron-phonon (e-ph) interaction. This gives rise to small polarons whose nature and dynamics is generally studied using the Lang-Firsov (LF) method based on the canonical LF transformation [2]. Recently, Ranninger and Thibblin [3] and de Mello and Ranninger [4] studied a two-site Holstein model using the numerical diagonalization technique and obtained non trivial results which are difficult to understand from the classical zero phonon averaging LF approach. In fact, in Ref. [4] the authors expressed doubts regarding the applicability of the LF approach and validity of the strong coupling perturbation expansion (in hopping) even in the strong coupling antiadiabatic limit where it is believed to be valid. Considering a similar two-site system Firsov and Kudinov [5] studied the energy levels and the wave functions of the system within the perturbation theory and concluded that the results are consistent with the exact numerical results obtained in Refs. [3] and [4] for large e-ph coupling strength and small hopping. Marsiglio [6] studied the Holstein model in one dimension with one electron up to 16 site lattices using numerical diagonalization technique
and concluded that neither the Migdal nor the usual small-polaron approximation is in quantitative agreement with the exact results for intermediate coupling strength. Kabanov and Ray and Alexandrov et al. performed the exact numerical diagonalization of two, four and six sites with one electron and observed that for \( t > \omega_0 \) the adiabatic Holstein small-polaron approximation, whereas for \( t < \omega_0 \) the LF approach describes the ground state energy of the system accurately except for a region of intermediate coupling strength. So no single conventional analytical method at present is known to us so as to describe the Holstein model for the entire range of the coupling strength either in the adiabatic or in the antiadiabatic limit. In a recent work we addressed this problem and considering a two-site system we developed a perturbation expansion using modified LF phonon basis. We calculated the perturbation corrections to the ground state energy and wave function up to the third and second order respectively. The results obtained thereby are in good agreement with the exact numerical results for the entire range of the coupling strength for the intermediate value of hopping (\( t \sim \omega_0 \)).

In this paper we have extended our previous work by calculating up to fifth order perturbation correction to the wave function and sixth order correction to the energy for the ground state of the two-site single polaron system using various standard phonon basis obtained through the LF, modified LF (MLF) and modified LF with squeezing transformations (MLFS). It may be mentioned that the role of squeezing is believed to be important for intermediate coupling and hopping regime and studies on a two-site and a four-site Holstein model using the MLFS transformation followed by zero phonon averaging show that the energy obtained within such method is very close to the exact result.

In the LF approach a phonon basis of fixed displacement at the electron residing site is chosen. Such a choice of basis diagonalizes the Holstein hamiltonian in absence of hopping. The hopping term is then treated as a perturbation. The perturbation
series is naturally expected to converge when hopping is weak and the e-ph coupling is strong. However, it is not precisely known the limit of the coupling strength as a function of hopping beyond which the LF approach is valid. Within the LF approach in the zeroth order of perturbation the effect of retardation between the electron and the lattice deformation produced by the electron cannot be obtained. Such a retardation becomes very important with smaller e-ph coupling strength and larger hopping. The phonon basis chosen in the MLF or MLFS approach have variational displacements and can produce the retardation effect even in the zeroth order of perturbation [12,14]. The ground state energy predicted within the MLF and MLFS method in the zeroth order of perturbation is much lower than that within the LF approach [13] except for large values of the coupling strength, where all the methods become equivalent. All these suggest that the MLF or MLFS phonon wave functions are proper choices for perturbative calculation when hopping is appreciable and the coupling strength is not very high. For weak hopping and large values of the coupling strength the MLF or MLFS phonon wave function reduces to that of the LF approach. Thus the perturbation methods based on the MLF and the MLFS phonon wave functions have the potentiality to be applicable for a wide range of the coupling strength.

The objective of this work is to develop perturbative expansions for the two-site single polaron system using phonon basis obtained through the LF, MLF and MLFS transformations and investigate the convergence of the perturbation series for different physical quantities of interest as a function of the e-ph coupling strength and hopping. Such study would provide direct answers to the important questions as (i) what is the region of e-ph coupling strength where the LF method is valid, (ii) whether the MLF and MLFS phonon wave functions are better than the LF wave function in the zeroth order of perturbation, (iii) in which region MLF and MLFS methods give better results than the LF method, (iv) which method within a few orders (one or
two) of perturbation could predict results closer to the exact one.

In Sec. II we define the model hamiltonian and describe different variational phonon basis states that we have considered. In sec. III we present the expressions for the energy, wave function and static correlation functions calculated within the perturbation theory for the ground state. In Sec. IV we shall present the results obtained by different methods and discuss about the convergence of the perturbation series, hence the applicability of the methods in different regions of the e-ph coupling strength for different values of hopping.

II. Formalism

The two-site single-polaron Hamiltonian is

\[
H = \sum_{i,\sigma} \epsilon n_{i\sigma} - \sum_{\sigma} t (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + g \omega_0 \sum_{i,\sigma} n_{i\sigma} (b_i + b_i^\dagger) + \omega_0 \sum_i b_i^\dagger b_i
\]

where \(i = 1, 2\), denotes the site. \(c_{i\sigma} (c_{i\sigma}^\dagger)\) is the annihilation (creation) operator for the electron with spin \(\sigma\) at site \(i\) and \(n_{i\sigma} (=c_{i\sigma}^\dagger c_{i\sigma})\) is the corresponding number operator, \(g\) denotes the on-site e-ph coupling strength, \(t\) is the usual hopping integral. \(b_i\) and \(b_i^\dagger\) are the annihilation and creation operators, respectively, for the phonons corresponding to interatomic vibrations at site \(i\), \(\omega_0\) is the phonon frequency. The hamiltonian (1) has spin degeneracy, hence for the one electron case the spin index is redundant. So spin indices are dropped in the following.

Introducing new phonon operators \(a = (b_1 + b_2)/\sqrt{2}\) and \(d = (b_1 - b_2)/\sqrt{2}\) the Hamiltonian is separated into two parts \((H = H_d + H_a)\) :

\[
H_d = \sum_i \epsilon n_i - t (c_1^\dagger c_2 + c_2^\dagger c_1) + \omega_0 g_+ (n_1 - n_2) (d + d^\dagger) + \omega_0 d^\dagger d
\]

and

\[
H_a = \omega_0 \tilde{a}^\dagger \tilde{a} - \omega_0 n^2 g_+^2
\]
where \( g_+ = g / \sqrt{2} \), \( \tilde{a} = a + ng_+ \) and \( \tilde{a}^\dagger = a^\dagger + ng_+ \).

\( \tilde{H}_a \) describes a shifted oscillator which couples only with the total number of electrons \( n (= n_1 + n_2) \), which is a constant of motion. The last term in Eq.(3) represents lowering of energy achieved through the lattice deformations of sites 1 and 2 by the total number of electrons.

\( \tilde{H}_d \) represents an effective e-ph system where phonons directly couple with the electronic degrees of freedom and its solution by any analytical method is a non trivial problem. We now use the MLF transformation where the lattice deformations produced by the electron are treated as variational parameters \([12,14,17]\). For the present system,

\[
\tilde{H}_d = e^R H_d e^{-R}
\]

where \( R = \lambda(n_1 - n_2)(d^\dagger - d) \), \( \lambda \) is a variational parameter related to the displacement of the \( d \) oscillator.

The transformed Hamiltonian is then obtained as

\[
\tilde{H}_d = \omega_0 d^\dagger d + \sum_i \epsilon_p n_i - t [c_1^\dagger c_2 \exp(2\lambda(d^\dagger - d)) \\
+ c_2^\dagger c_1 \exp(-2\lambda(d^\dagger - d))] + \omega_0(g_+ - \lambda)(n_1 - n_2)(d + d^\dagger)
\]

where

\[
\epsilon_p = \epsilon - \omega_0(2g_+ - \lambda)\lambda
\]

For a perturbation method it is desirable to use a basis where the major part of the hamiltonian becomes diagonal. When the hopping is appreciable a retardation between the electron and associated lattice distortion sets in and as mentioned before the MLF or the MLFS method would work better than the LF method for a wide region of e-ph coupling strength.

Now we will make a squeezing transformation \([18]\) to the Hamiltonian (5)

\[
\tilde{H}_{sd} = e^S \tilde{H}_d e^{-S}
\]
where \( S = \alpha (d_i d_i - d_i^\dagger d_i^\dagger) \). The new phonon basis is squeezed with respect to the previous basis. Squeezing parameter \((\alpha)\) partly reduces the polaronic narrowing effect and consequently enhances the hopping. However, the phonon energy increases with increasing \( \alpha \) and a competition between phonon energy and hopping delocalization (kinetic) energy determines the value of \( \alpha \) \[^{13}\]. The transformed hamiltonian (7) takes the form

\[
\tilde{H}_{sd} = \omega_0 d^\dagger d [\cosh^2(2\alpha) + \sinh^2(2\alpha)] + \omega_0 \cosh(2\alpha) \sinh(2\alpha)(d d + d^\dagger d^\dagger) \\
+ \sum_i \epsilon_p n_i - t[c_1^\dagger c_2 \exp(2\lambda_e(d^\dagger - d)) + c_2^\dagger c_1 \exp(-2\lambda_e(d^\dagger - d))] \\
+ \omega_0 (g_+ - \lambda)(n_1 - n_2)(d + d^\dagger) \exp(2\alpha) + \omega_0 \sinh^2(2\alpha)
\]

(8)

where \( \lambda_e = \lambda e^{-2\alpha} \)

(9)

For the single polaron problem we choose the basis set

\[
|\pm, N\rangle = \frac{1}{\sqrt{2}}(c_1^\dagger \pm c_2^\dagger)|0\rangle_e |N\rangle
\]

(10)

where |\(+\rangle\) and |\(-\rangle\) are the bonding and antibonding electronic states and \(|N\rangle\) denotes the \(N\)th excited oscillator state in the MLFS, MLF or LF basis depending on the method considered. It may be noted that the MLFS basis turns into the MLF basis if one puts \( \alpha = 0 \) and the MLF into the LF basis when \( \lambda = g_+ \).

The hopping term \( H_t \) in Eq. (8) has both diagonal and nondiagonal matrix elements in the chosen basis (10). The diagonal part of \( H_t \) is given by

\[
\langle N, \pm | H_t | \pm, N \rangle = \langle N, \pm | - t[c_1^\dagger c_2 \exp(2\lambda_e(d^\dagger - d)) + c_2^\dagger c_1 \exp(-2\lambda_e(d^\dagger - d))] |\pm, N \rangle \\
= \mp t e^{N} \sum_{i=0}^{N} \left[ \frac{(2\lambda_e)^2i}{i!}(-1)^i N_C_i \right]
\]

(11)

where \( t_e = t \exp(-2\lambda_e^2) \) and \( N_C_i = \frac{N!}{i!(N-i)!} \).

For the perturbation method we consider the diagonal part of the Hamiltonian (8) as the unperturbed Hamiltonian \( (H_0) \) and the remaining part of the Hamiltonian, \( H_1 = \tilde{H}_{sd} - H_0 \), as a perturbation.
The unperturbed energy of the state $|\pm, N\rangle$ is given by
\[
E_{\pm,N}^{(0)} = \langle N, \pm|H_0|\pm, N\rangle = \omega_0[\sinh^2(2\alpha) + N(\sinh^2(2\alpha) + \cosh^2(2\alpha))] \\
+ \epsilon_p \mp t_e \left[ \sum_{i=0}^{N} \frac{(2\lambda_e)^{2i}}{i!} (-1)^i N_i \right] 
\]  
(12)

The general off-diagonal matrix elements of $H_1$ between the two states $|\pm, N\rangle$ and $|\pm, M\rangle$ are calculated as (for $(N - M) > 0$)

\[
\langle N, \pm|H_1|\pm, M\rangle = P(N, M) + \frac{\omega_0}{2} \sqrt{N(N - 1)} \sinh(4\alpha) \delta_{N,M+2} 
\]  
for even $(N - M)$.

\[
\langle N, \pm|H_1|\mp, M\rangle = P(N, M) + \sqrt{N} \omega_0 (g_+ - \lambda) e^{2\alpha} \delta_{N,M+1} 
\]  
for odd $(N - M)$.

where

\[
P(N, M) = \mp t_e (2\lambda_e)^{N-M} \frac{\sqrt{N!}}{M!} \left[ \frac{1}{(N-M)!} + \sum_{R=1}^{M} (-1)^R \frac{(2\lambda_e)^{2R}}{(N-M+R)!R!} M(M-1)...(M-R+1) \right] 
\]

III. Perturbation corrections to the ground state

In this section we present the calculations of the perturbation corrections to the ground-state energy and wave function up to the sixth and fifth order, respectively using the LF, MLF and MLFS methods. The static correlation functions relating the electron and associated lattice deformations are also calculated using the corresponding perturbed wavefunctions.

For the chosen basis (10) the state $|+\rangle|0\rangle$ has the lowest unperturbed energy, $E_0^{(0)} = \epsilon_p - t_e + \omega_0 \sinh^2(2\alpha)$. The matrix element connecting this ground state and an excited state $|e, N\rangle$ is given by

\[
\langle N, e|H_1|+, 0\rangle = \left[ \frac{-t_e (2\lambda_e)^N}{\sqrt{N!}} + \omega_0 (g_+ - \lambda) e^{2\alpha} \delta_{e,1} \right] \delta_{e,-} \text{ for odd } N 
\]  
(15)

\[
= \left[ \frac{-t_e (2\lambda_e)^N}{\sqrt{N!}} + \sqrt{2} \omega_0 \sinh(2\alpha) \cosh(2\alpha) \delta_{N,2} \right] \delta_{e,+} \text{ for even } N 
\]
The first order correction to the ground state wave function is obtained as,

\[ |\psi_0^{(1)}\rangle = \frac{[\omega_0 (g+ - \lambda) e^{2\alpha} - 2\lambda e^{t_e}]}{(E_0^{(0)} - E_{+1}^{(0)})} |-, 1\rangle + \frac{[-t_e (2\lambda e)^2 + 2\omega_0 \sinh(2\alpha) \cosh(2\alpha)]}{\sqrt{2!} (E_0^{(0)} - E_{+2}^{(0)})} |+, 2\rangle \]

\[ - \sum_{N=3,4,5,..} t_e (2\lambda e)^N \sqrt{N!} |e, N\rangle \]  

(16)

where \( E_{\pm,N}^{(0)} \) is the unperturbed energy of the state \(|\pm, N\rangle\) as given in Eq.(12) and \( e = + \) or - for even and odd \( N \) respectively.

The first order correction to the energy \( (E_0^{(1)}) \) is zero since \( H_1 \) has no diagonal matrix element. The second order correction to the ground state energy is given by

\[ E_0^{(2)} = + \sum_{N=1,3..} \frac{|t_e (2\lambda e)^N|}{\sqrt{N!} (E_0^{(0)} - E_{e,N}^{(0)})} \left( \frac{\omega_0 (g+ - \lambda) e^{2\alpha} \delta_{N,1}}{|E_0^{(0)} - E_{-,N}^{(0)}|} \right)^2 \]

\[ + \sum_{N=2,4..} \frac{|t_e (2\lambda e)^N|}{\sqrt{N!} (E_0^{(0)} - E_{+,N}^{(0)})} \left( \frac{\sqrt{2} \omega_0 \sinh(2\alpha) \cosh(2\alpha) \delta_{N,2}}{|E_0^{(0)} - E_{-,N}^{(0)}|} \right)^2 \]  

(17)

Now one has to make a proper choice of \( \lambda \) and \( \alpha \) so that the perturbative expansion becomes convergent. Usually, within the MLF and MLFS approach zero phonon averaging is made [12,14] and the variational parameters \( \lambda \) and \( \alpha \) are found out by minimizing the ground state energy of the system. This corresponds to the minimization of the unperturbed energy in our calculation. Previously we have followed this procedure within the MLF approach [10] and found that the perturbation corrections to the energy converge rapidly. Here we will follow the same procedure to find out the variational phonon basis as a function of e-ph coupling for the MLF and MLFS methods. Minimizing the unperturbed ground state energy \( E_0^{(0)} \) with respect to \( \lambda \) and \( \alpha \) we obtain

\[ \lambda = \frac{\omega_0 g_+}{\omega_0 + 2t_e e^{-4\alpha}} \]

\[ \alpha = \frac{1}{4} \sinh^{-1} [2\alpha (g_+ - \lambda)] \]

It is interesting to note that these choices of \( \lambda \) and \( \alpha \) make the offdiagonal matrix elements between the states \(|+, 0\rangle\) to \(|-, 1\rangle\) and \(|+, 2\rangle\) equal to zero and consequently,
the coefficients of \(|-1, 1\) and \(|+2, 2\) in Eq. (16) and the terms corresponding to \(N = 1, 2\) in the r.h.s of Eq. (17) vanish. Since the first two terms in Eq. (16) are zero for the MLFS choice of the basis it is expected that the first order correction to the ground state wave function and second order correction (Eq. 17) to the energy would be smaller within the MLFS method. To examine the validity of the perturbation procedure one should calculate the higher order corrections and check whether the series is converging properly.

The second order corrections to the ground state wave function is given by

\[
|\psi^{(2)}_0\rangle = \sum_{k \neq 0} a^{(2)}_{0k} |k\rangle
\]

where \(a^{(2)}_{0k} = \sum_{m \neq 0} \left[ \frac{(H_1)_{km}(H_1)_{m0}}{(E_0^{(0)} - E_k^{(0)})(E_0^{(0)} - E_m^{(0)})} \right] \)

where \(|k\rangle\)'s denote the unperturbed states \(|\pm, N\rangle\) with the unperturbed energy \(E_{\pm, N}^{(0)}\) and the 0 refers to the ground state \(|+0\rangle\). \((H_1)_{km}\) is the off-diagonal matrix element of \(H_1\) between the states \(|k\rangle\) and \(|m\rangle\). These matrix elements are given in Eqs. (13) and (14). The third order correction \(E^{(3)}_0\) to the ground state energy is given by,

\[
E^{(3)}_0 = \sum_{k \neq 0} (H_1)_{0k} a^{(2)}_{0k}
\]

In general the nth order correction to the wave function and the \((n+1)\)th order correction to the energy are given by

\[
|\psi^{(n)}_0\rangle = \sum_{k \neq 0} a^{(n)}_{0k} |k\rangle
\]

\[
E^{(n+1)}_0 = \sum_{k \neq 0} (H_1)_{0k} a^{(n)}_{0k}
\]

where

\[
a^{(n)}_{0k} = \frac{1}{(E_0^{(0)} - E_k^{(0)})} \left[ -E_0^{(1)} a^{(n-1)}_{0k} - E_0^{(2)} a^{(n-2)}_{0k} - E_0^{(3)} a^{(n-3)}_{0k} - \ldots \ldots - E_0^{(n-1)} a^{(1)}_{0k} + \sum_{m \neq 0} \left[ (H_1)_{km} a^{(n-1)}_{0m} \right] \right]
\]
Using Eqs. (20) and (21) all the higher order corrections to the wave function and energy may be calculated step by step.

The ground state wave function may be written as,

\[ |\psi_G\rangle \equiv |+, 0\rangle + |\psi_0^{(1)}\rangle + |\psi_0^{(2)}\rangle + |\psi_0^{(3)}\rangle + \ldots \]

\[ = |+, 0\rangle + \sum_{N=1,3,\ldots} c_N|-, N\rangle + \sum_{N=2,4,\ldots} c_N|+, N\rangle \]  

(23)

The coefficients \(c_N\) are determined from the sum of the corresponding coefficients \(a_1^{(1)}\), \(a_2^{(1)}\), \(a_3^{(1)}\), etc., where \(N\) represents the state \(|k\rangle\). The normalized ground state wave function \(|\psi_G\rangle_N\) is

\[ |\psi_G\rangle_N = \frac{1}{\sqrt{N_G}} |\psi_G\rangle \]

where \(N_G\) is obtained as

\[ N_G \equiv \langle \psi_G | \psi_G \rangle = 1 + \sum_{N=1,3,\ldots} c_N^2 \]

- Correlation function

The static correlation functions \(\langle n_1 u_1 \rangle_0\) and \(\langle n_1 u_2 \rangle_0\), where \(u_1\) and \(u_2\) are the lattice deformations at sites 1 and 2 respectively, produced by an electron at site 1, are the standard measure of polaronic character and indicate the strength of polaron induced lattice deformations and their spread. The operators involving the correlation functions may be written as

\[ n_{1,2} = \frac{n_1}{2} [(a + a^\dagger) \pm (d + d^\dagger)e^{2\alpha} - 2 (n g_+ \pm \lambda (n_1 - n_2))] \]

(24)

The final form of the correlation functions are obtained as

\[ \langle n_1 u_1 \rangle_0 = \frac{1}{2} \left[ -(g_+ + \lambda) + \frac{A_0 e^{2\alpha}}{N_G} \right] \]

\[ \langle n_1 u_2 \rangle_0 = \frac{1}{2} \left[ -(g_+ - \lambda) - \frac{A_0 e^{2\alpha}}{N_G} \right] \]

(25)

where \(A_0 \equiv \langle \psi_G | n_1 (d + d^\dagger) | \psi_G \rangle = \sum_{N=1,3,5,\ldots} c_N \left[ \sqrt{N} c_{N-1} + \sqrt{N+1} c_{N+1} \right] \)
IV. Results and discussions

In this paper we present the results for \( t=0.5, 1.1 \) and 2.1 (in a scale of \( \omega_0 =1 \)). These values of \( (t/\omega_0) \) covers the cross-over region from the antiadiabatic to the adiabatic limits. Furthermore, exact results on some of the physical quantities are available for the above values of \( (t/\omega_0) \) which enables us to compare our results obtained within the perturbation methods with the exact results.

We estimate the perturbation corrections to the ground state energy and wave function up to the sixth and fifth orders respectively, within the LF, MLF and MLFS methods considering 25 phonon states (which is sufficient for \( g_+ \leq 2.2 \)) in the transformed phonon basis. Calculations of such successive orders of corrections would provide us the key features of the convergence of the perturbation series and the applicability of the method concerned.

For \( (t/\omega_0) = 0.5 \) we find a rapid convergence in the perturbation series for the ground state energy for all values of \( g_+ \). Fig. 1 shows the relative perturbation corrections i.e., the ratios of the perturbation corrections (to the ground state energy) of different orders to the unperturbed energy as a function of \( g_+ \). The energy corrections within the MLFS and the MLF methods are much smaller than that within the LF method for \( g_+ < 1.6 \). For \( (t/\omega_0) = 0.5 \) the fifth or sixth order correction to the energy is so small that the energy obtained with fifth or sixth order of perturbation within MLF method may be treated as the exact energy for all values of \( g_+ \). In Fig.2(a) we plot the exact energy thus obtained along with the unperturbed energies within different methods. It is seen that the MLFS or the MLF unperturbed energies are closer to the exact one than the LF unperturbed energy. In Fig. 2(b) we show the variation of \( |\langle \psi_0^{(0)} | \psi_G \rangle|^2 \), which gives the probability that the perturbed ground state \( (|\psi_G\rangle) \) lies in the unperturbed ground state \( |\psi_0^{(0)}\rangle \), with \( g_+ \) (\( |\psi_G\rangle \) is found out considering up to the fifth order correction to the wave function). This probability is closer to 1 for the MLFS and the MLF methods compared to that in the LF method. The results of Fig.
2 clearly indicate that the phonon basis, chosen within the MLFS or the MLF methods, are much better than the LF basis. It may be mentioned that the correlation function \( \langle n_1u_2 \rangle_0 \), which is a measure of the lattice deformation at site 2 produced by an electron at site 1 due to retardation effect vanishes for the LF unperturbed state. This correlation function is very sensitive to the higher order perturbation corrections to the wave function than the ground state energy. To examine the convergence of the perturbative expansion on this correlation function we plot \( \langle n_1u_2 \rangle_0 \), calculated up to different orders of perturbation corrections, as a function of \( g_+ \) in Fig. 3. It is found that for \( (t/\omega) = 0.5 \) this correlation function converges for all values of \( g_+ \). The curves corresponding to the correlation function calculated up to fourth and fifth order corrections to the wave function almost merge together (Fig.3) and specially for the MLF method they are almost identical in the entire region of \( g_+ \). Hence, the correlation function obtained considering up to the fifth order correction within the MLF method, may be considered as the exact one for \( (t/\omega) = 0.5 \). Fig. 3 also shows that even in the strong coupling limit one has to consider up to the second order corrections to the wave function to obtain (nearly) exact results. It is interesting to note that the MLF and the MLFS methods can predict non zero values of \( \langle n_1u_2 \rangle_0 \) even in the zeroth order of perturbation (i.e. with the unperturbed ground state wave function in the MLF or MLFS basis) for low and intermediate values of \( g_+ \) whereas the unperturbed LF wave function always predicts zero value for \( \langle n_1u_2 \rangle_0 \) and we find that in an appreciable region of low values of \( g_+ \) the predictions of the MLFS method with zeroth order of perturbation is very close to the exact one.

In Figs. 4-8 we have shown the results for \( t/\omega = 1.1 \) which is in between the adiabatic and antiadiabatic limits. In Fig. 4 the relative perturbation corrections to the unperturbed energy are plotted as a function of \( g_+ \). The perturbation corrections in energy are smaller within the MLF and MLFS than the LF method. For each method there is a range of \( g_+ \) where higher order corrections are appreciable and the
convergence is weak. For $t/\omega_0 = 1.1$ the range of $g_+$ where the convergence is weaker, is $0.4-1.2$ for the LF, $1-1.3$ for the MLF and $1.1-1.55$ for the MLFS method. For values of $g_+$ outside this range the perturbation corrections show rapid convergence. In the MLF method the perturbation corrections show satisfactory convergence in the entire region of $g_+$, while for the LF and MLFS methods there are small regions of $g_+$ where fifth or sixth order corrections are comparable or greater than the third and fourth order corrections and the convergence is not satisfactory in that region. The ground state energy calculated within the MLF method considering up to the sixth order correction, is shown in Fig. 5 as a function of $g_+$. This energy when compared with the exact results of Ref. [3], is found to be almost identical with the exact one. This is expected because the higher order corrections are successively smaller in magnitude and of alternate sign within the MLF method, so the net contributions from seventh to higher order terms to the energy would be negligibly small with respect to the unperturbed energy. The unperturbed ground state energy for the LF, MLF and the MLFS methods are also shown in the same figure. The MLFS unperturbed energy is closer to the exact energy and for low values of $g_+$ it is almost identical to the exact energy.

In Fig. 6 we plot the correlation function $\langle n_1 u_2 \rangle_0$ obtained by considering up to the different orders of perturbation corrections to the wave function against $g_+$. The MLFS method shows excellent convergence for low values of $g_+$ ($\leq 0.9$), the LF method shows very good convergence beyond $g_+ = 1.2$. The MLF method shows good convergence for the entire region of $g_+$, however the convergence is weaker in the range $0.9 \leq g_+ < 1.3$. When compared with exact results of $\langle n_1 u_2 \rangle_0$ (taken from the Ref. [3]), it is found that the MLF results up to the fifth order perturbation are identical to the exact results except in the region $0.9 < g_+ < 1.3$ where a slight departure in values from the exact results is seen. The correlation function $\langle n_1 u_1 \rangle_0$ would evidently show a much more rapider convergence than the convergence of $\langle n_1 u_2 \rangle_0$. 
To examine the nature of the cross-over from the delocalized (large) to localized (small) polaron we plot $\langle n_1(u_1 - u_2)\rangle_0/g_+$ against $g_+$ in Fig. 7 where the (nearly) exact plot (obtained from the MLF considering up to fifth order corrections to the wave function) and those obtained from the MLF and MLFS in the zeroth order of perturbations are shown. The standard LF approximation (zeroth order of perturbation or zero phonon averaging) always predicts the value of this quantity to be equal to 1, which is a characteristic of extremely localized polarons, and so a cross-over from small to large polaron cannot be obtained in the standard LF approximation. The MLF and MLFS methods can predict this cross-over even in the zeroth order of perturbation [12,14,15]. It may be mentioned that the value of $\langle n_1(u_1 - u_2)\rangle_0/g_+$ within MLF and MLFS methods in the zeroth order of perturbation is $\lambda/g_+$ (Eq. (25)). Fig. 7 shows that up to $g_+ = 1.0$ the results of MLFS with zero phonon averaging almost coincides with the exact results. The (nearly) exact plot shows a smooth cross-over from the delocalized to localized polaron with increase of $g_+$, whereas the zero phonon averaging results within MLF or MLFS procedure shows an abrupt feature which were noted before [12,14,15]. Löwen [20] pointed out that for a finite phonon frequency there cannot be any abrupt cross-over in the ground state of an e-ph system. The (nearly) exact plot of Fig. 7 is consistent with this conclusion.

In Fig. 8 we have shown the ground state wave function (within the MLF method considering up to fifth order correction to the wave function) for the $d$ oscillator as a function of position $x$ for different values of the e-ph coupling when the electron is located at site 1. For weak coupling the wave function shows displaced Gaussian like single peak. For intermediate values of $g_+$ an additional prominent shoulder appears in the wave function as seen in the curve for $g_+ = 1.3$. For higher values of $g_+$ this shoulder takes the form of a broad peak. These results are completely consistent with the results obtained by Ranninger and Thibblin by exact diagonalization study [3].

In Figs. 9-12 we have given the results of $t/\omega_0 = 2.1$, which is towards the adiabatic
limit where the LF method is not expected to work in this region. So it would be of general interest to examine whether the methods, dealt in this paper, show good convergence in any region of \( g_+ \). In Fig. 9 the relative perturbation corrections of different orders to the ground state energy are shown as a function of \( g_+ \). The figure shows that the perturbation corrections within the LF method are very large and do not converge at all in an appreciable region of \( g_+ \) (0.6-1.25). For the MLF and MLFS methods the perturbation corrections in energy are much smaller. The MLF method shows good convergence except in a region of 1.2 \( < g_+ < 1.6 \). For the MLFS method the corrections are negligible in a wide region of \( g_+ \) (0 \( < g_+ < 1.1 \)). However, in a region 1.25 \( < g_+ < 1.7 \) the perturbation corrections within the MLFS do not converge. For \( g_+ > 1.4 \) the convergence within the LF method is satisfactory and hence may be used.

In Fig. 10 we show the variation of \( |\langle \psi_0^{(0)} | \psi_G \rangle| \) with \( g_+ \) for different methods. The figure shows that for \( t/\omega_0 = 2.1 \) this value within the LF method is far from 1.0 for a broad region of \( g_+ \) (0.4–1.3) which signifies that the LF method is totally inapplicable in that region. However, in the same region the value of \( |\langle \psi_0^{(0)} | \psi_G \rangle| \) within the MLFS is close to 1 and thus MLFS should work exceedingly well there.

In Fig. 11 the convergence of the correlation function \( \langle n_1 u_2 \rangle_0 \) is shown. It is clearly found that the MLFS method shows excellent convergence for low values of \( g_+ \) (\( \leq 1.2 \)), the LF method shows good convergence beyond \( g_+ = 1.5 \). The MLF method shows a systematic good convergence for the entire region of \( g_+ \), however the convergence is weaker in an intermediate region of \( g_+ \).

In Fig. 12 the ground state phonon wave functions, evaluated by considering up to the fifth order perturbation correction within the MLF and LF methods, are shown for the \( d \) oscillator as a function of position \( x \) for \( g_+ = 1.6 \) and for different values of \( t/\omega_0 \) (0.5, 1.1, 2.1), when the electron is located at site 1. The LF and the MLF predictions are identical and hence cannot be distinguished in the plot.
These plots also exactly match with the phonon wave functions, calculated with exact diagonalization technique [4], for the corresponding set of parameters. The reason for such excellent agreement with the exact results is that for \( g_+ = 1.6 \) and for \( t/\omega_0 = 0.5, 1.1 \) and \( 2.1 \), a very good convergence is achieved in the wave function within the LF and MLF methods which is evident from Figs. (3), (6) and (11).

V. Conclusions

In the present work we examine the convergence of the perturbation expansions using the LF, MLF and MLFS phonon basis for a two-site one electron Holstein model for three values of \( t/\omega_0 \) (0.5, 1.1 and 2.1). For \( t/\omega_0 = 0.5 \) the perturbation series show very good convergence within all the three methods in the entire region of e-ph coupling strength. The perturbation corrections within the MLF and MLFS methods are much smaller than that of the LF method. For higher values of \( t/\omega_0 \) also good convergence is achieved for the major region of \( g_+ \). The perturbation expansion shows weak or bad convergence in an intermediate region of \( g_+ \), the range of which varies in different methods. The MLFS method yields negligible perturbation corrections and shows good convergence for a wide region of \( g_+ \) (from zero to an intermediate value) which increases with increasing value of \( t/\omega_0 \). In this region the LF method particularly shows bad convergence hence inapplicable. For large values of \( g_+ \) the LF method shows good convergence, as expected; the MLF and the MLFS methods also work satisfactorily there. The MLF method shows a systematic convergence in the whole region of \( g_+ \) even for higher values of \( t/\omega_0 \), as considered here. It is interesting to note that for strong coupling strength consideration of the second order correction to the energy as well as to the wave function reproduces almost the exact results for all the three methods. The calculated oscillator wave functions following our method match excellently with the exact oscillator wave functions, derived from the numerical diagonalization studies. Our study also shows that the region of \( g_+ \), where
no perturbation analytical method is applicable, is really very narrow in contrast to
the conclusions of some earlier works [3,4]. Although the analysis presented in this
paper is based on a two-site system, the approach may permit a better progress for
analytical studies of many-site systems.
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Figure captions:

FIG. 1. Variation of the relative perturbation corrections $E^{(n)}_0/E^{(0)}_0$ to the ground state energy as a function of the coupling strength $(g_+)$ for $t/\omega_0 = 0.5$ for (a) LF, (b) MLF and (c) MLFS method. $E^{(n)}_0$ is the nth order perturbation correction to the ground state energy and $E^{(0)}_0$ is the unperturbed ground state energy.

FIG. 2. (a): The plot of the ground state energy obtained by considering perturbation correction up to fifth order within the MLF method as a function of $g_+$ for $t/\omega_0 = 0.5$. The unperturbed energies (equivalent to the energy obtained with standard zero phonon averaging (ZPA)) within the LF and MLF methods are also shown. The MLFS (ZPA) results (not shown) lies in between the MLF and the exact curves. (b): The variation of $|\langle \psi^{(0)}_0 | \psi_G \rangle|^2$ with $g_+$ within LF, MLF and MLFS methods. $|\psi_G \rangle$ and $|\psi^{(0)}_0 \rangle$ are the corrected and the unperturbed wave functions, respectively.

FIG. 3. Plot of the correlation function $\langle n_1 u_2 \rangle_0$ calculated up to different order of perturbations in the wave function versus $g_+$ for $t/\omega_0 = 0.5$ within different methods (a) LF, (b) MLF and (c) MLFS. The labels (2), (3), .... denote the curve obtained by considering up to the second, third, .... order correction to the wave function, respectively.

FIG. 4. Variation of the relative perturbation corrections $E^{(n)}_0/E^{(0)}_0$ to the ground state energy as a function of the coupling strength $(g_+)$ for $t/\omega_0 = 1.1$ for (a) LF, (b) MLF and (c) MLFS method. $E^{(n)}_0$ is the nth order perturbation correction to the ground state energy and $E^{(0)}_0$ is the unperturbed ground state energy.

FIG. 5. The plot of the ground state energy obtained by considering perturbation correction up to fifth order within the MLF method as a function of $g_+$ for $t/\omega_0 = 1.1$. The unperturbed energies (or with zero phonon averaging results (ZPA)) within LF, MLF and MLFS methods are also shown.
FIG. 6. Plot of the correlation function $\langle n_1 u_2 \rangle_0$ calculated up to different order of perturbations in the wave function versus $g_+$ for $t/\omega_0 = 1.1$ within different methods (a) LF, (b) MLF and (c) MLFS. The labels (2), (3), .... denote the curve obtained by considering up to the second, third, ... order correction to the wave function, respectively.

FIG. 7. The variations of $\langle n_1(u_1 - u_2) \rangle_0/g_+$ with $g_+$ for LF, MLF and MLFS methods with zeroth order of perturbation for $t/\omega_0 = 1.1$. The solid curve corresponds to that obtained within the MLF method up to fifth order correction to wave function.

FIG. 8. Ground state oscillator wave function $G(x)$ as a function of $x$ for different values of the coupling strength when the electron is located at site 1 for $t/\omega_0 = 1.1$.

FIG. 9. Variation of the relative perturbation corrections $E^{(n)}_0/E^{(0)}_0$ to the ground state energy as a function of the coupling strength ($g_+$) for $t/\omega_0 = 2.1$ for (a) LF, (b) MLF and (c) MLFS method. $E^{(n)}_0$ is the nth order perturbation correction to the ground state energy and $E^{(0)}_0$ is the unperturbed ground state energy.

FIG. 10. The variation of $|\langle \psi_0^{(0)} | \psi_G \rangle|^2$ with $g_+$ within LF, MLF and MLFS methods for $t/\omega_0 = 2.1$. $|\psi_G \rangle$ and $|\psi_0^{(0)} \rangle$ are the corrected and the unperturbed wave functions, respectively.

FIG. 11. Plot of the correlation function $\langle n_1 u_2 \rangle_0$ calculated up to different order of perturbations in the wave function versus $g_+$ for $t/\omega_0 = 2.1$ within different methods (a) LF, (b) MLF and (c) MLFS. The labels (2), (3), .... denote the curve obtained by considering up to the second, third, .... order correction to the wave function, respectively.

FIG. 12. Ground state oscillator wave function $G(x)$ as a function of $x$ for $g_+ = 1.6$ when the electron is located at site 1 with different values of $t/\omega_0$. 
FIG. 1

(a) LF  
\[ t = 0.5 \]

(b) MLF  
\[ t = 0.5 \]

(c) MLFS  
\[ t = 0.5 \]

\[ \frac{E_0^{(n)}}{E_0^{(0)}} \]
FIG. 2
FIG. 3

(a)

(b)

(c)

MLF

MLFS
FIG. 5
FIG. 6
\[ \langle (u_1 - u_2)^2 \rangle_0 \]

\[ g_+ \]

FIG. 8
FIG. 9

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FIG. 10

(a) $E_0(n)/E_0^0$ vs. $g_+$ for LF at $t = 2.1$

(b) $E_0(n)/E_0^0$ vs. $g_+$ for MLF at $t = 2.1$

(c) $E_0(n)/E_0^0$ vs. $g_+$ for MLFS at $t = 2.1$
\[ |\langle \psi_0(0) | \psi_G \rangle |^2 \]

Fig. 11
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FIG. 13
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