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Effect of different site energies on polaronic properties

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Abstract. A two-site single polaron Holstein model is studied in presence of a difference in bare site energies ($\epsilon_d = \epsilon_2 - \epsilon_1$) using the perturbation theory with the variational modified Lang-Firsov (MLF) phonon basis. The polaronic ground-state wave function is calculated up to the fifth order of perturbation. The effect of ϵ_d (acts as a strength of diagonal disorder) on the polaron crossover, polaronic kinetic energy, oscillator wavefuncion and polaron localization are studied. Considering a double-exchange Holstein model with finite ϵ_d, role of disorder on the properties of the double-exchange system is also discussed.

PACS. 71.38.-k Polarons and electron-phonon interactions – 63.20.kr Phonon-electron and phonon-phonon interactions

1 Introduction

Study of narrow band electronic systems with strong electron-phonon (e-ph) interaction has long been an active research area in condensed matter physics. The field has drawn renewed interest following evidence of polaronic charge carriers in underdoped high-T_c cuprates [1], manganites [2], and organic superconductors. The one-dimensional polaron problem is also relevant in semiconductor physics, quantum dots [3] and linear conjugated organic polymer conductors [4]. The simplest model for studying polarons is the Holstein model [5] where an electron in a narrow band interacts locally with optical phonons. For large e-ph coupling the polaron is a small polaron with high effective mass, while for small coupling it becomes a large polaron having a much lower effective mass for a finite adiabatic parameter. The crossover from a large to a small polaron and the corresponding change in the polaronic properties in the ground state have been studied for the Holstein model by different groups [6–9] using various methods enlightening our understanding in this field. However studies on the nature and properties of polarons in presence of disorder are few and need much more attention. The imperfections or disorder may play an important role in complex materials (high-T_c oxides, manganites etc.) where signatures for polaronic carriers are found. Recently the small polaron concept has been used to explain the charge motion in DNA where the electronic band is very narrow and the presence of different kind of molecular units induces large disorder potential [10].

In absence of any disorder, translational symmetry ensures that the polaronic ground state is delocalized however large is the e-ph coupling strength provided other parameters (electronic hopping, phonon frequency) are finite. The large to small polaron crossover is a continuous one [8], which is consistent with the ground state properties, being analytic functions of e-ph coupling [11]. Localization requires a breakdown of the translational invariance which may be achieved through randomness of the site potential or hopping. The effect of site diagonal disorder on polaronic properties has been addressed by some authors. Shinozuka and Toyozawa [12] studied disorder induced self-trapping in a tight binding model in which the local site energies are randomly distributed between two values and found that the exciton-lattice interaction acts with the disorder to produce severe localization associated with a self-trapped exciton. In his study the lattice vibration was treated as classical oscillators. Bronold et al. [13] studied similar model but with an infinite coordination number within the dynamical coherent potential approximation. However the limitation of the coherent potential approximation is that it cannot fully distinguish between localized and itinerant states. Bronold and Fehske [14] improved the method to overcome the above shortcoming. They followed statistical dynamical mean field theory to predict localization of small polarons by extremely small disorder. However a proper study of the effect of disorder on the polaron crossover is not made in any of the above investigations. In the present work we consider a two-site cluster with different site energies. This is the minimal system to study the competition of the inter-site electronic hopping with the localization induced by the combined effect of the e-ph coupling and the site energy disorder. Difference in site energies would remove the two-fold degeneracy of the system in the absence of hopping and would tend to localize the electron in the lower potential site. *For convenience we will refer to the difference in site energies as disorder strength because it partly mimics the role of disorder in larger systems.* Another reason for choosing a two-site Holstein model is that almost exact

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results may be obtained for such a system by the perturbation method [15] using a modified Lang-Firsov (MLF) basis [16]. For the Holstein model the interaction is very short-ranged and the essential physics related to the polaronic behavior for a larger system is similar to that of a two-site system. In studying a Hubbard-Holstein model similar conclusion has been reached in reference [17]. The relevance of studying a two-site system in the context of Holstein and Holstein-double exchange models has been discussed in details in reference [18].

In Section 2 we discuss the formalism and perturbation calculations. In Section 3 we present the results obtained by MLF method and discuss the role of the disorder strength on the polaron crossover and the kinetic energy of the system. The localization of the polaron and ground state polaronic wavefunction are also discussed. Extension of this method to the double-exchange model is included in Section 4. Finally, a summary of the results are presented in Section 5.

2 Formalism

The two-site single-polaron Hamiltonian is

$$H = \epsilon_1 n_1 + \epsilon_2 n_2 - \sum_{\sigma} t(c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma}) + g\omega \sum_{i,\sigma} n_{i\sigma}(b_i + b_i^{\dagger}) + \omega \sum_i b_i^{\dagger} b_i \quad (1)$$

where i =1 or 2, denotes the site. ϵ_1 and ϵ_2 are the bare site-energies at site 1 and 2, respectively. $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) is the annihilation (creation) operator for the electron with spin σ 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 and ω is the phonon frequency. This Hamiltonian has spin degeneracy for the one electron case so the spin index is redundant.

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 ($H = H_d + H_a$):

$$H_d = \epsilon_1 n_1 + \epsilon_2 n_2 - t(c_1^{\dagger} c_2 + c_2^{\dagger} c_1) + \omega g_+ (n_1 - n_2)(d + d^{\dagger}) + \omega d^{\dagger} d \quad (2)$$

$$\text{and} \quad H_a = \omega \tilde{a}^{\dagger} \tilde{a} - \omega n^2 g_+^2 \quad (3)$$

where $g_+ = g/\sqrt{2}$, $\tilde{a} = a + n g_+$. H_a describes just a shifted oscillator, while H_d represents an effective e-ph system where phonons couple with the electronic degrees of freedom. In reference [15] we have shown that the MLF perturbation method works much better than the Lang-Firsov (LF) method for a large region of parameter space where the retardation is important. In the strong-coupling limit the MLF method reduces to the LF method and it works well there. We use the MLF transformation where the lattice deformations produced by the electron are treated as variational parameters [16,19]. For the present system, $\tilde{H}_d = e^R H_d e^{-R}$ where $R = \lambda(n_1 - n_2)(d^{\dagger} - d)$ and λ is a variational parameter describing the displacement of the d oscillator.

The transformed Hamiltonian is then obtained as

$$\tilde{H}_d = \omega d^{\dagger} d + (\epsilon_1 - \epsilon_p) n_1 + (\epsilon_2 - \epsilon_p) n_2 - t\,[c_1^{\dagger} c_2\, \exp(2\lambda(\mathrm{d}^{\dagger} - \mathrm{d})) + c_2^{\dagger} c_1 \exp(-2\lambda(d^{\dagger} - d))] + \omega(g_+ - \lambda)(n_1 - n_2)(d + d^{\dagger}) \quad (4)$$

where $\epsilon_p = \omega(2g_+ - \lambda)\lambda$.

For the single polaron problem we choose the basis set,

$$|+, N\rangle = (a_1 c_1^{\dagger} + a_2 c_2^{\dagger})|0\rangle_e |N\rangle_{\mathrm{ph}}$$
$$|-, N\rangle = (a_2 c_1^{\dagger} - a_1 c_2^{\dagger})|0\rangle_e |N\rangle_{\mathrm{ph}} \quad (5)$$

where $|+\rangle$ and $|-\rangle$ denote the electronic states and $|N\rangle$ denotes the Nth excited oscillator state in the MLF phonon basis. The normalization condition requires $a_1^2 + a_2^2 = 1$. The unperturbed part of the Hamiltonian is chosen as

$$H_0 = \omega d^{\dagger} d + (\epsilon_1 - \epsilon_p) n_1 + (\epsilon_2 - \epsilon_p) n_2 - t_e\,(c_1^{\dagger} c_2 + c_2^{\dagger} c_1) \quad (6)$$

where $t_e = t\ \exp(-2\lambda^2)$. The remaining part $H_1 = (\tilde{H}_d - H_0)$ is treated as a perturbation. The states $|\pm, N\rangle$ are the eigenstates of the unperturbed Hamiltonian (H_0) for $r = a_1/a_2 = [\epsilon_d + \sqrt{{\epsilon_d}^2 + 4{t_e}^2}]/2t_e$ where $\epsilon_d = \epsilon_2 - \epsilon_1$. The corresponding eigen energies are given by

$$E_{\pm,N}^{(0)} = N\omega + \frac{(\epsilon_1 + \epsilon_2)}{2} - \epsilon_p \mp \frac{1}{2}\sqrt{(\epsilon_1 - \epsilon_2)^2 + 4{t_e}^2} \quad (7)$$

The state $|+, 0\rangle$ has the lowest unperturbed energy, $E_0^{(0)} = \epsilon_1 + \frac{\epsilon_d}{2} - \epsilon_p - \frac{1}{2}\sqrt{{\epsilon_d}^2 + 4{t_e}^2}$.

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

$$\langle N, \pm|H_1|\pm, M\rangle = \mp t_e \frac{2r}{(1 + r^2)} \quad (8)$$

$$\langle N, \pm|H_1|\mp, M\rangle = -t_e \frac{(1 - r^2)}{(1 + r^2)} \quad (9)$$

for odd $(N - M)$,

$$\langle N, \pm|H_1|\pm, M\rangle = \mp\sqrt{N}\omega(g_+ - \lambda)\frac{(1 - r^2)}{(1 + r^2)}\delta_{N,M+1} \quad (10)$$

$$\langle N, \pm|H_1|\mp, M\rangle = \pm t_e + \sqrt{N}\omega(g_+ - \lambda)\frac{2r}{(1 + r^2)}\delta_{N,M+1} \quad (11)$$

It may be noted that for the ordered case (ϵ_d=0, hence r=1) the off-diagonal matrix elements $\langle N, \pm|H_1|\pm, M\rangle$ are nonzero only for even $(N - M)$ while $\langle N, \pm|H_1|\mp, M\rangle$ are nonzero only for odd $(N - M)$.

To find out the variational phonon basis as a function of e-ph coupling, the unperturbed ground state energy $E_0^{(0)}$ is minimized with respect to λ [15] and we obtain

$$\lambda = \frac{\omega g_+}{\omega + \frac{4{t_e}^2}{\sqrt{{\epsilon_d}^2+4{t_e}^2}}} \tag{12}$$

The perturbation corrections of different orders to the ground-state energy and the wavefunction may be calculated using the general off-diagonal matrix elements in equations (8–11). The ground-state wave function in the MLF basis may be written as,

$$|G\rangle = \frac{1}{\sqrt{N_G}}\left[|+,0\rangle + \sum_{N=1,2,..} c_N^+|+,N\rangle + \sum_{N=1,2,..} c_N^-|-,N\rangle\right] \tag{13}$$

The coefficients $c_N^{\pm}$ are obtained in terms of the off-diagonal matrix elements and unperturbed energies and N_G is the normalization factor.

The correlation functions involving the charge and the lattice deformations $\langle n_1 u_1\rangle_0$ 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. Following reference [15], the correlation functions may be written as

$$\langle n_1 u_1\rangle = \frac{1}{2}\left[-(g_+ + \lambda)\frac{B_0}{N_G} + \frac{A_0}{N_G}\right] \tag{14}$$

$$\langle n_1 u_2\rangle = \frac{1}{2}\left[-(g_+ - \lambda)\frac{B_0}{N_G} - \frac{A_0}{N_G}\right] \tag{15}$$

where $A_0 \equiv \langle G|n_1(d+d^\dagger)|G\rangle = \dfrac{2}{(1+r^2)}(rc_1^- + r^2 c_1^+)$
$$+ \sum_{N=1}^{\infty}\sqrt{N+1}\frac{2}{(1+r^2)}\left[r^2 c_N^+ c_{N+1}^+ + r(c_N^- c_{N+1}^+ + c_N^+ c_{N+1}^-) + c_N^- c_{N+1}^-\right]$$
and $B_0 \equiv \langle G|n_1|G\rangle = \dfrac{r^2}{(1+r^2)} + \sum_{N=1}^{\infty}\dfrac{1}{(1+r^2)}$
$$\times\left[2rc_N^- c_N^+ + r^2|c_N^+|^2 + |c_N^-|^2\right]$$

The static correlation functions in equations (14) and (15) are calculated for different ϵ_d to examine the role of the disorder on the polaron crossover.

The kinetic energy of the system in the ground state is obtained as

$$E_{K.E} = \langle G|H_t|G\rangle = \frac{1}{N_G}\left[-2t_e a_1 a_2 + 2\sum_{e=\pm}\sum_{N\neq 0} c_N^e\langle e,N|H_t|0,+\rangle + \sum_{e,e'=\pm}\sum_{N,M\neq 0} c_N^e c_M^{e'}\langle e,N|H_t|M,e'\rangle\right] \tag{16}$$

where $H_t = -t[c_1^\dagger c_2\ \exp(2\lambda(d^\dagger - d)) + c_2^\dagger c_1 \exp(-2\lambda(d^\dagger - d))]$ is the kinetic energy operator in the MLF basis. The occupation number $n(k)$ of the charge carrier for the ground state within MLF method is also calculated as

$$n_{0,\pi} = \frac{1}{2}(c_1^\dagger \pm c_2^\dagger)(c_1 \pm c_2) \tag{17}$$

$$\langle G|n_{0,\pi}|G\rangle = \frac{1}{2}\left[1 \pm \frac{E_{K.E}}{t}\right] \tag{18}$$

where $0, \pi$ denotes the values of the wave vector k. Therefore, it basically reflects the nature of the kinetic energy.

The ground-state wave function for the d-oscillator is obtained from equation (13) by using the wavefunction for the Nth excited (MLF-displaced) harmonic oscillator for $|\pm, N\rangle$.

$$\psi_n(x) = \langle x|n\rangle = \frac{1}{\pi^{1/4}\sqrt{2^n n!}} e^{-(x-x_0)^2/2} H_n(x - x_0) \tag{19}$$

where $H_n(x)$ is the Hermite polynomial of degree n and x_0 is the displacement of the oscillator due to the MLF transformation.

To study the localization effect due to disorder in site energy we calculate $|_e\langle 1|G\rangle|^2$ and $|_e\langle 2|G\rangle|^2$. These are the probabilities that the polaron in the ground state ($|G\rangle$) lies at site 1 and site 2, respectively.

$$|_e\langle 1|G\rangle|^2 = \frac{1}{N_G}\left[|a_1|^2 + \sum_{N\neq 0}|a_1 c_N^+ + a_2 c_N^-|^2\right] \tag{20}$$

$$|_e\langle 2|G\rangle|^2 = \frac{1}{N_G}\left[|a_2|^2 + \sum_{N\neq 0}|a_2 c_N^+ - a_1 c_N^-|^2\right] \tag{21}$$

3 Results and discussions

In this paper all the results are derived by calculating the ground-state wavefunction up to the fifth order of perturbation. Rongsheng et al. [20] compared our MLF-perturbation results for the ordered case [15] with their exact results and found that the MLF method up to the fifth order gives exact results for $t = 0.5$ (in a scale where $\omega = 1$) whereas for higher values of t (=1.1 and 2.1) very accurate results are produced by the MLF perturbation method for both strong and weak coupling regions. However in a narrow region of intermediate coupling the perturbation results for high values of t deviate from the exact results. These findings are fully consistent with our conclusions in reference [15]. In this paper we present the results mainly for the nonadiabatic regime ($t/\omega \leq 1.0$) for which the convergence of the MLF-perturbation series for both ordered and disordered cases is found to be very good in the entire region of the e-ph coupling strength. For the ordered case, the convergence in energy and correlation functions have already been reported in reference [15] and that for the wave function in reference [21].

In Figure 1 we plot the variation of the correlation functions $\langle n_1 u_1\rangle$ and $\langle n_1 u_2\rangle$ with g_+ for $t/\omega = 0.5$ and

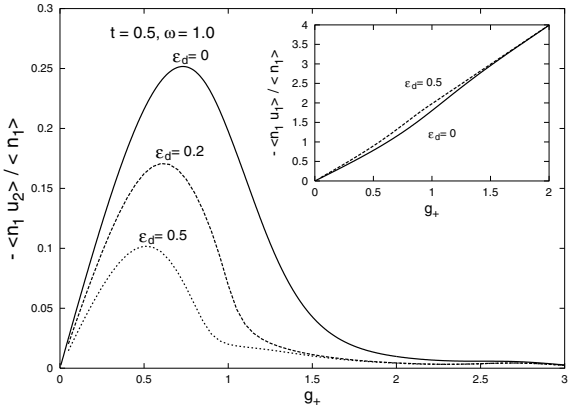

Fig. 1. Plot of the correlation function $\langle n_1 u_2 \rangle$ versus g_+ for $t/\omega = 0.5$ for different values of ϵ_d. Inset: on-site correlation function $\langle n_1 u_1 \rangle$.

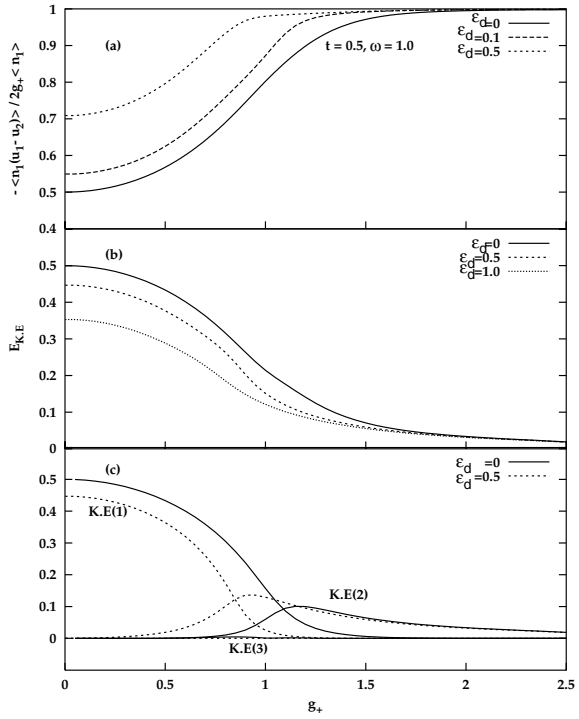

Fig. 2. (a) The variations of $\chi = \langle n_1(u_1 - u_2)\rangle/2g_+\langle n_1\rangle$ with g_+ for different values of ϵ_d for $t/\omega = 0.5$. (b) The variation of the kinetic energy $E_{K.E}$ with g_+ for $t/\omega = 0.5$ and $\epsilon_d = 0$, 0.5 and 1.0. (c) Different parts of the kinetic energy (see the three terms in Eq (16) referred as K.E(1), K.E(2) and K.E(3), respectively) vs. g_+ for different ϵ_d.

for different values of the disorder strength ϵ_d. For intermediate coupling, $\langle n_1 u_2 \rangle$ has appreciable values and $\langle n_1 u_1 \rangle / \langle n_1 \rangle$ (shown in inset) deviates downwards from its small polaronic LF value of $2g_+$. These are the signatures of retardation and directly show the delocalization of the polaron. With increasing ϵ_d the value of $\langle n_1 u_2 \rangle$ decreases and $\langle n_1 u_1 \rangle$ shows less deviation from its LF value. This signifies a reduced retardation effect with increasing disorder strength.

In Figure 2a we plot the correlation function $\chi = \langle n_1(u_1 - u_2)\rangle/2g_+\langle n_1\rangle$ as a function of e-ph coupling strength to examine the behavior of the large-to-small polaron crossover. In the small polaron limit the retardation effect is negligible and χ gets its standard LF value (=1). For a large polaron, the value of χ is lower. Figure 2a shows that the size of the polaron becomes more localized with increasing disorder strength. The polaron crossover is continuous, but a change in the curvature of χ vs. g_+ plot is observed at a point (in g_+ space) in the crossover region which may be taken as the crossover point. The crossover point shifts to lower value of g_+ as ϵ_d increases. Thus the disorder favors formation of small polarons.

In Figure 2b the kinetic energy of the polaron is plotted as a function of g_+. It is seen that the kinetic energy is suppressed by the disorder in the coupling range from low to intermediate values of g_+, while disorder has almost no effect on the kinetic energy for strong coupling. In general, it is well known that the polaronic kinetic energy shows three characteristic features [6,22]: (i) for small coupling the kinetic energy is very weakly suppressed from its non-interacting ($g = 0$) value, (ii) it shows a rapid (exponential) suppression in the crossover region and (iii) a much weaker suppression ($\propto 1/g^2$) at strong coupling. Same features are evident in Figure 2b. The kinetic energy in equation (16) has three terms. The first term is the contribution to the kinetic energy from the unperturbed ground state. This arises from the diagonal hopping and is significant in the range from low to intermediate couplings. The second term originates from the non-zero matrix elements of H_t between the unperturbed ground state and the polaronic states with higher phonon number, and the third term is due to the hybridization of polaronic states with higher phonon numbers through H_t. We plot these contributions separately as a function of g_+ in Figure 2c for $\epsilon_d = 0$ and 0.5. It is found that the first contribution, which is due to the diagonal (coherent) hopping, is suppressed substantially with increasing disorder strength. The second part of the kinetic energy (K.E(2)) originates from non-diagonal hopping. This part develops in the intermediate range of coupling and persists upto the strong coupling region. In fact this is the sole contribution to the kinetic energy for strong-coupling. It is seen from Figure 2c that this non-diagonal hopping contribution to the kinetic energy increases with disorder in the intermediate range of coupling, but is not affected by disorder in the strong coupling region. This leads to almost disorder independent kinetic energy at strong coupling. It may be mentioned that contribution from the third term is too small to show up in the figure for the range of our study.

In Figure 3, we have plotted the occupation number $n(k)$ of the polaron for the ground state with e-ph coupling. The difference between $n(k = 0)$ and $n(k = \pi)$ depends directly on the delocalization of the polaron (see Eq. (18)). In absence of hopping this difference vanishes. With increasing e-ph coupling the difference between $n(k)$ reduces as the kinetic energy is more and more suppressed. For the disordered case and in the range from weak to intermediate coupling, the difference in occupations reduces further owing to disorder-induced suppression of the

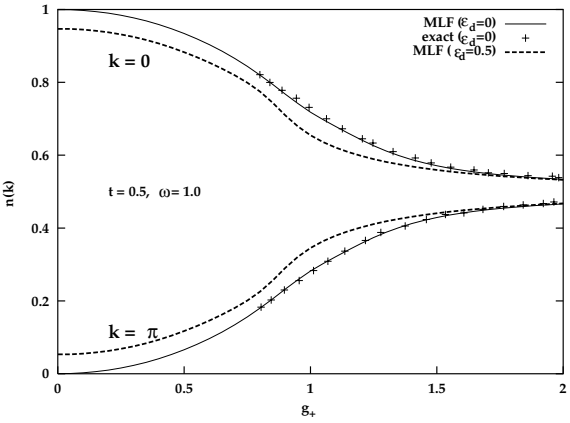

Fig. 3. The wave vector dependence of the occupation number $n(k = 0, \pi)$ of the charge carrier for the ground state with e-ph coupling within MLF method for ϵ_d=0 and 0.5. Exact results (for ϵ_d=0) from reference [23] is also plotted for comparison.

kinetic energy. In the strong-coupling regime, $n(k)$ does not show any change with ϵ_d because the kinetic energy is almost independent of ϵ_d in this region. The exact results for the occupation number [23] for the ordered case ($\epsilon_d = 0$) are also shown in Figure 3 for comparison with our MLF results.

In Figures 4a–d we have shown the ground-state wave functions of the d oscillator for different values of e-ph coupling for both the ordered and disordered cases considering that the electron is located at site 1. The results for the ordered case have been discussed in previous works [23,15,20]. The main changes, which are observed for the disordered case ($\epsilon_d = 1.0$) in the antiadiabatic regime, are as follows: (i) for weak coupling ($g_+ = 0.4$) the wave function, which shows displaced Gaussian-like single peak, is slightly more shifted; (ii) for intermediate coupling ($g_+ = 1.3$), the additional shoulder, which appears (at the right side of the main peak) for the ordered case, is absent in presence of disorder; (iii) for strong coupling ($g_+ = 2.0$) though the wavefunction around the main peak is identical for both cases, the additional small broad peak, observed for the ordered case, is not found for the disordered case. The first feature indicates that the on-site polaronic deformation is larger for the disordered case; while the second feature may be due to the reduced retardation effect. The third feature, i.e., disappearance of the additional broad peak for the disordered case, has a contradiction with the behavior of the kinetic energy. Both this broad additional peak and the kinetic energy in the strong-coupling regime are determined by the coefficients $c_N^{\pm}$ in equation (13). A logical question then arises why the broad peak in the oscillator wave function is modified by the disorder while the kinetic energy in that region is unaffected. In Figure 4e we plot $c_N^{\pm}$ versus N for $g_+ = 2.0$ for both ordered and disordered cases. For the ordered case c_N^- is nonzero for odd N, while c_N^+ is nonzero for even N. For the disordered case both the coefficients c_N^- and c_N^+ are nonzero for any N. For strong coupling, the reduced polaronic hopping makes the value of r (see the expression of r after Eq. (6)) very large in case of disorder. As a consequence we find that c_N^+ takes negligible value except for $N = 1$, while c_N^- is appreciable for both odd and even N. c_N^- changes sign alternately with N. However, the magnitude of the coefficients ($|c_N^e|$) for any N do not change much with disorder strength in the strong-coupling regime (shown in Fig. 4f). In this region we observe that the kinetic energy essentially depends on the magnitude of c_N^e rather than on its sign, hence it remains almost unaffected by disorder. However, the oscillator wavefunction which is given by $\sum_{N,e} c_N^e |N\rangle_{\rm ph}$, depends also on the sign of c_N^e and is affected by the disorder.

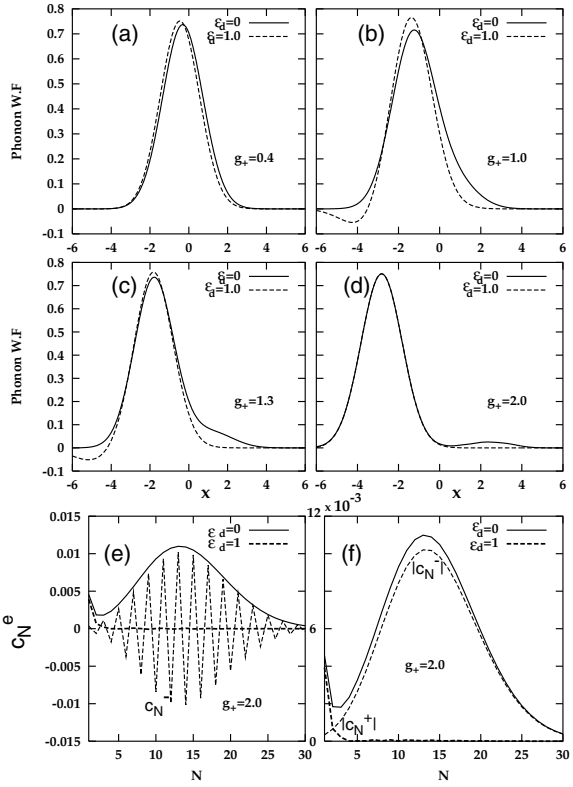

Fig. 4. Oscillator wave function (not normalized) vs. x with $t/\omega = 0.5$ for $\epsilon_d = 0$ and 1.0 for (a) $g_+ = 0.4$, (b) $g_+ = 1.0$, (c) $g_+ = 1.3$ and (d) $g_+ = 2.0$. (e) The coefficients c_N^e (see Eq. (13)) of the ground state wave function with phonon number N for $t/\omega = 0.5$ and $g_+ = 2$ for $\epsilon_d = 0$ and 1.0. Solid curve gives the value of c_N^- for odd N and c_N^+ for even N for the ordered case. For disordered case the thick dashed curve shows c_N^+ and the thin dashed curve shows c_N^-. (f) Magnitude of the coefficients ($|c_N^e|$) are shown for the same case as (e).

In Figure 5 we plot $|_e\langle 1|G\rangle|^2$ and $|_e\langle 2|G\rangle|^2$, which give the probabilities that the polaronic charge carrier in the ground state ($|G\rangle$) lies at site 1 and site 2, respectively. For the ordered case these probabilities are same (=0.5) for any value of the coupling. With increasing disorder strength these probabilities differ from 0.5; the site with lower site-energy has higher probability of being occupied than the other. This difference in the occupancy increases rapidly during polaron crossover as a consequence of rapid suppression of the polaronic hopping (t_e) with

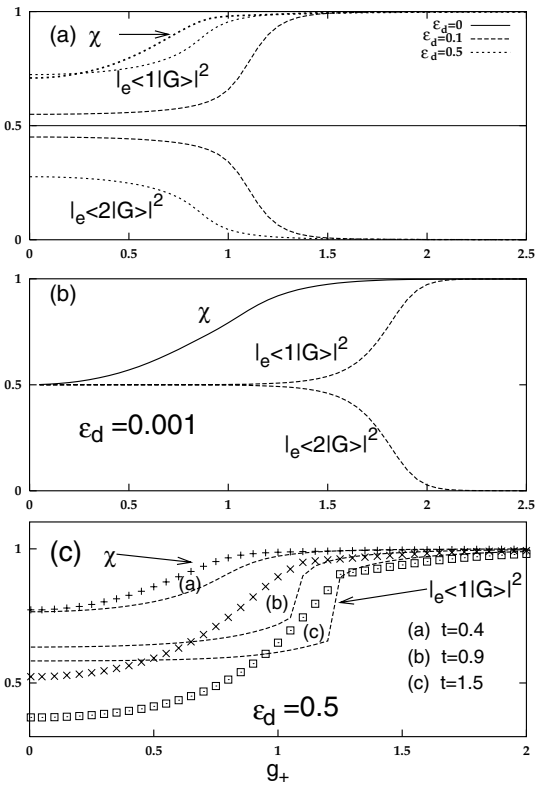

Fig. 5. Plots of $|_e\langle 1|G\rangle|^2$ and $|_e\langle 2|G\rangle|^2$ versus g_+ for $t/\omega = 0.5$. $|_e\langle 1|G\rangle|^2$ and $|_e\langle 2|G\rangle|^2$ are the probabilities of site 1 and site 2 being occupied by the electron, respectively. (a) The solid line for $\epsilon_d = 0$, thick dashed line for $\epsilon_d = 0.1$ and thin dashed line for $\epsilon_d = 0.5$; polaron crossover (χ) is also shown. (b) The same curves for $\epsilon_d = 0.001$. (c) Plots of χ and $|_e\langle 1|G\rangle|^2$ for different values of t. χ is denoted by different symbols and $|_e\langle 1|G\rangle|^2$ by broken line.

increasing g_+ in the crossover region. For strong-coupling regime $|_e\langle 1|G\rangle|^2$ becomes almost 1 while $|_e\langle 2|G\rangle|^2$ approaches to zero showing localization of the polaron at site 1. This localization as well as the correlation function χ are shown in Figures 5a and 5b for $\epsilon_d = 0.5$, 0.1 and 0.001. The figures show that the polaronic crossover precedes the localization for such values of ϵ_d. In Figure 5c similar plots are presented for different values of $t/\omega \leq 1.5$ and $\epsilon_d = 0.5$. With increasing t the polaron crossover and the localization occur at higher values of e-ph coupling as expected. The localization is abrupt but continuous for larger values of t while the polaron crossover is still very smooth for $t/\omega \leq 1.5$.

In Figure 6 we plot χ and $|_e\langle 1|G\rangle|^2$ as a function of disorder strength for different values of e-ph coupling with t/ω=0.5. For very weak coupling ($g_+ = 0.1$) the polaron crossover is induced by disorder potential and is very smooth. Here the localization and the polaron crossover occur almost simultaneously but none of them is complete even at $\epsilon_d = 2$. For $g_+ = 0.4$, which is also in the weak coupling range, the localization follows the polaron crossover and a large value of disorder strength is required for localization. For intermediate coupling ($g_+ = 1$) the

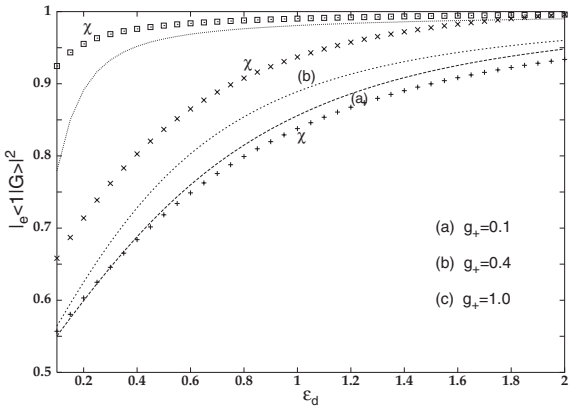

Fig. 6. Plots of χ and $|_e\langle 1|G\rangle|^2$ versus ϵ_d for different values of g_+ with $t/\omega = 0.5$. χ is denoted by different symbols and $|_e\langle 1|G\rangle|^2$ by broken line.

localization takes place in the small polaron region and 95% of the localization is achieved within $\epsilon_d/t \sim 1$. For higher values of coupling the polaron would be a small polaron even in absence of disorder and localization would occur for a small value of disorder strength. Our study points out that when the e-ph coupling is in the intermediate range, localization may be achieved with a disorder strength of the order of half (electronic) bandwidth of the system; this has also been pointed out in reference [24] in the context of manganites. For small e-ph coupling, disorder strength larger than the bandwidth is required for localization.

4 Two-site Holstein model with double exchange: effect of disorder

The relevant Hamiltonian for studying a two-site double exchange Holstein model in presence of antiferromagnetic interaction between core spins is given by [18,25]

$$H = \epsilon_1 n_1 + \epsilon_2 n_2 - \sum_\sigma t\ cos(\theta/2)(c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}) + g\omega \sum_{i,\sigma} n_{i\sigma}(b_i + b_i^\dagger) + \omega \sum_i b_i^\dagger b_i + JS_1.S_2 \quad (22)$$

where S_1, S_2 represent the local core spins (for manganites it is the spin of t_{2g} electrons) at sites 1 and 2, respectively and θ is the angle between them. J is the superexchange antiferromagnetic interaction between the neighbouring core-spins S. The transfer hopping integral (t) of the itinerant electron is modified to $t\cos(\frac{\theta}{2})$ because of the double exchange process which originates from strong Hund's coupling between the spins of the core electrons and itinerant electron [26]. Here we would treat the core spins classically. For manganites the core spins have $S = 3/2$. However, for small values of J/t, the qualitative behavior of the phase diagram of the two-site Holstein-double exchange model does not depend on the value of the spin or hopping as observed in reference [18]. Furthermore,

Edwards and his group [24] pointed out that for such models the resistivity and transition temperature T_c do not vary much with S, so that classical spin is a convenient approximation to $S = 3/2$ spins. Considering the out-of phase phonon mode which only couples with the electronic degrees of freedom and treating the spin classically, we obtain the MLF transformed Hamiltonian [25] as

$$\tilde{H}_d = \omega d^\dagger d + (\epsilon_1 - \epsilon_p)n_1 + (\epsilon_2 - \epsilon_p)n_2 - t\cos(\frac{\theta}{2}) \times \left[c_1^\dagger c_2 \exp(2\lambda(\mathrm{d}^\dagger - \mathrm{d})) + \mathrm{c}_2^\dagger \mathrm{c}_1 \exp(-2\lambda(\mathrm{d}^\dagger - \mathrm{d}))\right] + \omega(g_+ - \lambda)(n_1 - n_2)(d + d^\dagger) + JS^2\cos\theta \quad (23)$$

In our previous work [25] we studied the above Hamiltonian for a single polaron as a function of e-ph coupling for the ordered case (ϵ_1=ϵ_2) using perturbation theory with the variational MLF basis. We found that the nature of the ferromagnetic (FM) to antiferromagnetic (AFM) transition as well as that of the polaronic state depends on the relative values of J and t. For small values of JS^2/t the magnetic transition does not coincide with the polaronic crossover and a FM small polaronic state exists between a large polaronic FM state and extremely small polaronic AFM state. Similar phase diagrams have also been observed for both adiabatic and antiadiabatic limits in reference [18] for small values of JS^2/t. Here we will examine the effect of site-energy disorder on such polaronic state and crossover. We have followed the procedure of our previous work [25] to find out the ground state properties of the double exchange Holstein model with site disorder.

In manganites the ratio of the site energy disorder potential to the half band-width, when calcium is doped in $LaMnO_3$, is about 0.4 [24]. The value of the disorder strength used in the present work is of that order. It may be mentioned that previous studies [27] with a double exchange model have shown that the metal-insulator (MI) transition due to the off-diagonal disorder (associated with random spins in the paramagnetic phase) requires also a large diagonal disorder strength. This led to the conclusion that disorder alone cannot account for the MI transition in manganites and an e-ph coupling of intermediate range is needed for this purpose [24].

In Figures 7a and 7b we plot the angle (θ) between the core spins, the correlation function $\chi = \langle n_1(u_1 - u_2)\rangle/2g_+\langle n_1\rangle$ and the kinetic energy ($E_{K.E}$) as a function of g_+ to show the FM-AFM transition, polaron crossover and the polaron-delocalization energy for both the ordered and disordered cases. In presence of disorder, the FM-AFM magnetic transition and polaron crossover occur at lower values of g_+. The reason behind this behavior is that disorder effectively reduces the hopping, hence favors formation of the small polaron and the AFM phase. In the AFM phase, the polarons are small polarons with almost vanishing kinetic energy. However, the FM phase may have a large polaron character or a small polaron character depending on values of g_+. For low values of t (=0.7), it is difficult to distinguish between the regions of FM large polaron and FM small polaron since the change in χ is small and the curves for both χ and $E_{K.E}$ are very smooth for

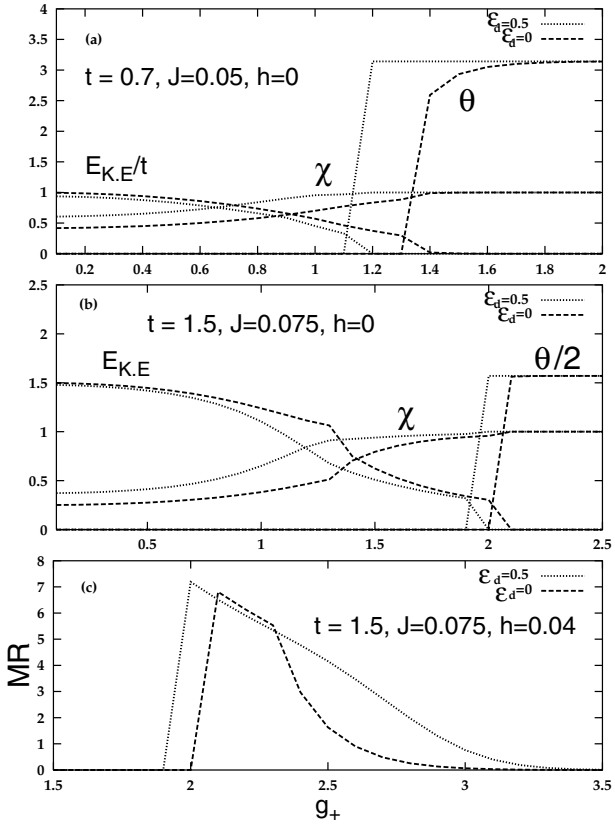

Fig. 7. Variation of θ, $\chi = -\langle n_1(u_1 - u_2)\rangle/2g_+\langle n_1\rangle$ and E_{KE} with g_+ for $\epsilon_d = 0$ and 0.5 in absence of magnetic field for (a) $t = 0.7$ and $JS^2 = 0.05$, and for (b) $t = 1.5$ and $JS^2 = 0.075$. (c) The magnetoresistance MR=$(E_{KE}(h) - E_{KE}(0))/h$ as a function of g_+ for $t = 1.5$, $JS^2 = 0.075$ and $h = 0.04$, h represents the applied magnetic field.

disordered case. In Figure 7b we consider a higher value of t (=1.5) with $JS^2/t = 0.05$ as relevant for manganite systems [28]. Here a crossover from the FM large polaronic state to a FM small polaronic state with reduced kinetic energy is seen for the disordered case, before the transition to the AFM state. So the site disorder does not make any drastic change to the qualitative features of the ground-state properties of the double-exchange Holstein model but smoothens the polaron crossover. In Figure 7c we plot the change in E_{KE} due to the magnetic field (h) as a function of g_+. This quantity may be related to the magnetoresistance for a system in the thermodynamic limit as pointed out in reference [25]. In general, the E_{KE} is a measure of delocalization of the polarons and its change with the magnetic field gives field-induced delocalization of the polaronic charge carriers. In reference [25] we reported for the ordered case that for $JS^2/t = 0.05$ the change in E_{KE} due to the field has a broad peak around the FM-AFM transition. We find that disorder makes the peak more broader but the value of the change in E_{KE} remains almost the same. We believe that the magneto-resistance of similar model system in the thermodynamic limit would show similar qualitative features. We do not present here the results for larger values of JS^2/t where the magnetic

transition coincides with the polaron crossover and the change in the E_{KE} shows a sharp peak at the FM-AFM transition [25] as we find that the site disorder does not change that behavior.

5 Conclusions

To summarize, we have presented the results on the two-site single polaron Holstein model in presence of a site energy disorder ϵ_d which appears as a difference in site energies. With increasing ϵ_d the retardation between the electron and associated deformation becomes weaker and the polaron crossover occurs at lower values of e-ph coupling. The polaronic kinetic energy is suppressed appreciably with disorder in the range from weak to intermediate couplings. However, in the strong-coupling region, where only the non-diagonal hopping processes contribute to the kinetic energy, it is independent of the disorder. For the oscillator wavefunction, a broad peak in strong-coupling region is observed for the ordered case ($\epsilon_d = 0$) in addition to the main peak. In presence of disorder ($\epsilon_d = 1.0$), this feature disappears. We find that even a small disorder ($\epsilon_d = 0.001$) can localize the electron in presence of e-ph coupling. The polaron crossover precedes the localization in the non-adiabatic regime for low to intermediate values of disorder ($\epsilon_d \leq t$).

For the double exchange Holstein model both the magnetic transition and polaron crossover shift toward lower values of e-ph coupling with increasing disorder strength. The qualitative features of the ground-state phase diagram does not change much with disorder. The magnetoresistance for the model shows up in a broader region of parameter space in presence of disorder.

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