Effect of different site energies on polaronic properties

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

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I. 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 [5-8, 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 aspect of choosing a two-site Holstein model is that almost exact results may be obtained for such a system with 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 relating polaronic behavior for a larger system is similar to that in a two-site system. In studying a Hubbard-Holstein model...
similar conclusion has been reached in Ref. [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 Ref. [18].

In Sec. II we discuss the formalism and perturbation calculations. In Sec. III we present the results obtained by MLF method and discuss the role of the disorder strength on the polaron crossover and the kinetic energy by MLF method and discuss the role of the disorder discussed in details in Ref. [18].

relevance of studying a two-site system in the context of electronic degrees of freedom. For a perturbation method it only with the total number of electrons \( n \) is a constant of motion. Consequently \( \langle \hat{H} \rangle \) is a Hamiltonian which is a constant of motion. Consequently.

II. Formalism

The two-site single-polaron Hamiltonian is

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

(1)

where \( i = 1 \) or \( 2 \), denotes the site. \( \epsilon_1 \) and \( \epsilon_2 \) are the bare site-energies at site 1 and 2, respectively. \( c_{1\sigma} \) (\( c_{2\sigma}^\dagger \)) 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 \( e^-\text{ph} \) 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 \( \omega \) 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 (\( H = H_d + H_a \)):

\[
H_d = \epsilon_1 n_1 + \epsilon_2 n_2 - t(c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) \\
+ \omega g_+(n_1 - n_2)(d + d^\dagger) + \omega d^\dagger d
\]

(2)

and \( H_a = \omega a^\dagger a - \omega n^2 g_+^2 \)

(3)

where \( g_+ = g/\sqrt{2}, a = a + ng_+ \). The \( a \)-oscillator couples only with the total number of electrons \( n = n_1 + n_2 \), which is a constant of motion. Consequently \( H_a \) describes just a shifted oscillator, while \( H_d \) represents an effective \( e^-\text{ph} \) system where phonons couple with the electronic degrees of freedom. For a perturbation method it is desirable to use a basis where the major part of the Hamiltonian becomes diagonal. When the hopping (\( t \)) is appreciable compared to the polaron energy (\( g^2\omega \)), a retardation between the electron and associated lattice distortion sets in. The retardation is important for low and intermediate values of \( g \); it produces a spread in the polaron size, the resultant polaron is a large one. In Ref. [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, \( H_d = e^R H_d e^{-R} \) where \( R = \lambda(n_1 - n_2)(d^\dagger - d) \) and \( \lambda \) is a variational parameter describing the displacement of the \( d \) oscillator.

The transformed Hamiltonian is then obtained as

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

(4)

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

For the single polaron problem we choose the basis set, \( |+; N\rangle = (a_1 c_1^\dagger + a_2 c_2^\dagger)|0\rangle c N\rangle_{\text{ph}} \)

\( |-; N\rangle = (a_2 c_1^\dagger - a_1 c_2^\dagger)|0\rangle c N\rangle_{\text{ph}} \)

(5)

where \( |+\rangle \) and \( |-\rangle \) denote the electronic states and \( |N\rangle \) denotes the \( N \)th 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

\[
H_0 = \omega d^\dagger d + (\epsilon_1 - \epsilon_p)n_1 + (\epsilon_2 - \epsilon_p)n_2 \\
- t_e (c_1^\dagger c_2 + c_2^\dagger c_1)
\]

(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 \( r = a_1/a_2 = |\epsilon_d + \sqrt{\epsilon d^2 + 4t_e^2}|/2t_e \) where \( \epsilon_d = \epsilon_2 - \epsilon_1 \).

The corresponding eigenenergies are given by

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

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

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 \( (N - M) \),

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

for odd \( (N - M) \),

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

(11)

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

Now one has to make a choice of \(\lambda\) so that the perturbation corrections are small and perturbative expansion becomes convergent. Here we will follow the procedure of our previous work \cite{15} to find out the variational phonon basis as a function of \(\epsilon\)-ph coupling. Minimizing the unperturbed ground state energy \(E_0^{(0)}\) with respect to \(\lambda\) we obtain

\[ \lambda = \frac{\omega g_+}{\omega + \frac{4r_e^2}{\sqrt{\omega^2 + 4r_e^2}}} \]  

(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 Eqs.(8-11). The ground-state wave function in the MLF basis may be written as,

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

\[ + \sum_{N=1,2,..} c_N^- |-, N\rangle \]  

(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 Ref. \cite{15}, the correlation functions may be written as

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

(14)

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

(15)

where \(A_0 \equiv \langle G | n_1 (d + d') | G \rangle = \frac{2}{(1 + r^2)} (r c_1^+ + r^2 c_1^{\dagger 2}) \)

\[ + \sum_{N=1}^{\infty} \sqrt{N+1} \frac{2}{(1 + r^2)} \left[ r^2 c_N^+ c_{N+1}^+ + r (c_N^+ c_{N+1}^2 + c_N^+ c_{N+1}) + c_{N+1} c_{N+1} \right] \]

and \(B_0 \equiv \langle G | n_1 | G \rangle = \frac{r^2}{(1 + r^2)} + \sum_{N=1}^{\infty} \frac{1}{(1 + r^2)} \left[ 2 r c_N^+ c_N^+ + r^2 |c_N^+|^2 + |c_N^-|^2 \right] \)

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

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

\[ E_{K,E} = <G | H_0 | G > \]

\[ = \frac{1}{N_G} \left[ -2 t_c a_1 a_2 + 2 \sum_{e=\pm \ N \neq 0} c_N^e \langle e, N | H_0 | 0, + \rangle \right. \]

\[ + \sum_{e,e' = \pm} \sum_{N,M,N \neq 0} c_N^e c_M^{e'} \langle e, N | H_0 | M, e' \rangle \]  

(16)

where \(H_0 = -t [c_1^e c_2^e \exp(2\lambda (d^+ - d)) + c_1^e c_1^e \exp(-2\lambda (d^+ - d))]\) 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

\[ n_{0,\pi} = \frac{1}{2} (c_1^e + c_1^{e'}) (c_1 \pm c_2) \]  

(17)

\[ \langle G | n_{0,\pi} | G \rangle = \frac{1}{2} \left[ 1 \pm \frac{E_{K,F}}{t} \right] \]  

(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 Eq. (13) by using the wavefunction for the N-th excited (MLF-displaced) harmonic oscillator for \(|\pm, N\rangle\).

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

(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 \(|\epsilon(1)|^2\) and \(|\epsilon(2)|^2\). These are the probabilities that the polaron in the ground state \(|G\rangle\) lies at site 1 and site 2, respectively.

\[ |\epsilon(1)|^2 = \frac{1}{N_G} \left[ |a_1|^2 + \sum_{N \neq 0} |a_1 c_N^+ + a_2 c_N^-|^2 \right] \]  

(20)

\[ |\epsilon(2)|^2 = \frac{1}{N_G} \left[ |a_2|^2 + \sum_{N \neq 0} |a_2 c_N^+ - a_1 c_N^-|^2 \right] \]  

(21)

III. Results and discussions

In this paper all the results are derived by calculating the ground-state wavefunction up to the fifth order of perturbation. For the ordered case a comparison of our MLF-perturbation results \cite{15} with the exact results by Rongsheng et al \cite{20} shows 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. 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 has already been reported in Ref. [12] and that for the wave function in Ref. [21].

In Fig. 1 we plot the variation of the correlation functions $\langle n_1 u_2 \rangle$ and $\langle n_1 u_2 \rangle$ with $g_+$ for $t/\omega = 0.5$ and for different values of the disorder strength $\epsilon_d$. 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 spread up of the polaron. With increasing $\epsilon_d$ 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 points to a reduced retardation effect with increasing disorder strength.

The polaron crossover from a large to a small polaron may be studied by the correlation function $\chi = \langle n_1 (u_1 - u_2) \rangle / 2g_+ \langle n_1 \rangle$. In the small polaron limit the retardation effect is negligible and $\chi$ gets its standard LF value (=1). For a larger size polaron the value of $\chi$ is lower. In Fig. 2(a) we plot $\chi$ as a function of $e$-$ph$ coupling strength. It is seen 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 $\chi$ vs. $g_+$ plot is observed at a point in the crossover region. This point (in $g_+$ space) where the curvature in $\chi$ vs. $g_+$ plot changes may be taken as the crossover point. The crossover point shifts to lower value of $g_+$ as $\epsilon_d$ increases. Thus the disorder favors formation of small polarons. In Fig. 2(b) we plot the kinetic energy of the polaron as a function of $g_+$. The kinetic energy is suppressed in presence of disorder in the range from low to intermediate values of $g_+$. But disorder has no significant effect on the kinetic energy for strong coupling where the polarons are small. The kinetic energy in Eq. (16) has three terms. The first term is the contribution to the kinetic energy from the unperturbed ground state which is significant for low to intermediate couplings. The second term is the contribution from the matrix elements of $H_t$ connecting the unperturbed ground state to higher phonon states. The third term is due to the hybridization of higher phonon states through $H_t$. We plot these contributions separately as a function of $g_+$ in Fig. 2(c) for $\epsilon_d=0$ and 0.5. It is found that the first contribution, which is dominant in the range from low to intermediate couplings and proportional to the product of the coeffi-

\[ \chi = \frac{\langle n_1 (u_1 - u_2) \rangle}{2g_+ \langle n_1 \rangle} \]

These are the signatures of retardation and directly show the spread up of the polaron. With increasing $\epsilon_d$ 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 points to a reduced retardation effect with increasing disorder strength.
coefficients $a_1$ and $a_2$ (see Eq.(16)), is suppressed substantially with increasing disorder strength. For strong-coupling regime the contribution to the kinetic energy comes only from the second term of Eq.(16) and that one is not affected by disorder in this region. 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 Fig. 3, we have plotted the occupation number $n(k)$ of the polaron for the ground state with $\epsilon$-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 $\epsilon$-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 kinetic energy. In the strong-coupling regime, $n(k)$ does not show any change with $\epsilon_d$ because the kinetic energy is almost independent of $\epsilon_d$ in this region. The exact results for the occupation number [22] for the ordered case ($\epsilon_d=0$) are also shown in Fig. 3 for comparison with our MLF results.

In Figs. 4(a-d) we have shown the ground-state wave functions of the $d$ oscillator for different values of $\epsilon$-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 [15, 20, 22]. The main changes, which are observed for the disordered case ($\epsilon_d=1.0$) in the antiadiabatic regime, are as follow:

(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 Eq.(13). A logical question then arises why...
observe that the kinetic energy essentially depends on the magnitude of $c_N^0$ rather than on its sign, hence it remains almost unaffected by disorder. However, the oscillator wave function which is given by $\sum_{N,e} c_N^0 |N\rangle_{ph}$ depends also on the sign of $c_N^0$ and is affected by disorder.

In Fig. 5 we plot $|\langle 1 | G \rangle|^2$ and $|\langle 2 | G \rangle|^2$, 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 increasing $g_+$ in the crossover region. For strong-coupling regime $|\langle 1 | G \rangle|^2$ becomes almost 1 while $|\langle 2 | G \rangle|^2$ approaches to zero showing localization of the polaron at site 1. This localization as well as the correlation function $\chi$ are shown in Fig. 5(a) and 5(b) for $\epsilon_d=0.5$, 0.1 and 0.001 to show that the polaronic crossover precedes the localization for $t/\omega = 0.5$. In Fig. 5(c) 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. However, the localization is abrupt but continuous for larger values of $t$ while the polaron crossover is still very smooth for $t/\omega \leq 1.5$.

It may be mentioned that when $t/\omega \geq 2$ and $\epsilon_d \geq 0.5$ we find that the polaron crossover and the localization occur almost simultaneously. However, for such large values of $t$ our perturbation method does not converge properly in a small range around intermediate coupling where polaron crossover takes place.

In Fig. 6 we plot $\chi$ and $|\langle 1 | G \rangle|^2$ as a function of disorder strength for different values of e-ph coupling with $t/\omega=0.5$. 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 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 Ref. 2 in the context of manganites. For small e-ph coupling, disorder strength larger than the bandwidth is required for localization.

IV. 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

\[ H = \epsilon_1 n_1 + \epsilon_2 n_2 - \sum_{\sigma} \left( t \cos(\theta/2) (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + g_{s} \sum_{i,\sigma} (b_{i\sigma}^\dagger b_{i\sigma} + \omega \sum_{i} b_{i\sigma}^\dagger b_{i\sigma} + JS_{1.S_{2}} \right) \tag{22} \]

where \( S_{1} \) and \( S_{2} \) represent the local core spins (for manganites it is the spin of \( t_{2g} \) electrons) at sites 1 and 2, respectively and \( \theta \) is the angle between them. \( J \) is the superexchange antiferromagnetic interaction between the neighboring core-spins \( S \). The transfer hopping integral \( (t) \) of the itinerant electron is modified to \( t \cos(\theta/2) \) because of the double exchange process which originates from strong Hund’s coupling between the spins of the core electrons and itinerant electron. 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 Ref. [24]. Furthermore, D. M. Edwards and his group [23] 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 [24] as

\[ \hat{H}_{d} = \omega d^\dagger d + (\epsilon_{1} - \epsilon_{p}) n_{1} + (\epsilon_{2} - \epsilon_{p}) n_{2} - t \cos(\theta/2) \left( c_{1}^\dagger c_{2} \exp(2\lambda(d^\dagger - d)) + c_{2}^\dagger c_{1} \exp(-2\lambda(d^\dagger - d)) \right) + \omega (g_{p} - \lambda) (n_{1} - n_{2})(d + d^\dagger) + JS^{2}\cos\theta \tag{23} \]

In our previous work [24] we studied the above Hamiltonian for a single polaron as a function of \( \epsilon_{ph} \) coupling for the ordered case \( (\epsilon_{1} = \epsilon_{2}) \) 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 Ref. [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 [24] 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 \( \text{LaMnO}_{3} \), is about \( 0.4 \) [23]. The value of the disorder strength used in the present work is of that order. It may be mentioned that previous studies [26] with a double exchange model have shown that the metal-insulator (MI) transition due to 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 cannot alone account for the MI transition in manganites and an \( \epsilon_{ph} \) coupling of intermediate range is needed for this purpose [26].

In Fig. 7(a) and 7(b) we plot the angle (\( \theta \)) between the core spins, the correlation function \( \chi = \langle n_{1}(u_{1} - n_{2}) \rangle / 2 + \langle n_{2} \rangle \) and the kinetic energy \( (E_{K,E}) \) as a function of \( g_{p} \) 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 \( g_{p} \). The reason behind this behavior is that disorder effectively reduces the hopping, hence favors formation of 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 \( g_{p} \). For low values of \( t \) (\( \approx 0.7 \)), it is difficult to distinguish between the regions of FM large polaron and FM small polaron since the change in \( \chi \) is small and the curves for both \( \chi \) and \( E_{K,E} \) are very smooth for disordered case. In Fig. 7(b) we consider a higher value of \( t \) (\( \approx 1.5 \)) with \( JS^{2}/t = 0.05 \) as relevant for manganite systems [27]. 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 po-
of the polarons and its change with the magnetic field [24]. In general, the system in the thermodynamic limit as pointed out in Ref. [1] J. P. Falck, A. Levy, M. A. Kastner, and R. J. Birgeneau, Phys. Rev. B 48, 4043 (1993); XiangXin Bi and Peter C. Eklund, Phys. Rev. Lett. 70, 2625 (1993).

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V. Conclusions

To summarize, we have presented the results on the two-site single polaron Holstein model in presence of a site energy disorder $\epsilon_d$ which appears as a difference in site energies. With increasing $\epsilon_d$ 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. But in the strong-coupling region where the hopping through multi-phonon process is dominant, kinetic energy is almost independent of $\epsilon_d$. 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 magneto-resistance for the model shows up in a broader region of parameter space in presence of disorder.

FIG. 7: Variation of $\theta$, $\chi = - < n_1(u_1 - u_2) > / 2g_+ < n_1 >$ and $KE$ 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 $MR=(KEE-E_{KE}(0))/\hbar$ as a function of $g_+$ for $t = 1.5$, $JS^2 = 0.075$ and $h = 0.04$, $h$ represents the applied magnetic field.
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