

Role of disorder in the two-site Holstein model with double exchange

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Date of Submission: 27th Jan, 2015

Date of Acceptance: 2nd Feb, 2015

Abstract

Using the perturbation method based on a variational phonon basis obtained by the modified Lang-Firsov (MLF) transformation, the two-site double-exchange Holstein model is studied in presence of a finite 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 ϵ_d (acts as a site-energy disorder) on the polaron crossover, polaronic kinetic energy and polaron localization are studied. Role of disorder on the properties of the double-exchange system is discussed.

Key words: electron-phonon interaction, polaron, double-exchange interaction, Holstein model, disorder

1. Introduction

Strong electron-phonon (e -ph) interaction in the narrow band electronic systems has drawn renewed interest following evidence of polaronic charge carriers in underdoped high- T_c cuprates¹, manganites², and organic superconductors. The one-dimensional polaron problem is also relevant in semiconductor physics, quantum dots³ and linear conjugated organic polymer conductors⁴. The simplest model for studying polarons is the Holstein model⁵ 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;7;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. The small polaron concept has been also used to explain

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the charge motion in DNA where the electronic band is very narrow and the presence of different kind of molecular units induces large disorder potential¹⁰.

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 one⁸, which is consistent with the ground state properties being analytic functions of e -ph coupling¹¹. 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^{12;13;14}. However a proper study of the effect of disorder on the polaron crossover is not made in those studies.

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 method¹⁵ using a modified Lang-Firsov (MLF) basis¹⁶. 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.

2. Formalism

The relevant Hamiltonian for studying a two-site double exchange Holstein model in presence of antiferromagnetic interaction between core spins is given by^{19;18}

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

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. 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 electron²⁰. 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.¹⁸. Furthermore, D. M. Edwards and his group²¹ 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 Hamiltonian¹⁹ as

$$\begin{aligned} \tilde{H}_d = \omega d^\dagger d + (\epsilon_1 - \epsilon_p)n_1 + (\epsilon_2 - \epsilon_p)n_2 - t \cos\left(\frac{\theta}{2}\right) & \left[c_1^\dagger c_2 \exp(2\lambda(d^\dagger - d)) \right. \\ & \left. + c_2^\dagger c_1 \exp(-2\lambda(d^\dagger - d)) \right] + \omega(g_+ - \lambda)(n_1 - n_2)(d + d^\dagger) + JS^2 \cos \theta \quad (2) \end{aligned}$$

where $d = (b_1 - b_2)/\sqrt{2}$, $g_+ = g/\sqrt{2}$, $\tilde{H}_d = e^R H_d e^{-R}$ with $R = \lambda(n_1 - n_2)(d^\dagger - d)$ and λ is a variational parameter describing the displacement of the d oscillator. In our previous work¹⁹ we studied the above Hamiltonian for a single polaron as a function of e -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 work¹⁹ to find out the ground state properties of the double exchange Holstein model with site disorder.

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.

The kinetic energy of the system in the ground state is obtained as $E_{K.E} = \langle G | H_t | G \rangle$ 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.

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. For the ordered case a comparison of our MLF-perturbation results¹⁵ with the exact results by Rongsheng *et. al*²² 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 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 ²¹. The value of the disorder strength used in the present work is of that order. It may be mentioned that previous studies²³ with a double exchange model have shown that the metal-insulator (MI) transition due to

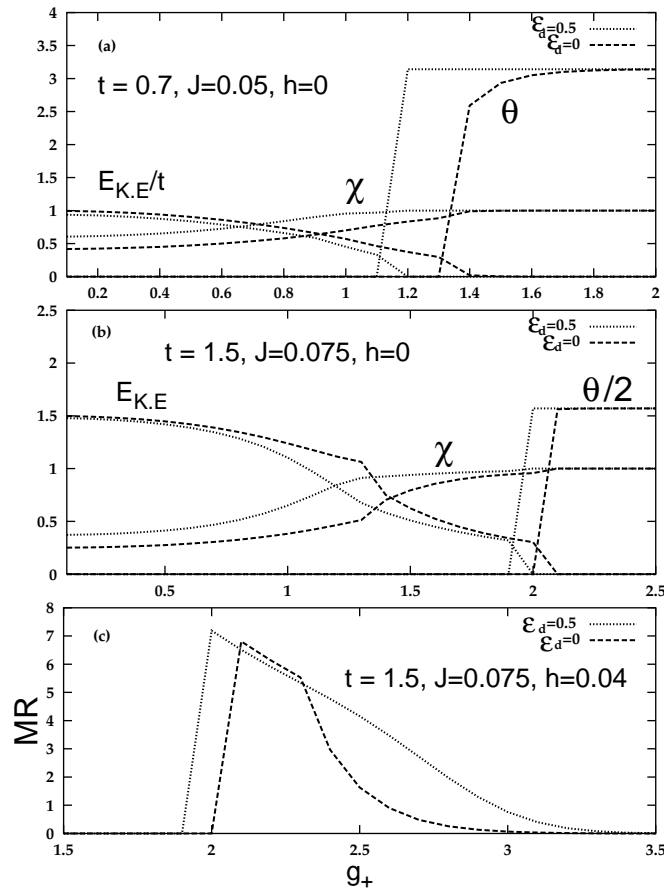


Figure 1: Variation of θ , $\chi = - \langle n_1(u_1 - u_2) \rangle / 2g_+ \langle n_1 \rangle$ and E_{KE} with g_+ for $\epsilon_d = 0$ and 0.5 in absence of magnetic field for (a) $t = 0.7$ and $JS^2 = 0.05$, and for (b) $t = 1.5$ and $JS^2 = 0.075$. (c) The magnetoresistance $MR = (E_{KE}(h) - E_{KE}(0))/h$ as a function of g_+ for $t = 1.5$, $JS^2 = 0.075$ and $h=0.04$, h represents the applied magnetic field.

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 e -ph coupling of intermediate range is needed for this purpose²¹.

In Fig. 1(a) and 1(b) we plot three parameters as a function of e-ph coupling (g_+) for both the ordered and disordered cases. These parameters are (i) the angle (θ) between the core spins, (ii) the correlation function $\chi = \langle n_1(u_1 - u_2) \rangle / 2g_+ \langle n_1 \rangle$ and (iii) the kinetic energy ($E_{K.E}$), which represent the FM-AFM transition, polaron crossover and the polaron-delocalization energy, respectively. 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 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 disordered case. In Fig. 1(b) we consider a higher value of t ($=1.5$) with

$JS^2/t = 0.05$ as relevant for manganite systems²⁴. 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 Fig. 1(c) 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 Ref.¹⁹. 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 Ref.¹⁹ 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 transition¹⁹ as we find that the site disorder does not change that behavior.

4. Conclusions

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. 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.

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