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Abstract

The ground state and finite-temperature properties of polarons are studied considering a two-site and a four-site Holstein model by exact diagonalization of the Hamiltonian. The kinetic energy, Drude weight, correlation functions involving charge and lattice deformations, and the specific heat have been evaluated as a function of electron–phonon (e–ph) coupling strength and temperature. The effects of site diagonal disorder on the above properties have been investigated. The disorder is found to suppress the kinetic energy and the Drude weight, and reduces the spatial extension of the polaron. Increasing temperature also reduces the kinetic energy, Drude weight and the polaron size when the e–ph interaction is weak or intermediate. For strong coupling the effect of temperature is small but opposite. For sufficiently strong coupling the kinetic energy arises mainly from the incoherent hopping processes owing to the motion of electrons within the polaron and is almost independent of the disorder strength. The specific heat shows a peak in the intermediate range of coupling, and the peak is suppressed in the presence of disorder. From the coherent and incoherent contributions to the kinetic energy, the temperature above which the incoherent part dominates is determined as a function of e–ph coupling strength.

1. Introduction

Study of different properties of polarons has been of great importance since the evidence of polaronic charge carriers in many materials of recent interest, namely high-T_c cuprates [1], CMR-manganites [2], biological materials like DNA [3], etc, which have large technological potential and importance. In the simplest Holstein model an electron in a narrow tight-binding band interacts locally with dispersionless optical phonons. For large e–ph coupling the resultant polaron is a small polaron with high effective mass [4, 5], while for weak coupling it becomes a large polaron having a much lower effective mass for a finite adiabatic parameter. The cross-over from a large to a small polaron and the corresponding changes in the polaronic properties in the ground state have been studied for the Holstein model by different groups [6–16] using various methods to enrich our understanding in this field. However, studies on the effects of finite temperature and disorder on polaronic properties are few and need more attention. Shinozuka and Toyozawa [17] 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 their study the lattice vibration was treated as a classical oscillator. Bronold *et al* [18] studied a similar model but with an infinite coordination number within the dynamical coherent potential approximation. Bronold and Fehske [19] followed statistical dynamical mean field theory to predict localization of small polarons by extremely small disorder. The effect of site diagonal disorder on the polaronic size and kinetic energy was investigated by us for a two-site system [20] and on a many-site system [21] by approximate methods only in the ground state.

In this paper we will consider a two-site and a four-site Holstein model and follow an exact diagonalization method to study the ground state as well as finite-temperature properties of the polarons and the effect of disorder on them. We will mainly study the kinetic energy, correlation functions involving charge and lattice deformations, Drude weight and the specific heat of the systems as a function of e–ph coupling for different temperatures and disorder strength. The temperature variation of the Drude weight and the part of the kinetic energy arising from incoherent hopping processes have also been studied.

This paper is organized as follows. In section 2 we have developed the formalism for the aforementioned study considering the Holstein model. We have presented the results and discussions for the two-site Holstein model in section 3.1 and those for the four-site system in section 3.2. The conclusion is given in section 4. In appendix A we have shown analytically, considering an infinite-size system and following strong coupling second-order perturbation theory, that the disorder has a weak or negligible effect on the kinetic energy for strong coupling.

2. Formalism

The Holstein Hamiltonian with site diagonal disorder in 1d is given by

$$H = \sum_i \epsilon_i c_i^\dagger c_i - \sum_i (t c_i^\dagger c_{i+1} + \text{h.c}) + g\omega \sum_i n_i (b_i^\dagger + b_i)$$
$$+ \omega \sum_i b_i^\dagger b_i \tag{1}$$

where $c_i^\dagger$ and c_i are the electron creation and annihilation operators at the site i, n_i $(= c_i^\dagger c_i)$ is the number operator, $b_i^\dagger$ and b_i are the creation and annihilation operators for the phonons corresponding to interatomic vibrations at site i, and ω is the phonon frequency. Electronic hopping takes place only between the nearest-neighbor sites with hopping strength t and g denotes the local e–ph coupling. The electronic site energy ϵ_i is independent of the site i for the ordered case. To study the effect of the site diagonal disorder we would put a different site potential at one of the sites of the two–four-site system. Spin index is not used for the electron, because a single polaron case has been studied here.

The third and fourth terms of equation (1) represent the electron–phonon interaction and phonon harmonic energy, respectively. These terms may be written in the momentum space defined by the phonon creation operators: $b_{\mathbf{q}}^\dagger = (1/\sqrt{N}) \sum_i b_i^\dagger e^{i\mathbf{q}\cdot\mathbf{R_i}}$ and the corresponding annihilation operators, where N is the number of sites in the system [7, 8, 16]. It can be easily shown that the in-phase ($\mathbf{q} = 0$) phonon mode does not couple with the electron dynamics but with the total number of electrons of the system. The harmonic term of this phonon mode along with its interaction with the electron may be separated out and written in a diagonal form [7, 8]. The rest of the Hamiltonian involving $(N-1)$ phonon modes and N electronic states (for a single-electron problem) are considered to form the basis states and construct the matrix elements. If one considers n_p number of phonon states per mode then the total number of basis states will be $n_{\text{Tot}} = N n_p^{(N-1)}$. Elimination of the in-phase mode thus reduces the states of the Hilbert space by a factor of n_p.

For the electron states we use the site space basis, which is convenient to take into account for the site disorder. For the phonon states we use the momentum space basis so that the in-phase ($\mathbf{q} = 0$) mode may be separated out. The Hamiltonian is then diagonalized to obtain the eigenstates and the eigenenergies. Thermodynamic expectation value of any

observable characterized by the operator O is then found out by

$$\langle O \rangle = \frac{1}{Z} \sum_{n=1}^{n_{\text{Tot}}} \langle n|O|n \rangle e^{-\beta E_n} \tag{2}$$

$$Z = \sum_{n=1}^{n_{\text{Tot}}} e^{-\beta E_n} \tag{3}$$

where E_n is the eigenenergy of the nth eigenstate $|n\rangle$, $\beta = 1/k_B T$ and T denotes the temperature. In this paper we are interested in evaluating the kinetic energy, static correlation function involving charge and lattice deformation, specific heat and the Drude weight. The operator corresponding to the kinetic energy is

$$H_t = -t \sum_{i,j}{}' c_i^\dagger c_j. \tag{4}$$

For the correlation functions involving charge and lattice deformations we calculate

$$\chi_m(i) = \langle n_i (b_{i+m}^\dagger + b_{i+m}) \rangle / 2g \tag{5}$$

which represents the lattice deformation produced at site $i+m$ when the electron is at site i. The Drude weight (D_n) in units of πe^2 for an eigenstate $|n\rangle$ of the polaronic system is obtained by introducing a phase factor to the hopping matrix element $(t \to t e^{i\phi})$ in order to break the time reversal symmetry and then finding out the response of the breakdown of the time reversal symmetry to the electric current as [22]

$$D_n = \frac{\partial^2 E_n(\phi)}{\partial \phi^2}\Big|_{\phi=0} \tag{6}$$

where $E_n(\phi)$ is the eigenenergy of the nth eigenstate in the presence of nonzero ϕ. The thermodynamic expectation value of the Drude weight (D) is found out by taking the thermal average of D_n over all the eigenstates

$$\langle D \rangle = \frac{1}{Z} \sum_n D_n e^{-\beta E_n}. \tag{7}$$

The specific heat may be expressed in terms of the energy fluctuation of the system at a finite temperature T as

$$C_v/k_B = \frac{1}{(k_B T)^2} [\langle E^2 \rangle - \langle E \rangle^2] \tag{8}$$
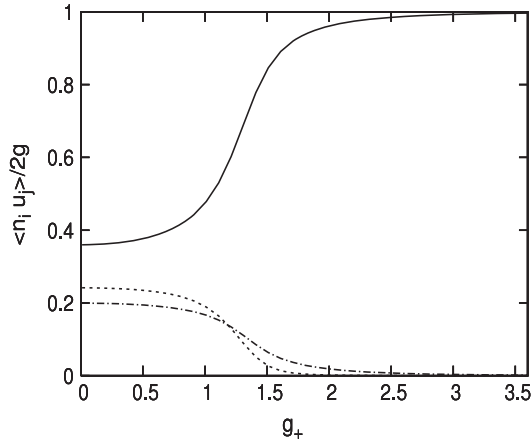
where $\langle E \rangle$ and $\langle E^2 \rangle$ are the thermal average of the energy and the square of the energy, respectively.

3. Results and discussions

3.1. Two-site system

For the two-site system the electron dynamics is coupled only to the out-of-phase ($\mathbf{q} = \boldsymbol{\pi}$) phonon mode. The Hamiltonian, which has to be considered for numerical diagonalization, is [20]

$$H_d = \sum_i \epsilon_i n_i - t(c_1^\dagger c_2 + c_2^\dagger c_1)$$
$$+ \omega g_+ (n_1 - n_2)(d + d^\dagger) + \omega d^\dagger d \tag{9}$$

Figure 1. Variation of $\langle n_i u_j \rangle / 2g$ with g_+ for $t = 2.1$ and $\epsilon_d = 0.5$ for the two-site Holstein model in the ground state. Solid line: $\langle n_1 u_1 \rangle / 2g$, dashed line: $\langle n_2 u_2 \rangle / 2g$ and dashed–dotted line: $\langle n_1 u_2 \rangle / 2g = \langle n_2 u_1 \rangle / 2g$. All the energy parameters are measured in units of $\omega = 1$.
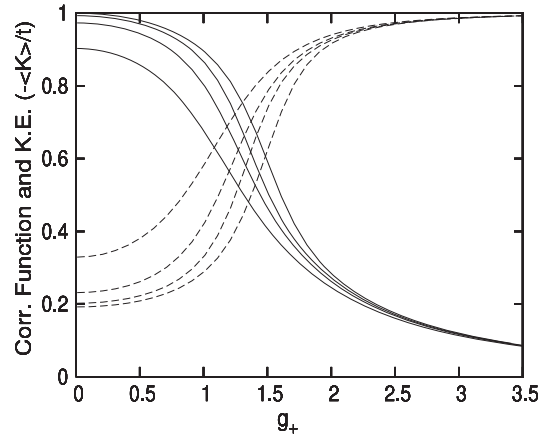
Figure 2. Variation of the kinetic energy $-\langle K \rangle / t$ (solid lines) and the correlation function χ_d^{avg} (dashed lines) with g_+ for $t = 2.1$ and different ϵ_d for the two-site Holstein model in the ground state. Solid lines from top to bottom and dashed lines from bottom to top are for $\epsilon_d = 0, 0.5, 1.0$ and 2.0, respectively.

where $g_+ = g/\sqrt{2}$ and $d = (b_1 - b_2)/\sqrt{2}$. We consider the basis states $c_i^\dagger |0\rangle_e |n_d\rangle_{ph}$, where $i = 1, 2$ and $n_d = 0, 1, 2, \ldots, n_d^m$, is the number of phonons in the d-oscillator. For this two-site system the results presented are obtained using $n_d^m = 50$. We find that the convergence in the physical quantities in the range of our study is achieved for n_d^m lower than 50. So the results for $n_d^m = 50$ may be considered as exact results.

In figure 1 we have presented the variation of the correlation function $\chi_m(i) = \langle n_i u_{i+m} \rangle / 2g$ for $i = 1, 2$ and $m = 0, 1$ (here $u_m = b_m + b_m^\dagger$) for the parameters $t = 2.1$ and $\epsilon_d = \epsilon_2 - \epsilon_1 = 0.5$ (all the energy parameters are expressed in units of $\omega = 1$). We will refer to ϵ_d for the two-site system as the disorder strength since it partly mimics the role of disorder in larger systems. For the ordered Holstein model it is well known that the on-site correlation involving charge and lattice deformation $\langle n_i u_i \rangle$ is larger than the intersite correlation $\langle n_i u_{i\pm1} \rangle$ and with increasing e–ph coupling $\langle n_i u_i \rangle$ increases while $\langle n_i u_{i\pm1} \rangle$ decreases. In the presence of disorder ($\epsilon_2 > \epsilon_1$), $\langle n_1 u_1 \rangle$ and $\langle n_1 u_2 \rangle$ show similar behavior with increasing e–ph coupling. However, for site 2, which have higher site energy, the on-site correlation $\langle n_2 u_2 \rangle$ decreases with increasing e–ph coupling and in the strong coupling region $\langle n_2 u_2 \rangle < \langle n_2 u_1 \rangle$ (figure 1). These are very different from the behavior of polarons in a ordered system. For disordered polaronic systems the average correlation functions may be defined as

$$\chi_0^{avg} = \frac{\sum_i \chi_0(i)}{\sum_i \langle n_i \rangle} \qquad (10)$$

$$\chi_1^{avg} = \frac{\sum_i \chi_1(i)}{\sum_i \langle n_i \rangle} \qquad (11)$$

$$\chi_d^{avg} = \frac{\sum_i (\chi_0(i) - \chi_1(i))}{\sum_i \langle n_i \rangle}. \qquad (12)$$

These average correlation functions show the usual characteristics, i.e. χ_0^{avg} increases while χ_1^{avg} decreases with increasing

g as expected when a polaron shrinks from a large to a small polaron with increasing coupling strength.

In figure 2 we have shown the variations of the kinetic energy and χ_d^{avg} with g_+ for different values of ϵ_d. It is seen that the kinetic energy is suppressed with increasing e–ph coupling as well as with increasing disorder strength. In the intermediate range of coupling the kinetic energy shows an exponential suppression. For strong coupling the kinetic energy reduces as $1/g^2$ and is almost independent of the disorder strength. The strong coupling behavior may be explained following an analytical calculation as shown in appendix A. With increasing disorder strength the correlation χ_d^{avg} increases (figure 2). The figure shows that the size of the polaron becomes smaller and the cross-over (from a large to a small polaron) occurs at a lower value of g_+ with increasing disorder strength. For strong coupling, disorder has almost no effect on χ_d^{avg}, similar to that observed for the kinetic energy.

To examine the effect of temperature on the properties of polarons, the kinetic energy and the correlation functions are evaluated for different temperatures. In figure 3 we have plotted the kinetic energy as a function of g_+ for different temperatures. For weak and intermediate coupling the kinetic energy decreases with increasing temperature, while for strong coupling the temperature has a smaller but opposite effect, i.e. the kinetic energy increases with increasing temperature. For very strong coupling the effect of temperature is almost negligible. Regarding the charge–lattice correlation we find that for weak and intermediate coupling χ_d^{avg} increases, i.e. the size of the polaron becomes smaller with increasing temperature, while for strong coupling the polaron size becomes larger with increasing temperature.

We have studied the specific heat (C_v) of the two-site polaronic system for different temperatures. In figure 4. we have presented the C_v of the ordered two-site system as a function of e–ph coupling for different temperatures. The figure shows that at low temperatures the specific heat shows a peak at intermediate coupling. With increasing temperature the
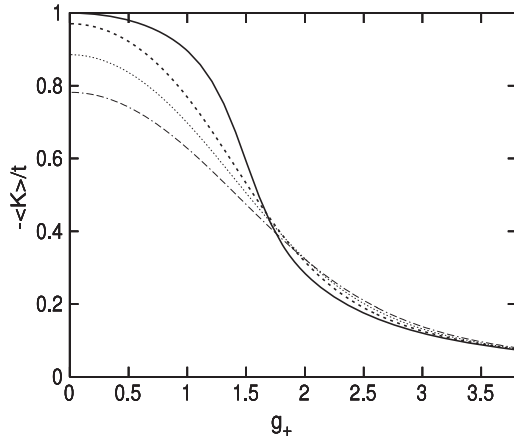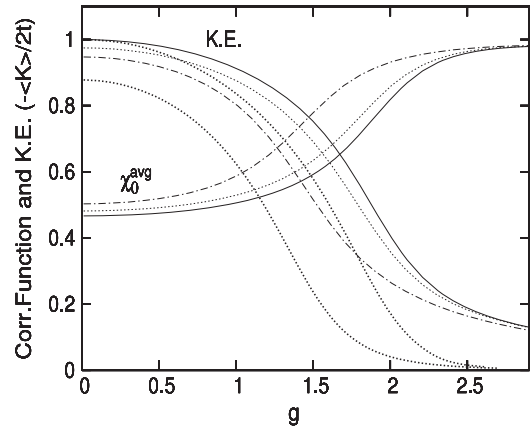
Figure 3. Variation of the kinetic energy $-\langle K \rangle/t$ with g_+ for the ordered case for different temperatures. Solid line: $k_B T = 0$, short dashed line: $k_B T = 1.0$, dotted line: $k_B T = 1.5$, dashed–dotted line $k_B T = 2.0$. $t = 2.1$ in the energy scale of $\omega = 1$.
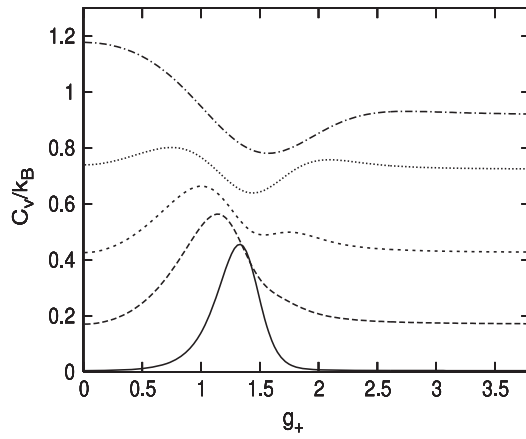
Figure 4. Variation of the specific heat (C_v/k_B) with g_+ for the ordered two-site Holstein model for different temperatures. Solid line: $k_B T = 0.1$, long dashed line: $k_B T = 0.2$, short dashed line: $k_B T = 0.3$, dotted line: $k_B T = 0.4$, dashed–dotted line $k_B T = 0.5$. $t = 2.1$ in the energy scale of $\omega = 1$.

peak shifts towards a lower value of g_+ and then disappears. At high temperatures a dip is developed in C_v in the intermediate coupling region.

It may be noted that at low temperatures the specific heat is mainly governed by the energy separation of the ground state and the first excited state of the two-site polaronic system. The specific heat for a system having only two energy levels with energy separation (ΔE), shows a peak at $\Delta E/k_B T = 2.58$, and C_v is very small when ΔE is far from $2.58 k_B T$. For the two-site Holstein model the energy separation (ΔE) between two lowest eigenenergy levels decreases monotonically with g_+ and becomes negligibly small at strong coupling [23, 24]. At a low temperature and weak e–ph coupling $\Delta E/k_B T$ is quite large and the corresponding specific heat has a small value. C_v attains a maximum at an intermediate coupling, when ΔE is $\sim 2.58 k_B T$, and becomes very small in the strong coupling region as $\Delta E \rightarrow 0$. At a higher temperature a higher value of ΔE is required to achieve the maximum value

Figure 5. Variation of the kinetic energy $-\langle K \rangle/2t$ and the correlation function χ_0^{avg} with g in the ground state for ordered and disordered four-site Holstein model. Solid lines: ordered case, dashed lines: disordered with site potentials $(1, 0, 0, 0)$, dashed–dotted curves: site potentials $(-1, 0, 0, 0)$. Dotted lines represent the Drude weight for ordered lattice (top dotted line) and disordered lattice with site potentials $(-1, 0, 0, 0)$ (bottom dotted line). Value of the hopping parameter used $t = 1.0$ in the energy scale of $\omega = 1$.

in C_v. Since ΔE increases with decreasing g_+ for the two-site Holstein model, the peak in C_v is obtained at a lower value of g_+ for a higher temperature. At high temperatures the higher energy states, in addition to the ground and first excited states, have significant contributions to the specific heat. This leads to the absence of the peak and formation of a dip in C_v.

3.2. Four-site system

For the four-site Holstein model, out of the four phonon modes there are three modes with $\mathbf{q} \neq 0$ which couple to the electron dynamics. These three phonon modes along with the four electronic states are considered for diagonalization of the matrix. We have done the numerical diagonalization with $n_p = 9$ per phonon mode and checked that this gives fairly accurate results in the range of our study presented here.

The kinetic energy and the static correlation function $\chi_m^{\text{avg}} = \sum_i \chi_m(i)/\sum_i n_i$ for $m = 0, 1, 2$ are evaluated as a function of g for a fixed temperature or as a function of temperature for different values of g for the four-site system. In figure 5 the kinetic energy and χ_0^{avg} are plotted against g for the ordered case and for disordered cases with site potentials $(1, 0, 0, 0)$ and $(-1, 0, 0, 0)$. The potential $(1, 0, 0, 0)$ means the values of ϵ_i for $i = 1, 2, 3, 4$ are $1, 0, 0$ and 0, respectively. Figure 5 shows that χ_0^{avg} is higher for disordered cases compared to the ordered case, implying that the polaron becomes a smaller polaron on introduction of the disorder. The suppression of the kinetic energy due to disorder is also seen in the figure. For the $(-1, 0, 0, 0)$ case the value of χ_0^{avg} is higher and the kinetic energy is lower than those for the $(1, 0, 0, 0)$ case. In the former case the electron will tend to be trapped at the site of the negative potential while for the latter case the electron would try to avoid the positive potential site. The trapping potential would suppress the kinetic energy more drastically and favor small polaron
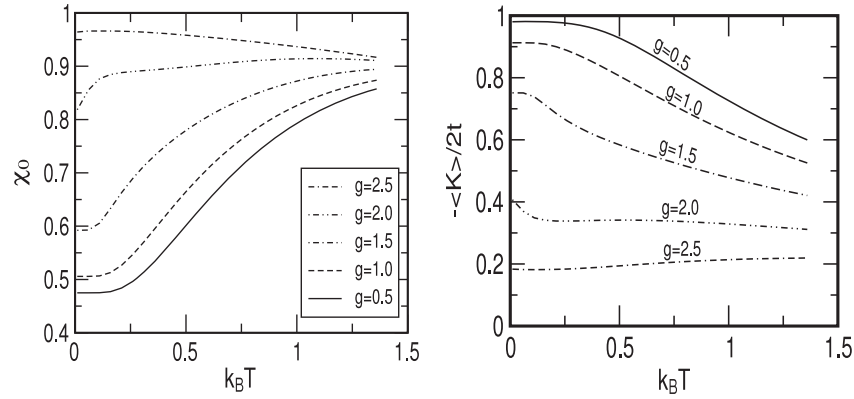
Figure 6. Variation of χ_0 and the kinetic energy $-\langle K \rangle /2t$ with temperature for the ordered four-site Holstein model for different values of g. Value of the hopping parameter used $t = 1.0$ in the energy scale of $\omega = 1$.

formation in the presence of e–ph coupling. In the strong coupling limit the dependence of the kinetic energy and the correlation function on the disorder strength is very weak. The reasons are explained in appendix A.

Figure 6 shows the variation of the on-site correlation function (χ_0) and the kinetic energy ($-\langle K \rangle$) with temperature for different g values. For weak and intermediate coupling χ_0 increases with increasing temperature. For strong coupling the effect of temperature is small but opposite (figure 6(a)). This shows that the lattice deformation associated with the polaron gets more and more localized with increasing temperature in the regime of weak and intermediate e–ph coupling, while for strong coupling the on-site deformation decreases and the polaron size gets larger with increasing temperature. The kinetic energy, on the other hand, decreases with increasing temperature for weak and intermediate coupling and increases for strong coupling (figure 6(b)). Our results agree with those of Hohenadler *et al* [25] who studied the 1d Holstein model by the quantum Monte Carlo method and observed the same variation of the kinetic energy with increasing temperature. We have also studied the ground state and the excited states of the polaronic system separately. It is found that for small or intermediate coupling the excited states have lower kinetic energy and smaller polaronic size than those of the ground state. For strong coupling, on the other hand, the ground state is a small polaron with smaller polaronic size and lower kinetic energy compared to most of the excited states. These result in lowering of the kinetic energy with increasing temperature for small and intermediate coupling and enhancement of the kinetic energy for strong coupling.

In figure 7 we have shown the variation of C_v as a function of g for the ordered and disordered systems for $k_B T = 0.1$. The specific heat shows a peak at intermediate coupling, which is suppressed with increasing disorder strength. Similar suppression of the specific heat peak due to disorder has also been observed for the two-site system. In figure 7 we have also shown the plots of χ_0^{avg} to show that the specific heat peak occurs in the region of g where χ_0^{avg} also undergoes a sharp change. However, the peak position in C_v, as mentioned previously, would be mainly decided by the tuning of the energy separation of two lowest levels of the system with the thermal energy at low temperatures.
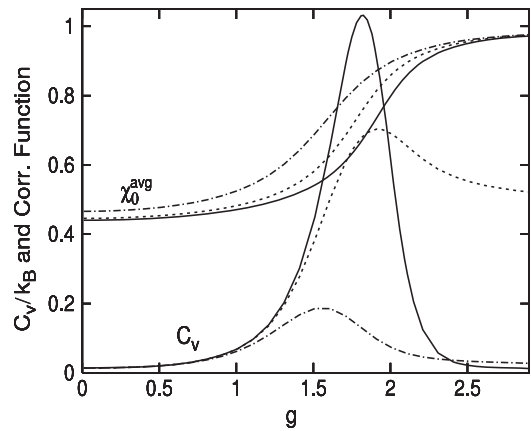
Figure 7. Variation of the specific heat (C_v/k_B) and the correlation functions χ_0^{avg} with g at a temperature $k_B T = 0.1$ for $t = 1.2$ for a different set of site potentials for the four-site Holstein model. Solid lines: ordered case, dashed line: disordered case with site potentials $(-0.5, 0, 0, 0)$, and dashed–dotted line: disordered case with site potentials $(-1, 0, 0, 0)$.

The kinetic energy contains contributions from both the coherent and incoherent hopping processes [26]. The Drude weight (in units of πe^2) represents the coherent part of the kinetic energy. The contribution from the incoherent hopping processes may be found out from the total kinetic energy and the Drude weight by using the f-sum rule (see appendix B):

$$-\frac{\langle K \rangle}{2} = \frac{\langle D \rangle}{2} + \langle S^{\text{reg}} \rangle \qquad (13)$$

where $\langle K \rangle$ and $\langle D \rangle$ are the thermal average of the kinetic energy and the Drude weight, respectively, and

$$S^{\text{reg}} = t^2 \sum_{n' \neq n} \frac{|\langle n| \sum_i (c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i)|n'\rangle|^2}{E_n - E_{n'}} \qquad (14)$$

is proportional to the contribution to the kinetic energy from the incoherent hopping processes.

We have studied the effect of e–ph interaction and the disorder on the Drude weight of the four-site Holstein model. The variation of the Drude weight with g for the ordered
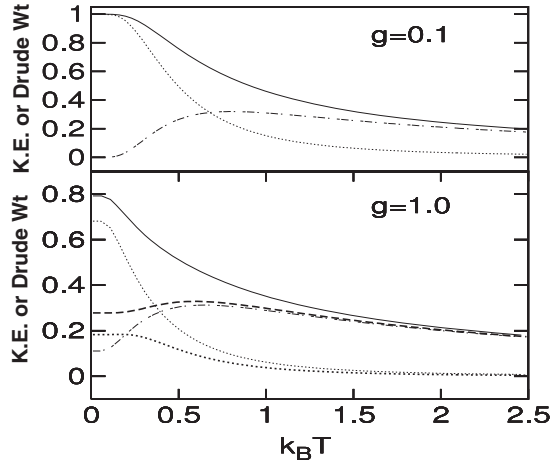
Figure 8. Plot of the kinetic energy $-\langle K\rangle/2t$ (solid lines), Drude weight $(D/2t)$ (dashed lines) and incoherent part of the kinetic energy (dotted–dashed lines) with $k_B T$ for the ordered lattice for $g = 0.1$ and 1. The dotted line and the thick dashed line show the variation of the Drude weight and the incoherent part of the kinetic energy, respectively, with temperature for the disordered lattice with site potential $(-1, 0, 0, 0)$ for $g = 1$. The value of the hopping parameter used $t = 0.5$.

Figure 9. Variation of the cross-over temperature (T_{cross}) with g for $t = 0.5$ for the ordered case.

and disordered (with site potentials $(-1, 0, 0, 0)$) systems are shown in figure 5 to make a comparison with corresponding plots of the kinetic energy. For the ordered case, the Drude weight and the kinetic energy have the same values at $g = 0$. This indicates that, in the absence of e–ph interaction and disorder, the entire part of the kinetic energy comes from coherent hopping. In the range of intermediate to strong coupling the Drude weight shows an exponential suppression with increasing g. The kinetic energy, on the other hand, shows an exponential suppression only in the range of intermediate coupling and a $1/g^2$ behavior in the strong coupling region. For the disordered case, the Drude weight is smaller than the kinetic energy even at $g = 0$ because of disorder-induced incoherent hopping. For strong coupling the Drude weight almost vanishes for both the ordered and the disordered cases, and the kinetic energy, consisting of only incoherent hopping, becomes very weakly dependent on the disorder strength.

We have investigated the effect of temperature on the coherent and incoherent parts of the kinetic energy by evaluating the kinetic energy and the Drude weight as a function of temperature for different values of g. Some representative plots (for $g = 0.1$ and 1) are given in figure 8. At low temperature the kinetic energy as well as the Drude weight show negligible dependence on temperature, represented by the flat region of the curves. This flat region is larger for smaller g. After the flat region the kinetic energy reduces exponentially with temperature. At high temperatures, where the Drude weight is very small, the kinetic energy may be fitted to a function $a/T + bT$. For a small value of g the value of b is very small and the kinetic energy varies approximately as $1/T$. In the temperature range $1.5 \leqslant k_B T \leqslant 2.5$ the values of a and b are, respectively, 0.477 and 0.003 for $g = 0.1$, and 0.376 and 0.012 for $g = 1.0$. The Drude weight shows almost exponential dependence on temperature both in the intermediate and high temperature ranges. A good fit
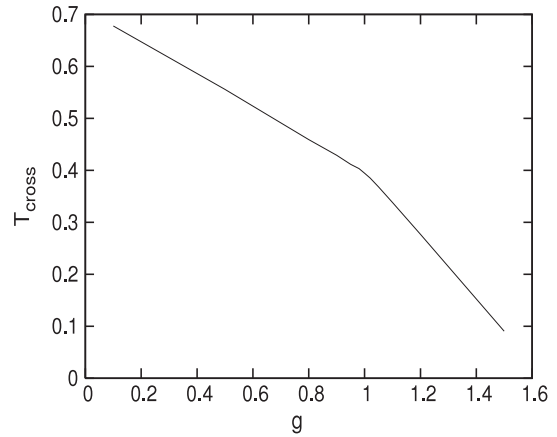
to the Drude weight is obtained with a function $a\mathrm{e}^{-bT}$, but with different values of the parameters a and b in the two (intermediate and high temperature) ranges. The part of the kinetic energy arising from incoherent processes increases with temperature, reaches a peak and then decreases with increasing temperature.

In figure 8 we have also shown the variation of the Drude weight and the incoherent part of the kinetic energy with temperature in the presence of disorder with site potentials $(-1, 0, 0, 0)$ for $g = 1$. It is seen that at low temperatures the effect of disorder is very large on both the Drude weight and the incoherent part of the kinetic energy. The Drude weight is rapidly suppressed while the incoherent part is enhanced a lot with the application of the disorder site potential. At high temperatures the Drude weight becomes very small for both the ordered and disordered cases. The disorder has little effect on the incoherent part of the kinetic energy at high temperatures.

For the ordered case we have determined the cross-over temperature (T_{cross}) from the intersection of the curves for the coherent and the incoherent part of the kinetic energy such that for $T < T_{\mathrm{cross}}$ the coherent part is dominant and for $T > T_{\mathrm{cross}}$ the incoherent part is dominant. The variation of T_{cross} with g is shown in figure 9. The cross-over temperature decreases with g. The T_{cross} versus g curve shows a sudden change in the gradient at $g = 1$ for $t = 0.5$ (this corresponds to the scaled e–ph coupling $\lambda = g^2 \omega/zt = 1$). The rate of fall of T_{cross} with g is higher in the region $g > 1$ than that for $g < 1$.

We would address now the possible size effect on the results. In appendix A we have derived a strong coupling effective polaronic Hamiltonian where the different coefficients (in equation (A.2)) have no size dependence provided the number of nearest neighbors (z) is the same. For a four-site system, $z = 2$, which is the same as that for an infinite 1d chain. The kinetic energy in the ground state, obtained from equation (A.2), for $z = 2$ is given by

$$K_G = -2t_p - 4\frac{t_p^2}{\omega} \sum_{n,m=0;n+m\geqslant 1}^{\infty} \frac{g^{2(n+m)}}{n!\, m!\, (n+m)}$$

$$-4\frac{t_p^2}{\omega} \sum_{n=1}^{\infty} \frac{g^{2m}}{m!\, m} \tag{15}$$

where $t_p = t e^{-g^2}$. The above expression clearly shows that for strong coupling the kinetic energy in the ground state should not have any size dependence if the number of nearest neighbors is the same, hence the kinetic energy for $N = 4$ will be the same as that for an infinite lattice, where N is the number of lattice sites. This is completely consistent with the results obtained in a recent numerical study by Hohenberg *et al* [25]. They obtained the same kinetic energy for $N = 4, 8, 16, 32$ for large g while a small size effect is observed for small and intermediate coupling. With increasing temperature the size effect is even smaller, as noted in [25]. Other authors [27, 28] have also pointed out that the size effect is not very significant in shaping different polaronic properties for the ordered Holstein model. However, the system size effect on the Drude weight of the polaronic system in the presence of disorder is not known to our knowledge and may be the subject of an interesting study.

4. Conclusions

We have investigated the effect of disorder and temperature on the properties of a polaron for a two- and four-site Holstein model. The disorder reduces the polaron size and suppresses the kinetic energy and the Drude weight. For strong coupling the polarons are practically immobile and the kinetic energy arises mainly from the to-and-fro motion of the (bare) electron between nearest-neighbor sites, keeping the center of the polaron fixed. In this regime the effects of disorder on the correlation functions and the kinetic energy are very small.

Increasing temperature also reduces the polaron size and suppresses the kinetic energy and the Drude weight for weak and intermediate e–ph coupling, while for strong e–ph coupling temperature has the opposite effect, i.e. the polaron size and the kinetic energy increases with increasing temperature.

The polaronic specific heat shows a peak in the intermediate coupling regime at low temperatures. The peak is suppressed in the presence of disorder.

The polaronic kinetic energy has contributions from the coherent and the incoherent hopping processes. The contribution from the coherent hopping (Drude weight) shows an exponential suppression in the region of intermediate to strong e–ph coupling. For strong coupling the Drude weight is very small and the kinetic energy, consisting of the incoherent part mainly, shows a $1/g^2$ dependence. For small and intermediate coupling the Drude weight shows an exponential suppression with temperature both in the intermediate and high temperature range. At high temperature the Drude weight is very small and the kinetic energy, dominated by the incoherent contributions, shows approximately a $1/T$ dependence. We have also identified a cross-over temperature below which the coherent part of the kinetic energy is dominant and above which the incoherent part is dominant. This cross-over temperature decreases with the increase of the electron–phonon coupling.

Appendix A

Applying the standard Lang–Firsov (LF) transformation to the Holstein model in equation (1) one obtains

$$
\begin{aligned}
\bar{H} &= e^R H e^{-R} \\
&= \sum_i (\epsilon_i - \epsilon_p) c_i^\dagger c_i - \sum_{i,j}' t_p c_i^\dagger c_j e^{g(b_i^\dagger - b_j^\dagger)} e^{-g(b_i - b_j)} \\
&\quad + \omega \sum_i b_i^\dagger b_i
\end{aligned} \tag{A.1}
$$

where $R = \sum_i g n_i (b_i - b_i^\dagger)$, $\epsilon_p = g^2 \omega$ is the polaron binding energy, $t_p = e^{-g^2}$ is the polaronic hopping strength and j is a nearest neighbor of i.

The second term of equation (A.1) represents the kinetic energy operator which involves zero-phonon as well as multiphonon processes (in the LF phonon basis) associated with the hopping of a polaron between nearest-neighbor sites. In the strong coupling limit, where t_p is very small, following a second-order strong coupling perturbation theory an effective expression for the kinetic energy terms (within the phonon ground state) may be obtained as [29]

$$
\begin{aligned}
H_{kin} &= -t_p \sum_{i,j}' c_i^\dagger c_j \\
&\quad - 2z t_p^2 \sum_{n,m=0;n+m\geqslant 1}^\infty \frac{g^{2(n+m)}}{n!\, m!\, (n+m)\omega} \sum_i c_i^\dagger c_i \\
&\quad - 2t_p^2 \sum_{n=1}^\infty \frac{g^{2m}}{m!\, m\omega} \sum_{i,k}'' c_i^\dagger c_k
\end{aligned} \tag{A.2}
$$

where z is the number of nearest neighbors. The first term of H_{kin} represents the coherent hopping of polarons without emission or absorption of phonons, while the second term originates from virtual hopping of a polaron from site i to a nearest-neighbor site j and back. This hopping is associated with virtual emission of multiphonons at the sites i and j followed by absorption of all the emitted phonons while hopping back. In this process the (bare) electron within the polaron undergoes forward and backward motion between nearest-neighbor sites, keeping the polaron immobile. The third term represents an effective hopping of a polaron from site i to a second nearest-neighbor site k via a common nearest-neighbor site j where multiphonons are created and then absorbed. For strong coupling the coefficients of the first and third terms in equation (A.2) become negligible and only the second term ($\sim t^2/\epsilon_p$) contributes to the kinetic energy. In the presence of disorder $(n+m)\omega$ in the denominator of the second term modifies to $(n+m)\omega \pm \epsilon_d$, where ϵ_d is the difference between the site potentials at sites i and j. The major contributions of this term for strong coupling comes from multiphonon processes with high values of $(n+m)\omega$ such that $(n+m)\omega \gg \epsilon_d$. As a consequence of the above reasons the coefficient of the second term in (A.2) as well as the kinetic energy in the strong coupling region becomes very weakly dependent on the disorder potential.

It may be mentioned that equation (A.2) is valid for any dimension and size of the system. The value of z would be different for different dimensions.

Appendix B

The Hamiltonian of the system in the broken time reversal symmetry may be written as

$$H(\phi) = -\sum_i (t e^{i\phi} c_i^\dagger c_{i+1} + \text{h.c}) + V \quad (B.1)$$

where V is composed of the electronic potential and interaction of electrons with the lattice. Let H_0 be the Hamiltonian of the system when $\phi = 0$, and the corresponding eigenenergies and eigenstates be E_n^0 and $|\psi_n^0\rangle$, respectively. If $E_n(\phi)$ be the eigenenergy of the Hamiltonian $H(\phi)$, the Drude weight for the nth eigenstate of the Hamiltonian H_0 is [22]

$$D_n = \left.\frac{\partial^2 E_n(\phi)}{\partial \phi^2}\right|_{\phi=0}. \quad (B.2)$$

Considering the terms involving ϕ as a perturbation in the Hamiltonian (B.1) a second-order perturbation calculation gives

$$E_n(\phi) = E_n^0 - i\phi t \langle \psi_n^0 | \left(\sum_i c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i \right) | \psi_n^0 \rangle$$
$$+ \phi^2 t^2 \sum_{n' \neq n} \frac{|\langle \psi_n^0 | (\sum_i c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i) | \psi_{n'}^0 \rangle|^2}{E_{n'}^0 - E_n^0}$$
$$+ \frac{\phi^2 t}{2} \langle \psi_n^0 | \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) | \psi_n^0 \rangle + \cdots. \quad (B.3)$$

Therefore

$$D_n = 2t^2 \sum_{n' \neq n} \frac{|\langle \psi_n^0 | (\sum_i c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i) | \psi_{n'}^0 \rangle|^2}{E_{n'}^0 - E_n^0} - K_n \quad (B.4)$$

where

$$K_n = -t \langle \psi_n^0 | \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) | \psi_n^0 \rangle \quad (B.5)$$

is the expectation value of the kinetic energy for the nth eigenstates of the Hamiltonian H_0. Taking the thermal average over all the eigenstates at a temperature T establishes the sum rule

$$-\frac{\langle K \rangle}{2} = \frac{\langle D \rangle}{2}$$
$$+ t^2 \left\langle \sum_{n' \neq n} \frac{|\langle \psi_n^0 | \sum_i (c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i) | \psi_{n'}^0 \rangle|^2}{E_n - E_{n'}} \right\rangle. \quad (B.6)$$

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