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Small polaron formation in many-particle states of the Hubbard-Holstein model: The one-dimensional case

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Abstract. We investigate polaron formation in a many-electron system in the presence of a local repulsion sufficiently strong to prevent local-bipolaron formation. Specifically, we consider a Hubbard-Holstein model of interacting electrons coupled to dispersionless phonons of frequency ω_0. Numerically solving the model in a small one-dimensional cluster, we find that in the nearly adiabatic case $\omega_0 < t$, the necessary and sufficient condition for the polaronic regime to occur is that the energy gain in the atomic (*i.e.*, extremely localized) regime $\mathcal{E}_{\rm pol}$ overcomes the energy of the purely electronic system $\mathcal{E}_{\rm el}$. In the antiadiabatic case, $\omega_0 > t$, polaron formation is instead driven by the condition of a large ionic displacement $g/\omega_0 > 1$ (g being the electron-phonon coupling). Dynamical properties of the model in the weak and moderately strong coupling regimes are also analyzed.

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1 Introduction

There is increasing evidence that polarons are formed in the lightly doped insulating phase of the high temperature superconducting cuprates [1,2] and in the high-temperature paramagnetic phase in doped manganites [3]. On the theoretical side, simple polaronic models like the Holstein and the Su-Schrieffer-Heeger models have attracted intensive studies in the last few years. However, whereas the cases of one or two polarons have been carefully investigated both numerically [4–10] and analytically [11,12], the case of many polaronic carriers is still incompletely understood. The relevance of electronic correlations in the materials mentioned above provides a strong motivation to study the combined effect of the electron-phonon coupling which leads to polaronic features and the strong electron-electron interaction. The main goal of the present work is to numerically investigate strongly correlated many-particle systems interacting with phonons in order both to identify a simple criterion for the formation of a polaronic state and to characterize the static and dynamical properties of such a state. We will only be concerned with the Hubbard-Holstein and the tJ-Holstein models, as minimal systems with local electron-electron (e-e) and electron-phonon (e-ph) interactions. In order to focus on the physics of unbound polarons (as opposed to bipolarons), we will always consider the limit of strong local e-e repulsion to prevent the formation of a local bipolaron [13]. The short-range character of the bare interactions considered in this model greatly simplifies the numerical analysis on finite clusters. Furthermore, the strong coupling limit of the e-ph interaction gives rise to small (single-site) polarons, which are individually rather well understood, thus providing a simple limit of the model. Since we focus on metallic states, we purposely avoid specific conditions (like, *e.g.*, quarter-filling) leading to ordered insulating states. Finally we confine our analysis to the one-dimensional case. This choice is an inescapable consequence of the smallness of our numerical clusters, but also allows for useful comparisons with the wealth of well-established physical results available in $d = 1$.

The model reads

$$\mathcal{H} = -t \sum_{\langle ij\rangle,\sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + h.c. \right) + U \sum_i c^\dagger_{i,\uparrow} c_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} + g \sum_{i,\sigma} \left[c^\dagger_{i,\sigma} c_{i,\sigma} - \langle c^\dagger_{i,\sigma} c_{i,\sigma} \rangle \right] \left(a_i + a^\dagger_i \right) + \omega_0 \sum_i a^\dagger_i a_i. \quad (1)$$

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We use units such that the lattice spacing $a = 1$ and also $\hbar = c = 1$. To make our analysis more complete, we also investigate the tJ-Holstein model, where the U term in (1) is replaced by an Heisenberg interaction $\mathcal{H}_J = J\sum_{\langle ij\rangle}(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4}n_i n_j)$, with the additional constraint of no double occupancy $\sum_\sigma c^\dagger_{i,\sigma}c_{i,\sigma} \leq 1$.

2 The small polaron criterion

A polaronic state can be characterized as a bound state of electrons and phonons, in which the electronic motion is accompanied by a significant lattice displacement. The strong coupling between the electron and the lattice strongly suppresses the electronic mobility. The carriers are therefore self-trapped in the potential well that they generated. The polaronic state is therefore characterized by two conditions: (a) the energy gain associated with the self-trapping must be larger than the loss of kinetic energy, and (b) the local lattice displacement must be sizeable, in order to significantly reduce the electronic hopping amplitude.

In previous analyses in the single-particle case of the Holstein model [8,9,12], emphasis was put on the difference in the criteria for polaron formation in the adiabatic ($\omega_0 < t$) or antiadiabatic ($\omega_0 > t$) regimes. In the adiabatic regime the crossover to polarons is dictated by the condition (a), since in this limit, as soon as a bound state is energetically favorable, the electron mobility is automatically reduced due to the large mass of the lattice. In the single particle case the energy of the strong-coupling polaronic state is $\mathcal{E}_{\rm pol} = -g^2/\omega_0$, while the free electron energy $\mathcal{E}_{\rm el} = -2dt$. Then the condition for single polaron formation in the nearly adiabatic ($\omega_0/t < 1$) case reads (see, *e.g.* Ref. [8]).

$$\lambda \equiv g^2/(2dt\omega_0) > 1. \tag{2}$$

In the antiadiabatic regime the crossover for the single-particle case is instead given by the condition (b), which in the Holstein model is expressed as $\alpha \equiv g/\omega_0 > 1$.

In the presence of many carriers and e-e correlations the electronic energies and the e-ph coupling are affected, so that the criterion for polaron formation in the adiabatic regime (which involves a condition on the energies) will be different in the many particle case with respect to the single particle one. On the other hand condition (b) ruling polaron formation in the antiadiabatic regime is not substantially changed by increasing the number of particles. In particular the slow dynamics of the electronic degrees of freedom when $\omega_0 \gg t$ strongly suppresses electronic screening processes. Therefore in the antiadiabatic regime the single-particle condition $\alpha = g/\omega_0 > 1$ of large ion displacement is expected to hold also in the many particle case.

For these reasons we mostly investigate here the physically relevant case of the adiabatic regime where the phonon frequency ω_0 is smaller than the electronic energy scale t (the typical electronic energy scale stays t even in the presence of correlations). The same analysis has also been applied to the antiadiabatic case, where it is confirmed that the single-particle condition $\alpha > 1$ holds in the many-particle case as well for all the considered values of parameters and fillings. Therefore we will only present results for the adiabatic regime. In this case the energetic balance condition rules the crossover. A polaronic bound state can therefore be realized only if the energy of such a state $\mathcal{E}_{\rm pol}$ is lower than the energy of the electrons in the absence of electron-phonon interaction $\mathcal{E}_{\rm el}$.

It is quite natural to generalize the condition (2) to the many-particle case by comparing the energy of the strongly coupled e-ph system, $\mathcal{E}_{\rm pol}$, where the polarons are strongly localized and the kinetic energy is negligible, with the energy of the purely electronic system (*i.e.* of the simple Hubbard or tJ models). In other words, we identify the value of the coupling for which the polaronic crossover occurs, $g = g_{\rm c}$, with the e-ph coupling above which the energy of the strongly polaronic state is lower than the energy of the purely electronic state. In this framework it is useful to generalize the definition of λ by defining the quantity

$$\tilde{\lambda} \equiv \mathcal{E}_{\rm pol}(g)/\mathcal{E}_{\rm el} \tag{3}$$

that reduces to λ for a single particle, and show that the criterion for small polaron formation in the general case of finite densities and in the presence of e-e correlation is $\tilde{\lambda} > 1$. Of course this criterion can only be significant provided the crossover between the purely electronic and the polaronic regimes is sufficiently sharp, as is indeed the case in the adiabatic regime [9].

The criterion $\tilde{\lambda} \equiv \mathcal{E}_{\rm pol}(g)/\mathcal{E}_{\rm el} > 1$ would be of little use if simple expressions in terms of the bare parameters or at least simple estimates of $\mathcal{E}_{\rm pol}(g)$ and $\mathcal{E}_{\rm el}$ were not available. Therefore, we now turn to the explicit evaluation of $\mathcal{E}_{\rm pol}(g)$ and $\mathcal{E}_{\rm el}$. Unfortunately, while some simple arguments allow an easy estimation of the energy in the strongly polaronic regime, the knowledge of the purely electronic energy (*i.e.* of the Hubbard model) is a much more difficult task. However, we point out that our goal is *not* to investigate the Hubbard model by itself, but rather to analyze the many-body effects of interaction on polaron formation, once a full knowledge of the purely electronic system (no matter how complicated) is assumed.

In order to evaluate the strong coupling energy $\mathcal{E}_{\rm pol}(g)$ we start from the atomic limit of zero hopping $t = 0$, in which the Hubbard-Holstein model can be exactly solved. In this case a Lang-Firsov canonical transformation allows the elimination of the linear e-ph coupling by introducing a shift $\alpha \equiv g/\omega_0$ of the ionic equilibrium position. An effective non-retarded attraction between the particles arises $U_{\rm attr} = -2g^2/\omega_0$, which must be compensated by a larger repulsion U to avoid (local) bipolaron formation. In this atomic limit each site is independent and each electron individually shifts the ionic site on which it resides forming a strong-coupling polaron of energy $\mathcal{E}_{1-{\rm pol}} = -g^2/\omega_0$. An opposite shift, but with identical energy gain, is induced by holes, so that, for $N_{\rm s}$ sites at average filling n the total energy is $\mathcal{E}^{t=0}_{\rm pol} = -N_{\rm s}n(1-n)g^2/\omega_0$. As soon as a finite hopping is introduced, a coherent kinetic energy

contribution arises, which, even in the absence of e-e interaction is exponentially small ($t^* = t\exp(-\alpha^2)$) and can safely be neglected in our estimate of the energy. However, more relevant additional corrections arise, which are due to incoherent virtual hopping processes of the electrons to neighboring sites. These processes naturally depend on the occupancy of the neighboring sites. If the site is unoccupied, the electron can hop onto it without paying any electronic repulsion U. However, this hopping occurs instantaneously without allowing the lattice time to relax. Therefore an intermediate virtual state of higher energy proportional to $g^2/\omega_0 \gg t$ is reached, before a second hop restores the initial configuration. In the limit of very strong e-ph coupling and accounting for the probability for a singly occupied site to have at least one empty site nearby, the virtual double-hopping process lowers the total energy by an amount of the order [14]

$$\mathcal{E}_{1/\lambda} \approx -2N_{\rm s}n(1-n)t^2/(g^2/\omega_0). \tag{4}$$

On the other hand a second incoherent correction to the polaronic energy occurs when the neighboring site is already occupied by an electron with opposite spin (for parallel spins this process is forbidden by the Pauli principle). In this case a virtual state is reached where an e-e interaction is also present giving rise to a superexchange coupling. In the case of finite e-e repulsion U, this term provides an additional incoherent contribution to the energy of the polaronic state. In a recent work [15] we showed that the e-ph coupling dresses the effective magnetic coupling J leading to an increase of its value. However, for a Holstein-like e-ph coupling no corrections to the purely electronic J arise up to order g^2/U. For the sake of simplicity we therefore estimate this contribution $\mathcal{E}_{\rm el}^J$ by using the value for $g = 0$ calculated by exact diagonalization.

As a result, the energy of the polaronic state can be estimated as

$$\mathcal{E}_{\rm pol} \approx -N_{\rm s}n(1-n)g^2/\omega_0 + \mathcal{E}_{1/\lambda} + \mathcal{E}_{\rm el}^J. \tag{5}$$

It is worth noting that in the above expression the bare e-ph coupling and phonon frequency appear. This is because in the strong-coupling regime, where the coherent motion of the polarons is suppressed, no screening occurs due to the very massive carriers. This situation is different from the case of a Fermi liquid, where the presence of the e-e interaction leads to a dressing of the e-ph coupling [16] and is complementary to the case of an interacting electron system near the Mott-Hubbard transition (or near the Luther-Emery point for one-dimensional systems), where Umklapp processes render the e-ph interactions ineffective: If a system is localized by the e-e interaction, this latter screens out the effects of the e-ph coupling and, conversely, if a system is localized by strong e-ph interactions (as in the present case), the e-e interactions have no effect on the phonon parameters.

The evaluation of the purely electronic energy $\mathcal{E}_{\rm el}$ of the Hubbard model is not possible in general unless one resorts to numerical methods. However, for the sake of simplicity, we consider a one-dimensional system for which we can evaluate the energy in a simple way using well-known results. In the $U = \infty$ limit an exact mapping exists between the Hubbard model and a system of free spinless fermions [17], and in the more general case of finite U the Bethe ansatz solution of the Hubbard model provides the exact results (see, *e.g.*, Ref. [18]). To make our calculation similar for the Hubbard and the tJ model, the alternative we chose is to directly carry out a numerical evaluation of the ground state energy of the purely electronic models on a one-dimensional cluster as a function of U or J and n.

We are now in a position to check the validity of the criterion $\tilde{\lambda}_{\rm c} \equiv \mathcal{E}_{\rm pol}(g_{\rm c})/\mathcal{E}_{\rm el} \sim 1$ by means of exact diagonalization of finite clusters. Due to the infinite set of accessible phonon states on each site, we need to truncate the phonon Hilbert space by allowing for a finite maximum number $N_{\rm ph}^{\rm Max}$ of phonons on each site. The crossover between quasi-free electrons and a polaronic state is signaled by rather abrupt changes in the behavior of most physical quantities; many quantities can be used to identify the crossover coupling, some examples of which are the electronic kinetic energy or effective mass, the electron-lattice correlation function or the average number of phonons per site, and so on. We identify the crossover value $g = g_{\rm c}$ separating the two regimes with the value of g for which the slope of the average number of phonons per site $\langle n_{\rm ph}(g)\rangle$ is maximum [20]. We always limited the calculation to values of g such that $\langle n_{\rm ph}(g)\rangle < N_{\rm ph}^{\rm Max}$ and checked that the result was well converged by changing $N_{\rm ph}^{\rm Max}$.

We performed calculation for various fillings in 5 and 6 sites clusters for $\omega_0/t = 0.2$. In Table 1 we report, besides the electronic energy and the magnetic energy, the crossover values of λ and $\tilde{\lambda}$ obtained using the numerically calculated values of $g_{\rm c}$.

As far as $\tilde{\lambda}$ is concerned, we report results obtained both neglecting the incoherent $1/\lambda$ contribution $\mathcal{E}_{1/\lambda}$ (sixth column, $\tilde{\lambda}_{\rm c}$) and considering such contribution (seventh column, $\tilde{\lambda}'_{\rm c}$)

Note that for $U = \infty$ an additional symmetry appears around quarter-filling ($n = 1/2$), making the filling $n = 1/5$ equivalent to $n = 4/5$ and $n = 2/5$ equivalent to $n = 3/5$.

It is evident from Table 1 that the criterion $\tilde{\lambda}_{\rm c} \approx 1$ is quite well satisfied, even neglecting the incoherent term, whereas the values of $\lambda_{\rm c}$ are significantly different for different parameters. This result is particularly remarkable since the energies $\mathcal{E}_{\rm pol}(g_{\rm c})$ and $\mathcal{E}_{\rm el}$ entering in the numerator and the denominator of $\tilde{\lambda}$ respectively, vary significantly with filling and Coulomb repulsion U (or J). Various observations are in order. First of all it is apparent that the calculation of $\tilde{\lambda}_{\rm c}$ without including the incoherent contribution $\mathcal{E}_{1/\lambda}$ to $\mathcal{E}_{\rm pol}$ gives quite homogeneous values of $\tilde{\lambda}_{\rm c} \sim 1$ (within 10%) for systems with different values of U or J, but similar filling. Larger discrepancies (but always smaller than 20%) exist between different classes of fillings. We notice that the values of $\tilde{\lambda}_{\rm c}$ for finite U or J are slightly underestimated because we estimated the magnetic energy in $\mathcal{E}_{\rm pol}$ taking the purely electronic contribution, which is known to be lower

Table 1. Filling (first column) and interaction (second column) dependencies of the total purely electronic energy (third column), of the purely magnetic energy (fourth column), of λ_c found with the maximum derivative of $\langle n_{ph}(g)\rangle$ (fifth column), and of the $\tilde{\lambda}_c$'s calculated *without* ($\tilde{\lambda}_c$) and *with* ($\tilde{\lambda}'_c$) the $\mathcal{E}_{1/\lambda}$ correction in $\mathcal{E}_{pol}$ for $\omega_0/t = 0.2$.

n	U	$\mathcal{E}_{el}$	$\mathcal{E}^J_{el}$	λ_c	$\tilde{\lambda}_c$	$\tilde{\lambda}'_c$
1/6	∞	−2.00000	0.	1.187	0.989	1.340
1/5	∞	−2.00000	0.	1.228	0.983	1.308
2/6	∞	−3.46410	0.	1.069	0.823	1.183
2/5	∞	−3.23607	0.	1.076	0.798	1.143
2/5	10	−3.48806	−0.14253	1.269	0.910	1.187
2/5	20	−3.35407	−0.06861	1.136	0.826	1.143
2/5	$J = 0.4$	−3.35407	−0.12572	1.182	0.883	1.186
2/5	$J = 0.2$	−3.29317	−0.05896	1.102	0.821	1.152
3/5	10	−3.71681	−0.30940	1.099	0.793	1.087
3/5	20	−3.46485	−0.14124	1.079	0.788	1.109
3/5	$J = 0.4$	−3.50730	−0.28743	1.002	0.767	1.109
3/5	$J = 0.2$	−3.36766	−0.13559	1.040	0.781	1.124
4/5	10	−3.22487	−0.92167	1.463	1.012	1.181
4/5	20	−2.60681	−0.45633	1.343	0.999	1.228
4/5	$J = 0.4$	−2.90651	−0.91216	1.201	0.975	1.204
4/5	$J = 0.2$	−2.45174	−0.45336	1.215	0.978	1.246

than in the presence of e-ph coupling [15]. This underestimation is proportionally more crude for larger J or smaller U values. Correcting for this effect should produce an even more uniform value for $\tilde{\lambda}_c$. The magnetic energy in the strongly polaronic regime is also different from $\mathcal{E}^J_{el}$ because the reduced itinerancy of the carriers obviously affects the spin correlations. Therefore a further refinement of the estimate of $\mathcal{E}_{pol}$ could be obtained by calculating the magnetic energy in the polaronic state taking $\mathcal{E}^J_{el}$ from the purely electronic model with $t = 0$. Also in this case a larger magnetic contribution would be found (when the carriers are localized the magnetic correlations are obviously stronger) and this would go in the direction of rendering the values for $\tilde{\lambda}_c$ more uniform.

An additional important ingredient in the estimate of $\tilde{\lambda}_c$ turns out to be the contribution $\mathcal{E}_{1/\lambda}$ of the incoherent hopping processes to $\mathcal{E}_{pol}$ (see Eq. (5)). The estimated filling dependent contribution (4) leads to a sizable modification of the criterion from $\tilde{\lambda}_c \sim 1$ to $\tilde{\lambda}'_c \sim 1.2$. However, despite this purely quantitative change, which was not considered in our previous single-polaron work [8], and which arises from a simple refinement of the estimate of the polaron energy, the physical meaning of the criterion stays the same. As a result of this latter filling-dependent improvement in the estimate of the polaron energy, the crossover values $\tilde{\lambda}_c$'s reported in the last column of Table 1 turn out to be more homogeneous with varying filling within each class of interaction values and the criterion $\tilde{\lambda}'_c \approx 1.2$ seems to be generically satisfied within a few percent.

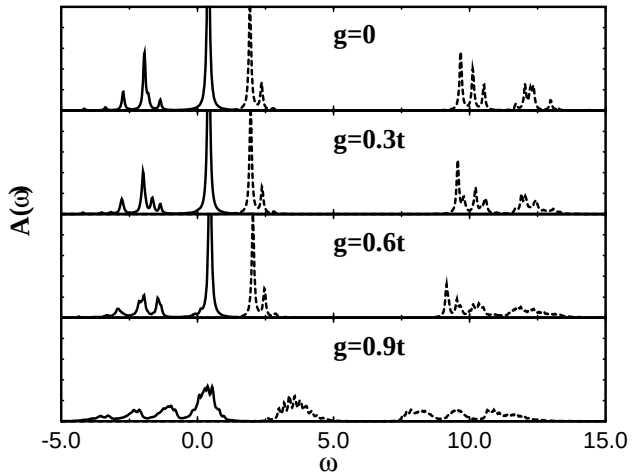

Fig. 1. Spectral density (solid line for PE, dashed line for IPE) for $U = 10\ t$ and $\omega_0/t = 0.4$, for various values of g and $n = 4/5$.

3 Dynamical properties

In the previous section, we characterized the crossover from weak to strong coupling regimes through the analysis of static properties, namely the average number of phonons. In this section we consider the effects of this polaron-formation crossover on dynamical properties such as the spectral densities $A(\omega)$ and the dynamical conductivity $\sigma(\omega)$. Here we report on this investigation for the specific but typical case of the Hubbard-Holstein model with $U = 10\ t$.

3.1 Spectral function

In this section we study the spectral density associated with the injection of an electron (inverse photoemission, IPE)

$$A^+_\sigma(\omega) = \frac{1}{N}\sum_{k,n} |\langle \phi^{M+1}_n | c^\dagger_{k\sigma} | \phi^M_0 \rangle|^2 \delta(\omega - (E^{M+1}_n - E^M_0)), \tag{6}$$

and the corresponding quantity for the emission of an electron (photoemission, PE)

$$A^-_\sigma(\omega) = \frac{1}{N}\sum_{k,n} |\langle \phi^{M-1}_n | c_{k\sigma} | \phi^M_0 \rangle|^2 \delta(\omega + (E^{M-1}_n - E^M_0)). \tag{7}$$

In Figure 1 we show the PE (solid line) and IPE (dashed line) spectral densities for a 5-site cluster and four electrons with $U = 10\ t$, for different values of g ranging from $g = 0$ to $g = 0.9\ t$.

A recent k-resolved spectral analysis in the two-dimensional tJ model with two holes [21], shows a markedly different behavior between the incoherent (local) excitations at high energies, not substantially affected by e-ph coupling, and the dispersive "quasiparticle" states

near the Fermi level, which become very massive with increasing g [22]. On the contrary this behavior is not present in our one-dimensional cluster, where the fact that electrons are composites of holons and spinons leads to all electronic excitations in the upper and lower Hubbard bands being incoherent. These are only marginally affected by the e-ph interaction and mainly display a broadening, which is particularly evident in the upper Hubbard band. A closer inspection also allows one to detect the effects of multiphonon excitations dressing the purely electronic states by forming "shoulders" or "combs" with excitation energies spaced by ω_0.

The presence of a phonon-induced retarded local attraction also reduces the local instantaneous Hubbard repulsion U. For the moderate $g = 0.3\ t$ and $g = 0.6\ t$, this attractive effect is not large enough ($\lesssim 2g^2/\omega_0 \lesssim 2$) to be clearly visible in a marked reduction of the gap between the lower and upper Hubbard bands. Rather a small leaking of spectral weight at the edges of the gap results from the much more evident broadening mentioned above. The effective phonon-mediated attraction increases the amount of doubly occupied sites in the ground state thus modifying the relative weight of the spectral densities related to the injection (inverse photoemission, IPE) or to the emission (photoemission, PE) of electrons, represented by the dashed and solid lines in Figure 1 respectively. For the large value of $U = 10\ t$ and for $g = 0.3\ t$ and $g = 0.6\ t$, which are substantially smaller than those leading to bipolaron formation, the amount of doubly occupied sites in the ground state is always small and its small changes do not significantly affect the relative weight of the photoemission and inverse photoemission spectral features. As a consequence one observes an approximate, but quite well-satisfied conservation of the spectral weight in the PE and IPE parts of the spectrum *separately* for moderate values of g. As the e-ph coupling is further increased to $g = 0.9\ t$ the energy gap between the upper and the lower Hubbard band is substantially reduced and the weight conservation no longer holds separately for the PE and IPE parts of the spectrum.

On the other hand, for the largest values of g we observe a substantial transfer of spectral weight from the upper Hubbard band, which is broadened and lowers its overall intensity, to the lower Hubbard band. This latter acquires weight essentially because the possibility of exciting phonons allows more states to be reached by injecting one electron in the system by conserving the momentum and without increasing the number of doubly occupied sites in the final state.

3.2 Optical conductivity

The real part of the conductivity for a one-dimensional tight-binding model at zero temperature may be expressed in terms of the Kubo formula

$$\sigma(\omega) = D\delta(\omega) + \sum_{n\neq 0} |\langle\phi_n|\mathrm{J}|\phi_0\rangle|^2 \delta(\omega - (E_n - E_0^M)), \quad (8)$$

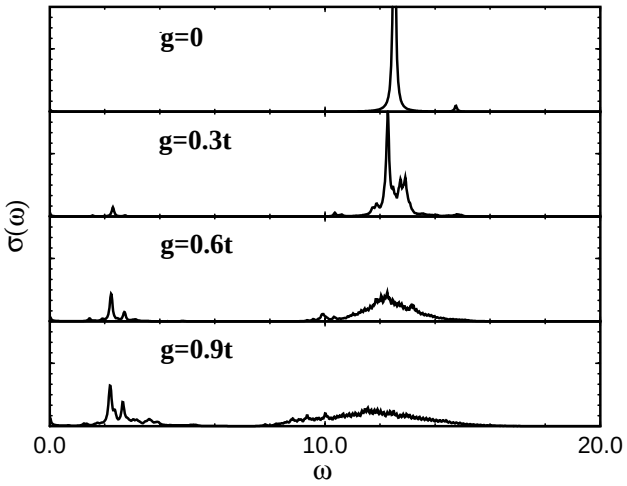

Fig. 2. Finite frequency optical conductivity for $U = 10\ t$ and $\omega_0/t = 0.4$, for various values of g and $n = 4/5$.

where J is the current operator. The finite frequency part (second term) can be straightforwardly calculated by means of the Lanczos algorithm. The coefficient of the zero frequency delta function contribution D is usually called the Drude weight and can be evaluated by combining the above with the well known sumrule for the total conductivity in terms of the kinetic energy $\langle H_\mathrm{t}\rangle$,

$$\int_0^\infty \sigma(\omega)\mathrm{d}\omega = -\frac{\pi e^2}{2}\langle H_\mathrm{t}\rangle. \quad (9)$$

In Figure 2 we show the behavior of the finite-frequency part of the dynamical conductivity for the same parameters as in Figure 1. Again the most apparent effect of the coupling with the phonons is a substantial broadening of the high-energy excitations. A second remarkable feature is represented by the marked increase of spectral weight at low frequencies. As in the case of the single-particle spectral density, this occurs because the possibility of phonon excitations accompanying electron particle-hole excitations allows for a large number of intraband transitions (*i.e.* between states with the same number of doubly occupied sites). This effect is made particularly apparent by the comparison with the $g = 0$ case ("uppermost panel" in Fig. 2), where the small number of sites and of holes strongly suppresses the weight at frequencies of order t [23].

As far as the zero-frequency contribution is concerned, although quasiparticle transport is absent in $d = 1$, there is still coherent charge (holon) transport. At $T = 0$ this leads to the presence of a δ-like Drude conductivity at zero frequency. It is noticeable that this ideal conductance behavior persists at finite values of g at least at $T = 0$ despite the non-integrable character of the model with $g \neq 0$.

The suppression of coherent charge transport *via* phonon dressing of the holon excitations leads to a strong decrease of the Drude spectral weight in the dynamical conductivity. As shown in Figure 3, the Drude weight related to absorption from coherent excitations at $\omega = 0$ decreases slowly in the weak-coupling regime ($\lambda \lesssim 1$)

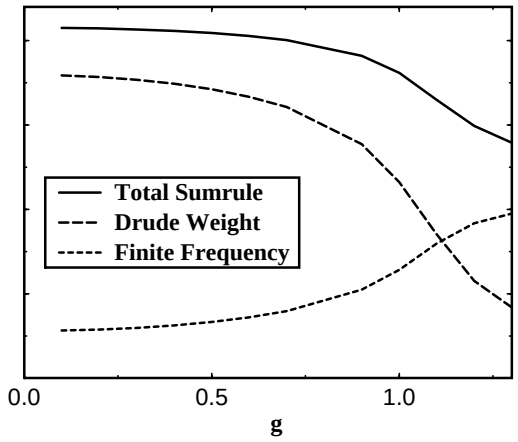

Fig. 3. Integrated optical conductivity (Total Sumrule), Drude weight and finite frequency weight as functions of g for $U = 10$ t, $\omega_0/t = 0.4$ and $n = 4/5$.

whereas it is strongly suppressed for larger e-ph coupling when the polaronic crossover sets in. In the latter case the rapid decrease is consistent with the usual exponential decrease of the charge-carrier band-width $v \to v \exp -\alpha^2$. The only difference is now that in $d = 1$, v no longer is to be interpreted as the Fermi velocity of quasiparticles, but is related to the holon dispersion. On the other hand, by increasing g, spectral weight is transferred to higher energies, as indicated by the increase of the finite frequency weight in Figure 3.

Although we cannot easily access the very strong coupling regime, we also checked in a few cases that for stronger couplings than those reported in the figure, this incoherent high-energy part of the absorption also decreases, but more slowly, according to the expected $1/g$ behavior. The overall decrease of the total absorption is a natural consequence of the sum rule (9) relating the frequency integrated dynamical conductivity to the average kinetic energy.

4 Conclusions

In this work, we have investigated the electron-polaron crossover in the many-particle case. We mainly considered the adiabatic regime, in which the condition for polaron formation is modified with respect to the single-particle case. The main result is that a clear criterion has been identified determining the strength of e-ph coupling leading to polaron formation. Remarkably, a simple physical interpretation of the criterion is still possible in the many-particle case provided that the single electron energy is replaced by the many-body purely electronic energy and the magnetic energy contribution is considered in the polaronic phase.

The effects of the intermediate polaronic regime have also been investigated on the dynamical properties. In particular, both in the single-particle spectral density and in the optical conductivity, we find that the electron-to-polaron crossover leads to a broadening of the high energy ($\omega \sim U$) features. At the same time the increase of momentum conserving processes due to the mixed electron-multiphonon character of the excitations substantially increases the weight of intraband ($\omega \sim t$) processes.

The above scenario was investigated by numerical exact diagonalization of a 5-site cluster. This leads to several limitations. First of all the presence of finite size effects in such a small system forces the analysis to be limited to short-range models. Even the analysis of models with a nearest-neighbor intersite e-ph coupling like the Su-Schrieffer-Heeger model lead to substantially larger finite-size effects. Another quite interesting problem, which we could not address within our small-cluster analysis is related to the competition with other phonon-driven instabilities like charge-density-waves (CDW), phase separation or incommensurate stripe formation. Even in the case of these latter two instabilities, which are not Fermi-surface instabilities, the small size of our system does not allow for a systematic comparison with the polaron formation within our numeric analysis. On the other hand, some information can be gained by comparing our results with different analyses. In particular as far as phase separation and (with the inclusion of long-range Coulomb interactions) stripe formation, the analyses of references [16,24] indicate that they occur for e-ph couplings that are smaller than those leading to polaron formation. The approximate character of these analyses, however, still leaves room for further work in this direction. As far as commensurate CDW formation is concerned, the recent density-matrix renormalization group analysis of reference [25] in the infinite-U Hubbard-Holstein model at $n = 1/4$ indicates that the CDW instability competes strongly with polaron formation. However, in the adiabatic regime the CDW and the polaron instability occur nearby in the phase diagram (whereas polarons are favored in the antiadiabatic regime), so it is likely that the polaronic instability will win for fillings far from 1/4, which are less favorable for CDW.

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13. Strictly speaking, the local e-e repulsion only prevents the formation of on-site bipolarons, but allows for the formation of non-local bound states resulting from retardation and giving rise to interesting effects like charge-density waves or superconductivity.
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19. We choose periodic or antiperiodic boundary conditions in order to have a closed shell ground-state for every filling.
20. Obviously a sligthly different value for the crossover e-ph coupling could be obtained by calculating different physical quantities like, *e.g.*, the (electron-density)–(ionic shift) correlation function, but this would not affect our general conclusions.
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22. In this regard we notice in passing, that the e-ph coupling would be a natural probe to identify the different (propagating *vs.* incoherent) character of the excitations of electronic systems in more than one dimension.
23. We explicitly checked that, in the purely electronic case with five sites and four electrons, no transitions are permitted at frequencies of order t. This feature is not generic, and changes with system size and/or filling, but this does emphasize the role of phonons in opening new momentum-conserving channels available for optical transitions.
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