Small-polaron formation and optical absorption in Su-Schrieffer-Heeger and Holstein models

M. Capone, W. Stephan,* and M. Grilli
Istituto Nazionale di Fisica della Materia and Dipartimento di Fisica, Università di Roma ''La Sapienza,'' Piazzale Aldo Moro 2, 00185 Roma, Italy

(Received 7 June 1996; revised manuscript received 2 April 1997)

The conditions leading to small-polaron formation for a single charge carrier in the Su-Schrieffer-Heeger (SSH) model are compared with the Holstein model. From analytic perturbation theory and exact numerical diagonalization of small clusters different criteria are established, which however have a common physical origin: Polaron formation requires a sizable mass enhancement and a lattice deformation energy gain larger than the loss in the bare electron kinetic energy in both models. The optical absorption of the Su-Schrieffer-Heeger model in the polaronic regime is also shown to exhibit an additional feature not present in the Holstein model. This additional feature arises due to the bond nature of small polarons in the SSH model, and is determined by transitions from the ground state of the bonding character on a shortened bond to excited states of the antibonding character on the same shortened bond. [S0163-1829(97)02032-8]

I. INTRODUCTION

Electrons acquire polaronic character in the presence of a sufficiently strong electron-phonon (e-ph) coupling when they displace the ions around them and move carrying along the lattice deformation. Being accompanied by the much heavier lattice degrees of freedom, in the polaronic regime the carriers acquire large effective masses and, in some cases, may even be trapped in the potential well arising from the ionic displacement that they created.

In the present work we investigate the Su-Schrieffer-Heeger (SSH) model[1] in comparison with the Holstein model.[2] Due to their relative simplicity these models are the most frequently considered models for electrons and phonons interacting via a short-range potential and may well be taken as a suitable paradigmatic basis for investigating the physics of strongly interacting e-ph systems.

The concepts underlying polaron theory in these models are long standing and have found various theoretical substantiations over the last decades.[3] More recently the discovery of polarons in the insulating phases of high-temperature superconductors[4,5] has triggered numerical exact diagonalization analyses on models with strong e-e interactions.[6–8] However, the strong-coupling nature of the polaronic state does not allow reliable analytic approaches in the intermediate crossover region, which is of the greatest interest in order to quantitatively investigate the conditions for polaron formation. On the other hand, the multiphononic essence of polarons makes it difficult to approach the strong-coupling regime from the numeric point of view. A landmark in this context was provided by quantum Monte Carlo calculations in Ref. 9 where an interpolation formula was presented describing the critical e-ph coupling leading to polaron formation in the Holstein model.

The polaronic properties of the Holstein model, where the electron density is coupled to an optical phonon mode, have been much studied, and a remarkable part of the work has been devoted to the study of the optical response, which is reasonably well understood.[10–13] On the other hand, the SSH or nonlocal coupling model has received little attention in this regard. In general both forms of e-ph coupling are present in real materials, with the relative importance of each depending on the detailed structure of the material.[14]

One goal of this paper is to provide a picture of small-polaron formation in the SSH model and to show that this picture and the analogous one for the Holstein model can be understood in terms of the same physical concepts. We show that polaron formation in both models occurs when two physical criteria are satisfied: A sizable mass enhancement, and lattice deformation energy gain larger than the loss in the bare electron kinetic energy.

The second major goal of this paper is to demonstrate that the optical response of the SSH model exhibits some features which are quite distinct from those of the Holstein model.

The SSH model is described by the Hamiltonian

$$\mathcal{H}=-t\sum_{\langle ij\rangle} c_i^\dagger c_j+\omega_0\sum_i a_i^\dagger a_i+g\sum_i [(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i) \times(a_{i+1}^\dagger+a_{i+1}-a_i^\dagger-a_i)] \quad (1)$$

and the Holstein model by

$$\mathcal{H}=-t\sum_{\langle ij\rangle} c_i^\dagger c_j+g\sum_i c_i^\dagger c_i(a_i+a_i^\dagger)+\omega_0\sum_i a_i^\dagger a_i . \quad (2)$$

We use units such that the lattice spacing $a=1$ and also $\hbar=c=1$.

Since we will restrict ourselves to the single-electron case we will not consider electron spin indices throughout this paper. Moreover, in short-range models, where only small polarons can be formed in the strong-coupling regime, dimensionality is not a qualitatively relevant parameter.[9] Therefore, for simplicity and for restrictions in our numerical analysis, we confine ourselves to the one-dimensional case. The first term in Eqs. (1) and (2), proportional to the nearest-neighbor hopping integral t (which we will take as our unit of energy) gives rise to a tight-binding band structure of the form $E(k)=-2t\cos(k)$. A dispersionless $[\omega(q)=\omega_0]$ Einstein phonon is created by the field $a_i^\dagger$ and is coupled to the

covalent bond variable $c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i$ in the SSH model and to the local electronic density in the Holstein model. For the Holstein model, the coupling arises from the dependence of the local atomic energy (i.e., the Madelung energy) on the ionic position. This coupling is relevant when the screening of the Madelung potential is poor, and is believed to be nonnegligible in the superconducting cuprates.[15] On the other hand, the covalent e-ph coupling in the SSH model is due to the dependence of the hopping integral on the relative distance between two adjacent ions.[1] Notice that our SSH model differs from the conventional one in having optical (instead of acoustic) phonons like the Holstein model: To clarify more easily the common mechanisms underlying the polaron formation in the two models we avoided unnecessary differences between them, thus focusing on the role played by the different e-ph couplings. Moreover, despite the completely different origin of the e-ph coupling in the two models, we choose the same notation g to emphasize the generic character of the physical processes that we are going to present.

II. CRITERION FOR POLARON FORMATION

A. General considerations

Before addressing the problem of the single polaron formation in a more formal way within the above models, we first would like to provide simple and intuitive arguments (all the following general arguments apply in a generic dimensionality d). As mentioned above, the setting in of a polaronic regime is characterized by *both* a strong reduction of the effective hopping matrix element due to a sizable local displacement of the ionic positions *and* a lattice deformation energy gain larger than the loss of bare kinetic energy.

Before considering the SSH model, we consider how the fulfilling of these two conditions occurs in the Holstein model. For the Holstein model, these effects are directly related to two parameters which are often introduced in this field: $\lambda \equiv g^2/(2dt\omega_0)$ and $\alpha \equiv g/\omega_0$. λ represents the ratio between the polaronic binding energy $E_p=-g^2/\omega_0$ in the strong-coupling limit and the *bare* average kinetic energy of the electrons of the order of half the bandwidth ($\sim -2td$). Notice that the bare hopping t has to be used here. In fact this is of the order of the kinetic energy actually lost when the polaron is formed. Then the value of λ determines the convenience for the system to give up the kinetic energy gain arising from the hopping to gain the lattice deformation energy induced by the local e-ph potential. On the other hand, as is clear from a standard Lang-Firsov transformation of the Holstein model,[16] α represents half the ionic displacement in units of $(2M\omega_0)^{-1/2}$, where M is the ionic mass. It is intuitive that the strong reduction of the effective hopping matrix element is governed by the amount of lattice displacement. However, a crucial role in this regard is played by the adiabatic ratio ω_0/t. In particular, in the antiadiabatic regime $\omega_0 > t$, phonons are energetically costly and only their vacuum state couples effectively to the low-energy hopping processes. Then the small overlap of phononic ground-state wave functions on neighboring sites exponentially reduces the hopping amplitude.[17] In this case it is apparent that α governs the mass enhancement. The energetic ratio $\lambda=\alpha^2\omega_0/2td \gg 1$ is also in favor of the lattice deformation, so that polarons in the antiadiabatic regime of the Holstein model are formed as soon as $\alpha \approx 1$. Notice that the condition $\lambda > 1$ in this specific case is not sufficient to determine a polaronic crossover.

On the other hand, a sizable lattice displacement is not enough to give rise to a large mass enhancement in the nearly adiabatic regime ($\omega_0 < t$), because phonons can be created rather easily. Then the effective hopping matrix element no longer arises only from the overlap of the phonon vacuum states on adjacent sites, but to a large extent it involves the overlap of excited states also, whose spatial extension is larger. Therefore, in this regime the reduction of the hopping matrix element is less severely affected by large values of α. In this case, where $t > \omega_0$, the more restrictive condition on the ratio between deformation energy gain and kinetic energy loss ($\sim t$) plays a relevant role and $\lambda \approx 1$ determines the onset of polaron formation. This also establishes a direct connection[3] between the polaronic intermediate-coupling regime and the standard Fermi-liquid perturbation theory[18] where the mass enhancement is given by $m^*=m(1+\lambda)$.

In summary, *the simultaneous occurrence of the two conditions* $\lambda > 1$ *and* $\alpha > 1$ *is needed to characterize and to determine polaron formation in the Holstein model*. In particular, one can immediately recognize from the definition of λ and α that a crucial role is played by the adiabatic ratio ω_0/t. If ω_0/t is small, the condition for a large $\lambda=\alpha^2\omega_0/2td$ is more difficult to realize than $\alpha > 1$, and polaron formation will be determined by the more restrictive $\lambda > 1$ condition. The opposite is true when the system is in the antiadiabatic regime $\omega_0/t > 1$.

This intuitive argument was already implicit in the interpolation formula Eq. (4.1) in Ref. 9 once this is expanded in the two opposite limits $\omega_0/t \gg 1$ and $\omega_0/t \ll 1$.

On the other hand, it will be shown that in the SSH model the value of λ still determines the energetic advantage in deforming the lattice and losing kinetic energy. However, the mass enhancement is ruled by a different mechanism with respect to the Holstein model [see Eq. (14) below] and is directly related to λ regardless of the value of the adiabatic ratio ω_0/t. Therefore λ determines *both* the energetic advantage in deforming a bond *and* the suppression of the hopping integral associated with the lattice distortion and it will be the relevant parameter for the description of the system for any value of ω_0/t. All these intuitive arguments will be substantiated below by analytic calculations and numerical exact diagonalization of small clusters.

B. A first insight from perturbative calculations

The above arguments may be made more formally precise within a perturbative analytic calculation in the limit of small e-ph coupling ($g \ll t, \omega_0$). In this case we evaluated the second-order correction to the electronic self-energy represented in the diagram of Fig. 1.

To explore both the adiabatic and the antiadiabatic regimes, we cannot apply Migdal's theorem to discard vertex corrections: Our approximation only relies on the small value of g. This also allows for the simplification of using the bare electronic Green function instead of carrying out a

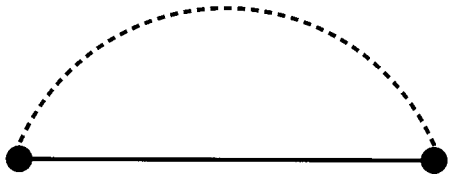

FIG. 1. Lowest-order self-energy diagram of the electron propagator. The solid line is the bare electron Green function; The dashed line is the bare phonon propagator. The dots represent the e-ph coupling.

self-consistent evaluation including the full Green function inside the self-energy diagram.

For the sake of simplicity and to allow for a more direct comparison with the numerical results on small clusters, we only deal with one-dimensional systems. Nevertheless, we explicitly checked in the easier case of the Holstein model that our analytic results apply to multidimensional cases as well.

For our purposes we only need the perturbative corrections to the effective mass

$$\frac{m^*}{m}=\frac{1-\partial Re\Sigma(k,\omega)/\partial\omega|_{\omega=-2t,k=0}}{1+\partial Re\Sigma(k,\omega)/\partial E_k|_{\omega=-2t,k=0}}. \tag{3}$$

It is quite obvious that the polaronic regime cannot be attained within our lowest-order perturbative approach: The cloud dressing the electrons in a polaronic excitation involves multiphononic processes, which are not included in the diagram of Fig. 1. Nevertheless valuable indications on the beginning of the polaronic crossover can be extracted from the above expression. In particular, one can determine the parameters for which the effective mass starts to grow $[(m^*-m)/m\sim 1]$, also marking the region where perturbation theory is no longer applicable.

In the SSH model the bare e-ph vertex in $d=1$ associated with scattering of an electron from a k to a $k+q$ Bloch state has the following form:

$$g_{k,k+q}=2ig[\sin(k+q)-\sin(k)]. \tag{4}$$

Consequently, once a frequency integration is carried out, the self-energy is given by

$$\Sigma(k,\omega)=4g^2/N\sum_q \frac{1}{\omega-\omega_0-\epsilon_{k+q}+i\delta} \times[\sin^2(k+q)+\sin^2(k)-2\sin(k)\sin(k+q)]. \tag{5}$$

To obtain the effective mass and the ground-state energy of a single electron in the bottom of the band, we only need to evaluate $\mathrm{Re}\Sigma(k=0,\omega)$ and its derivatives in the $k=0$ state and for $\omega=E(k=0)=-2t$, finding

$$\frac{m^*}{m}=1+\lambda\left[\frac{8\omega_0}{\sqrt{\omega_0^2+4t\omega_0}}+\frac{2\omega_0}{t}\left(\frac{2t+\omega_0}{\sqrt{\omega_0^2+4t\omega_0}}-1\right)\right]. \tag{6}$$

By expanding the perturbative correction in Eq. (6) in the two opposite, adiabatic ($\omega_0\ll t$) and antiadiabatic[19] ($\omega_0\gg t$) limits, we get

$$m^*=m\left(1+6\lambda\sqrt{\frac{\omega_0}{t}}\right)\quad \omega_0\ll t, \tag{7}$$

$$m^*=m(1+8\lambda+2\alpha^2)\quad \omega_0\gg t. \tag{8}$$

The electrons in the SSH model in the fully adiabatic limit $\omega_0=0$ are completely free ($m^*=m$). This is due to the vanishing of the bare e-ph vertex for small transferred momenta q [cf. Eq. (4)], which overcompensates the divergent density of states in the integral of Eq. (5). Physically this effect arises because many electronic states lie close to the $k=0$ point, but the phonon-mediated scattering between them occurs at low momentum transfer, which is less effective in the SSH model, where phonons decouple from the electrons in the long-wavelength limit.

Equation (7) shows that the effective mass enhancement is governed by λ in the adiabatic limit. The extra factor of $\sqrt{\omega_0/t}$ arises from the vanishing value of the e-ph vertex (4) at the bottom of the one-dimensional band, as can be checked by considering a finite density of electrons with a Fermi energy μ away from the bottom of the band. We will come back to this point when we will compare this behavior with the Holstein model. In the antiadiabatic limit the mass enhancement in the SSH model [Eq. (8)] involves both α^2 and λ. In this limit $\lambda\gg\alpha^2$ and therefore the mass correction is dominated by λ also in the antiadiabatic regime. This behavior is a consequence of the specific localization mechanism that occurs in the SSH model (we defer the discussion on this point after the numerical analysis presented in the next section) and can be contrasted with the different behavior of the Holstein model, for which the self-energy for a single particle in $d=1$ is given by[20]

$$\Sigma(\omega)=\frac{\lambda\omega_0}{\sqrt{[(\omega-\omega_0)/2t]^2-1}}, \tag{9}$$

where the real part of the square root has the same sign as $(\omega-\omega_0)$. Notice that the self-energy is momentum independent because the bare e-ph vertex is also momentum independent. This feature allows the introduction of the density of states in the momentum integrals, thus leading to a straightforward extension of our results above one dimension.

From Eqs. (9) and (3) we find

$$\frac{m^*}{m}=1+\frac{2\lambda t(2t+\omega_0)}{\sqrt{\omega_0}(4t+\omega_0)^{3/2}}. \tag{10}$$

Also in this case we evaluate the mass correction in the adiabatic and in the antiadiabatic limits

$$m^*=m\left(1+\frac{\lambda}{2}\sqrt{\frac{t}{\omega_0}}\right)\quad \omega_0\ll t, \tag{11}$$

$$m^*=m(1+\alpha^2)\quad \omega_0\gg t. \tag{12}$$

In agreement with the intuitive arguments presented at the end of the previous section, the antiadiabatic result shows that the mass enhancement is driven by the condition $\alpha>1$, which is more restrictive than $\lambda>1$.

On the other hand, as expected, the adiabatic result for the mass enhancement is proportional to λ. This contribution is also proportional to $\sqrt{t/\omega_0}$, which is large in this limit, which seems to contrast with the usual perturbative calculations within Fermi-liquid theory,[18] where only a correction of order λ is predicted. This feature arises from the singular density of states at the bottom of a one-dimensional band, as can be checked by considering a finite density of electrons with a finite Fermi energy μ away from the bottom of the band. In this latter case the coefficient of the mass correction becomes $\sqrt{t/(\omega_0+\mu)}$ and is no longer singular in the adiabatic limit.[21] This specific, nongeneric result is the price that we have to pay in order to take advantage of the simpler analytic treatment in one dimension, but it does not hide the important finding that only the λ parameter rules the polaron formation when $\omega_0 < t$. Moreover it is worth noting that our simple, lowest-order perturbative calculation already gives a strong indication that one electron in a fully adiabatic[22] (i.e., $\omega_0 \equiv 0$) one-dimensional Holstein lattice is localized ($m^* \to \infty$). In light of our calculation, this well-known result[23] can easily be attributed to the singular density of states.[24]

C. Exact diagonalization analysis

In order to set the above scheme for the single-polaron formation in the SSH model on more solid ground, we performed exact numerical calculations on small clusters by means of the Lanczos algorithm. As usual,[20] we truncate the phononic Hilbert space so as to include only a finite number of phonons per lattice site. To reliably explore the strong-coupling regimes, we had to include up to 50 phonons per site (and check the convergence of the results by varying the phonon number). Due to the huge enlargement of the Hilbert space induced by the presence of the lattice degrees of freedom, we have only been able to investigate small clusters up to four sites.[25] In such small clusters finite-size effects are obviously relevant. However, we checked that as far as the criterion for polaron formation is concerned, our results are rather insensitive to the boundary conditions and no qualitative changes occur in passing from three- to four-site lattices: In the short-range models considered here, polaron formation is a local, high-energy phenomenon. Small bond-polaron formation in the SSH model is characterized by the shrinking of the bond on which the electron is localized due to the enhancement of the effective hopping between the two sites. At the same time the neighboring bonds are stretched and the hopping between the two occupied sites and the surrounding ones is reduced resulting in a tendency towards localization. Eventually the hopping between the two sites and the rest of the lattice vanishes and may even change sign. This pathological situation is a well-known feature of the SSH model, which in real systems never occurs due to higher-order corrections to the expansion of the hopping parameter t in terms of the ionic displacement. For all couplings where we find polaron formation in the SSH model, we checked that these pathologies do not occur. We also notice that, by increasing the phonon frequency, the effective hopping is relatively less affected, so that larger values of λ can be reached before the zero-hopping pathology is found. As a consequence, the region with substantial polaronic character is enlarged.

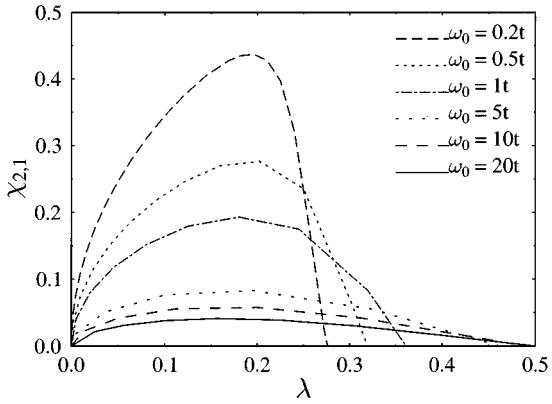

FIG. 2. Local density-displacement correlation function $\chi_{2,1}$ for the SSH model and one electron in a four-site lattice with periodic boundary conditions. The curves are labeled by ω_0/t: Curves with larger maxima correspond to smaller values of ω_0/t.

To extract information on the values of g at which the polaron crossover begins we analyzed the correlation function between the electronic density on a site i and the ionic displacement on the site $i-\delta$

$$\chi_{i,\delta} \equiv \langle \phi_0 | c_i^\dagger c_i (a_{i-\delta} + a_{i-\delta}^\dagger) | \phi_0 \rangle, \tag{13}$$

where $|\phi_0\rangle$ is the ground state of the system.

For the SSH model we specifically investigated the behavior of the density-displacement correlation functions $\chi_{i,0}$ and $\chi_{i,1}$ for different values of the adiabatic parameter ω_0/t as a function of the e-ph coupling constant. The calculation was performed on a four-site lattice with open boundary conditions. The density-displacement correlation functions, as all physical quantities, are smooth functions of the e-ph coupling for all finite phonon frequencies. Whereas $\chi_{i,0}$ always increases with g, $\chi_{i,1}$ first increases and then decreases in the strong-coupling regime. This agrees with the well-known result that polarons are small in models with short-range e-ph interactions: Well formed polarons are so local that the presence of a fermion on a site is uncorrelated with the ionic displacements on neighboring sites. We also found that the adiabatic regime is characterized by a rather sharp crossover, whereas the crossover for larger phonon frequency is increasingly smooth as the phonon frequency increases. Since polaron formation is a crossover without symmetry changes between two phases, some arbitrariness is unavoidable in defining a criterion separating the free-electron and the polaronic regimes. In particular we choose the critical g from the point of maximum of the nearest-neighbor density-diplacement correlation function $\chi_{i,1}$. We checked that different criteria (like, e.g., the maximum slope of the local density-displacement correlation function $\chi_{i,0}$) provide the same qualitative results.

In Fig. 2 we display the result for $\chi_{i,1}$ as a function of λ in the SSH model for various values of ω_0/t. It is apparent that, while the position of the maximum is substantially independent of the phonon frequency, the width of the curve substantially broadens with increasing ω_0/t.

The phase diagram of Fig. 3(a) is calculated using the results for the correlation functions as shown in Fig. 2. The critical λ as a function of ω_0/t is indicated with a solid line. We also show the crossover region, defined as the range of

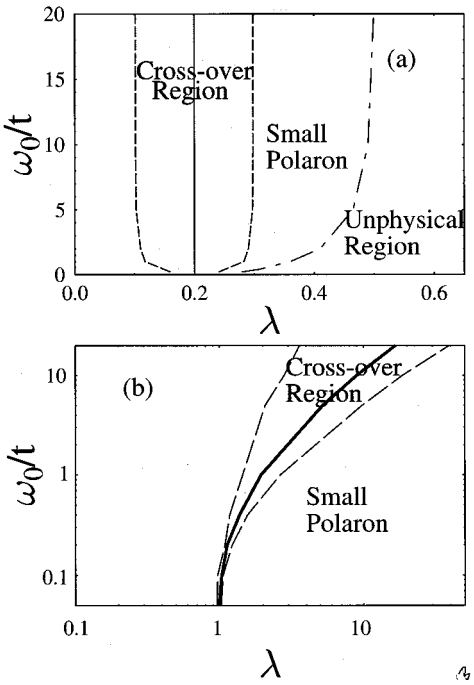

FIG. 3. Phase diagram for one electron in a four-site (a) lattice with open boundary conditions for the SSH model; (b) for the Holstein model (periodic boundary conditions). The solid line is the critical value of λ for the polaronic crossover; The crossover region is shaded and its boundary is indicated by the dashed lines. The dot-dashed line in (a) is the boundary of the pathological region for the SSH model.

parameters for which $\chi_{i,1}$ significantly changes. This region is estimated by the ''width'' at half the maximum of the same function. The pathological region of parameters at large g's is associated with the negative value of $\chi_{i,1}$, as a consequence of the unphysical negative value of the effective hopping matrix element.

As expected from the perturbative calculation, we find that the polaronic regime is determined by the condition $\lambda_c=$constant both in the adiabatic and the antiadiabatic regimes.[26] The specific mechanism of hopping reduction giving rise to localization in the SSH model, accounts for this difference with respect to the Holstein model.

For clarity we begin this discussion by considering the fully adiabatic limit.[22] In this case, at first order the hopping is reduced by the stretching of the bonds by $t^*=t-gu$, where u is the (dimensionless) value of the bond length variation in units of $(2M\omega_0)^{-1/2}$ (notice that for $\omega_0\to 0$, g has to vanish but gu stays finite).[22] We can write $u=\gamma g/\omega_0$ for the SSH model even if the Lang-Firsov result $u=g/\omega_0$ is not valid for this model. Numerical calculations show that γ is a weakly decreasing function of ω_0/t, so that, at least to leading order the reduction of the effective hopping matrix element is governed by the value of λ

$$t^*=t-gu=t\left(1-\gamma\frac{g^2}{2\omega_0 t}\right)=t(1-\gamma\lambda). \tag{14}$$

In the-strong coupling regime the electron is localized on a single bond and the many-site model becomes equivalent to a two-site cluster. Then, for such a small system, an analytic solution is possible giving $\gamma=4$ for the constant appearing in Eq. (14). Thus λ determines the reduction of the effective hopping when the lattice displacement is sizable.

As for the Holstein model case, another condition needs to be satisfied in order to have a polaronic regime: The energy gain due to the polaron formation, i.e., the typical energy of a self-trapped carrier has to be larger than the loss in bare kinetic energy associated with the self-trapping. Since in the strong-coupling regime the electron localizes on a single bond the polaronic binding energy is given by the strong-coupling energy of a two-site cluster. The solution of the two-site cluster shows that the polaron energy for the SSH model still contains a contribution from the free-electron hopping, arising from the delocalization of the electron between the two sites of the bond. Then the ground-state energy is given by $E_0=-t-2g^2/\omega_0$. We divide this energy by the free-electron energy $-2t$ to obtain the ratio of the energy gain associated with polaron formation to the energy loss associated with the decrease of electronic mobility.[27] If we explicitly evaluate the range of λ values for which

$$(-t-2g^2/\omega_0)/(-2t)>1, \tag{15}$$

we readily obtain $\lambda>0.25$. This value coincides with the value at which the hopping matrix element vanishes according to Eq. (14) and to the adiabatic limit of the parameter $\gamma=4$. This implies that when $\omega_0\to 0$, the system will have no energetic advantage in localizing the electron on a bond, unless the pathological condition $t^*=0$ is reached. According to the physical idea that *both* a sizable lattice displacement *and* an energy gain from deformation larger than the kinetic energy loss are required to realize a polaronic state, one should not expect polarons in the adiabatic limit of the SSH model. Indeed, we carried out the exact diagonalization of large clusters (100 sites) in the extreme adiabatic limit finding that the SSH model does not present any marked polaronic behavior for couplings smaller than the ''pathological'' g's at which the hopping changes sign.

For finite phonon frequencies this picture is modified by the lattice dynamics. The numerical study shows that the ground-state energy is not strongly effected by the lattice dynamics: regardless of the value of ω_0/t, λ larger than 0.25 remains the condition to obtain an energetic advantage from localization. On the other hand, the effective hopping matrix element is less severely reduced by the coupling to the lattice fluctuations and the value of λ for which the effective hopping becomes zero increases with ω_0/t [from Fig. 3(a), one sees that $\gamma\approx 2$ for $\omega_0/t\approx 20$]. Therefore, for finite ω_0, it is always possible to find a regime where the lattice deformation becomes energetically favorable and a substantial lattice displacement (i.e., hopping reduction) is present without having a nonphysical vanishing of the hopping. In this region, which is larger for large phonon frequencies [see Fig. 3(a)], the electron has a polaronic character for values of λ larger than $\lambda_c\approx 0.2$. Finite-size effects easily account for the small quantitative discrepancy between this value and the fully adiabatic estimate $\lambda_c\approx 0.25$.

The above result shows that λ determines both the reduction of the hopping integral associated with the lattice distortion and the tendency towards localization driven by the energetic advantage in deforming the lattice. It is then natural

to consider λ as the relevant parameter for polaron formation regardless of the value of the adiabatic ratio ω_0/t. Notice that this finding was also suggested by the perturbative result (7) and (8), showing that the main corrections to the effective mass are proportional to λ both in the adiabatic and in the antiadiabatic regime.

For the numerical analysis also, the results for the SSH model can be contrasted with the findings in the Holstein model, for which the phase diagram is reported in Fig. 3(b). In this case one sees that the condition leading to a polaronic regime is given by $\lambda>\lambda_c\approx 1$ only when $\omega_0<t$. At larger values of the adiabatic ratio polarons are formed for $\lambda>(\omega_0/t)_c$ thus implying $\alpha>1$. Also in the case of the Holstein model, then, the numerical analysis provides a substantiation to the general arguments of Secs. II A and II B.

III. OPTICAL ABSORPTION

A. Formalism

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

$$\sigma(\omega)=D\,\delta(\omega)+\Im\left\langle 0\left|J^{\dagger}\frac{1}{\omega-H+E_0-i\delta}J\right|0\right\rangle, \quad (16)$$

where J is the current operator.

The coefficient of the zero-frequency δ-function contribution D is usually called the Drude weight: it is given by

$$D=-\frac{\pi e^2}{2}\langle H_t\rangle-\sum_{n\neq 0}\frac{|\langle\phi_0|J|\phi_n\rangle|^2}{E_n-E_0}. \quad (17)$$

If the Drude weight D is nonzero the system is a perfect conductor;[28] this will generally be the case in such models with periodic boundary conditions (PBC) and no disorder at zero temperature.

In the Holstein model J is

$$J_H=iet\sum_i\,(c_{i+1}^{\dagger}c_i-c_i^{\dagger}c_{i+1}), \quad (18)$$

while for the SSH model it is

$$J_{\rm SSH}=ie\sum_{i\sigma}\,[t-g(a_{i+1}^{\dagger}+a_{i+1}-a_i^{\dagger}-a_i)](c_{i+1}^{\dagger}c_i-c_i^{\dagger}c_{i+1}). \quad (19)$$

The fact that $J_{\rm SSH}$ contains an explicit coupling to the phonon degrees of freedom is physically simple to understand: in this case the bond length is modified by the lattice distortion, so that the change in electric dipole moment associated with the hopping of an electron is modified proportionally. Here we have neglected in both cases the direct coupling of the electric field to the ions which is of order $\sqrt{m/M}$, where m and M are the electron and ion masses. We are interested only in the features resulting from the e-ph coupling, not in the direct excitation of the bare phonons. Equations (16)–(19) may be derived following the standard approach used, for example, in the case of the Hubbard model.[29]

The use of the Lanczos algorithm to evaluate correlation functions such as Eq. (16) is well established.[30] The finite-frequency part of Eq. (16) has previously been studied by Alexandrov *et al.*[12] for the Holstein model.

We have used both periodic and open boundary conditions for our numerical calculations. With open boundary conditions (OBC) the system is like a molecule; in this case free acceleration is impossible and the Drude weight D is always zero. With PBC D may be determined either by studying the dependence of the ground-state energy on an adiabatic change of boundary condition, equivalent to a static uniform vector potential,[28] or by making use of the f sum rule which relates the integrated conductivity to a ground-state expectation value. For the Holstein model the latter is

$$\int_0^{\infty}\sigma(\omega)d\omega=-\frac{\pi e^2}{2}\langle H_t\rangle, \quad (20)$$

while, given the explicit form for the current for the SSH model Eq. (19) the sum rule for the SSH model is given by

$$\int_0^{\infty}\sigma(\omega)d\omega=-\frac{\pi e^2}{2}\langle H_t+H_{e-\rm ph}\rangle. \quad (21)$$

The e-ph coupling term appears in the sum rule for the SSH model in the same way the hopping term does: this is a direct consequence of the origin of this term, arising from a modulation of the hopping integral. We have made use of the sum rule to determine D.

B. The optical excitation of small polarons: simple limits

The optical excitation of a small polaron for the Holstein model has been studied by Emin[11] by means of general arguments in the adiabatic limit and calculated by means of exact diagonalization by Alexandrov *et al.*[12] for the more general case. The physical origin of the optical absorption of a small polaron can be easily described in the adiabatic limit $\omega_0=0$ invoking the Franck-Condon principle. The ground state is given by an electron localized on a single site, which is strongly displaced from its equilibrium position, while all the other sites are not displaced. The electron can be excited to a neighboring site without changing the lattice configuration by the application of the current operator. The difference in energy between the two states is the lowering of the electronic energy associated with the small-polaron formation $2E_p$, where $E_p=2\lambda t$ is the small-polaron binding energy.

The physical mechanism we have described is not peculiar to the extreme adiabatic limit $\omega_0=0$, and is not strongly affected by the introduction of the lattice dynamics via a finite value of the phonon energy ω_0. Note that the current operator (18) acts only on the electronic degrees of freedom. Hence the current operator connects only states having the same lattice configuration, or at least having a nonzero overlap as far as the phononic state is concerned. Thus the physical picture we introduced for the extreme adiabatic limit can be extended to finite frequencies.

The SSH model optical conductivity can also be studied starting from adiabatic arguments invoking the Franck-Condon principle, but now taking into account the bond nature of the polaronic state. The ground state is characterized by a short bond on which the electron is localized. The short bond is generated by the shift of two neighboring sites to-

wards one another by equal amounts. The electronic ground state is the even combination of the two local states.

The optical absorption can happen in two different channels: a ''Holstein-like'' one in which the electron is excited onto a different bond that is not shortened, and a local channel in which the electron is excited from the even symmetry ground state into the local odd symmetry state on the short bond. The first kind of excitation is analogous to the excitation of the Holstein polaron and is expected to generate a band similar to the one previously described, centered at $2E_p$ (even if in this case E_p is not simply given by the Lang-Firsov result g^2/ω_0). The local excitation energy is given by the difference in electronic energy between the even-parity ground state and the odd-parity state, keeping the lattice configuration fixed. While the ''Holstein-like'' excitation is characterized by the fact that the electron is excited from a state in which it gains an energy $2E_p$ from the local distortion to a state in which the electron energy is not affected by the lattice configuration, the ''local'' transition carries the electron from a state in which the distortion lowers the energy by an amount $2E_p$ to a state in which the electron energy is raised by the same amount $2E_p$. Hence the energy difference involved in the optical transition is $4E_p$. If we introduce a finite phonon frequency this absorption peak broadens into a ''band'' exhibiting phonon features separated by the typical phonon frequency ω_0.

For the special case of only two sites the SSH model can be analytically solved for arbitrary ω_0 by means of a modified Lang-Firsov transformation that acts on the bond variable. After performing the modified Lang-Firsov transformation we obtain for the two-site cluster

$$\sigma_{2s}(\omega)=\frac{\pi e^2}{4}\sum_{n=0}^{\infty}(2t+n\omega_0)e^{-8\alpha^2}\frac{(8\alpha^2)^n}{n!}\times\delta(\omega-(2t+n\omega_0)). \tag{22}$$

The conductivity of the two-site cluster given by Eq. (22) consists of a succession of Dirac delta functions at frequencies separated by the phonon frequency ω_0. Once the Dirac delta functions are substituted by Lorentzians the analytic formula (22) gives the same result as the numerical calculations: a single absorption band centered at $\omega=2t+8g^2/\omega_0$, with width proportional to g/t and intensity proportional to $t/g+4g/\omega_0$. Of course, the other ''Holstein-like'' absorption feature, which we argued should be present due to the transfer of the electron from the shortened bond to a neighboring undistorted one, cannot occur for a two-site system where there is only one bond. This implies that the sum rule (21) which is given by

$$\int_0^{\infty}\sigma(\omega)d\omega=\frac{\pi e^2}{2}\left(t+\frac{4g^2}{\omega_0}\right) \tag{23}$$

is exhausted by this feature. This is consistent with the width and intensity described above.

We expect the physics of the polaronic absorption for the SSH model to be much more dependent on the adiabatic ratio than is the case for the Holstein model. The dependence of the current operator on the phonon operators makes it possible to have an optical transition which does not leave the lattice configuration unaltered, expecially if the phonon frequency is comparable to or even greater than the hopping integral. This point will be discussed further in light of the numerical results.

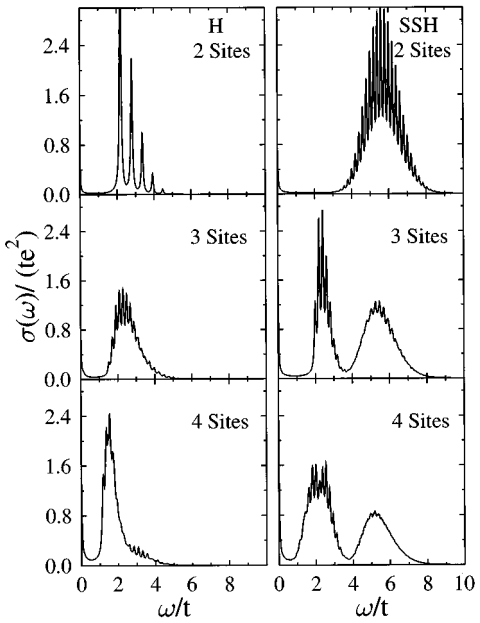

FIG. 4. Finite frequency optical conductivity for $\omega_0/t=0.2$ for the Holstein model (H, left column) with $g/t=0.55$ and the SSH model with $g/t=0.3$ (SSH, right column) for one electron on OBC clusters of different lattice sizes: from top to bottom two, three, and four sites.

C. Exact diagonalization results

In Fig. 4 we show the optical conductivity for the Holstein and SSH models for different lattice sizes for a phonon frequency $\omega_0=0.2t$. We have chosen the coupling for the two different models in order to have the low-energy feature for the SSH model centered at the same frequency as the feature in the Holstein model. For the Holstein model this coupling is intermediate, which can be seen both from the asymmetry of the absorption band and the significant size dependence of the spectrum.[12] With a further increase in the coupling strength this absorption band becomes very similar to that expected from simple analytic approaches[10,11] as was previously found in Ref. 12. For the SSH model on the other hand, we are already deeper in the polaronic regime. This is clear from the fact that the low-energy feature for the SSH model does not change significantly from 3 to 4 sites, while the one in the Holstein case changes more noticeably. If one increases the coupling strength further, however, there is the risk of obtaining unphysical results for the SSH model as discussed in Sec. II C. We avoid the unphysical region of this simple version of the model by restricting the coupling strength. The numerical calculations have been performed with a maximum allowed number of phonons $n_{\max}=50$ for the two- and three-site calculations and $n_{\max}=20$ for the four-site calculations.

While the results for the Holstein model do not depend qualitatively on the number of sites, the SSH two-site model has a very different behavior compared to the larger systems.

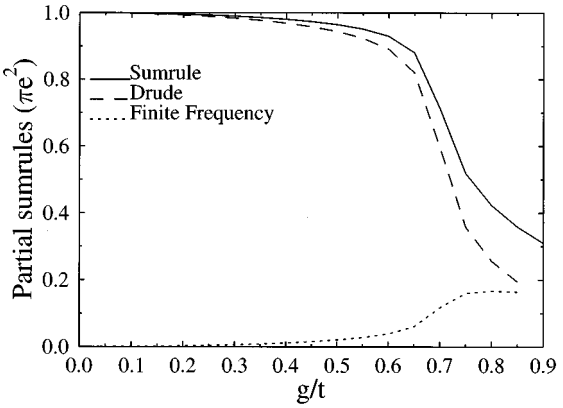

FIG. 5. Spectral weights for the Holstein model with $\omega_0/t=0.2$ for a four-site cluster with PBC. The solid line is the total sum rule Eq. (20); the dashed line is the Drude weight; the dotted line is the integrated weight of the finite frequency polaronic absorption feature.

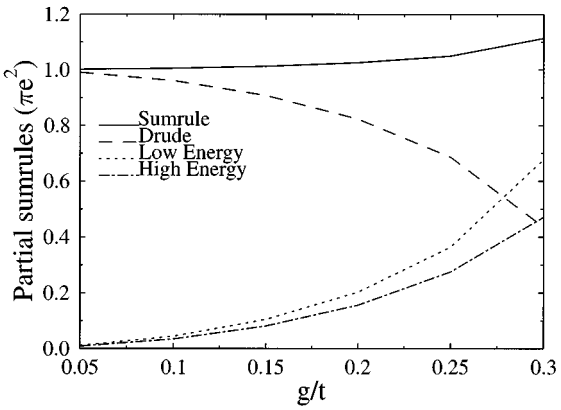

FIG. 6. Spectral weights for the SSH model for a four-site cluster with PBC and phonon frequency $\omega_0=0.2t$. The solid line is the total sum rule Eq. (21); the dashed line is the Drude weight; the dotted line is the integrated weight of the low energy ''Holstein-like'' polaronic absorption feature; the dot-dashed line is the high-energy local bonding-antibonding transition.

The two-site SSH model, as we have anticipated in the preceding section shows just a single feature centered at $\omega=2t+8g^2/\omega_0$, associated with a local transition from the even-parity ground state to odd-parity excited states. Increasing the number of sites a lower energy feature appears centered at half the center of the high-energy ''local'' feature. It is generated by the excitation of the electron from one bond to a neighboring one. It is worth noting that the two features do not change significantly going from three sites to four sites, despite the fact that the model has a nonlocal e-ph coupling.

To summarize the results up to this point: the most noticeable feature of the optical conductivity of a single SSH polaron in the (quasi-)adiabatic limit is the presence of two optical absorption bands generated by different optical excitation processes, one corresponding to the feature found in the Holstein model, and the other at twice the energy corresponding to a local excitation on the distorted bond.

Further information about the different way in which the polaron excitation occurs in the two models can be extracted from an analysis of the optical spectra as functions of the e-ph coupling. This may be most clearly seen by examining the various contributions to the sum rule. As a consequence of the self-trapping, the electronic kinetic energy is strongly suppressed in the strong-coupling limit; Eq. (20) implies that the total weight of optical excitations decreases with increasing coupling for the Holstein model. On the other hand, the optical sum rule for the SSH model Eq. (21) also involves the e-ph term, which increases with increasing coupling constant.

In Fig. 5 we show for the Holstein model the total sum rule, the Drude weight, and the incoherent integrated weight as a function of the e-ph coupling for $\omega_0=0.2t$. The total sum rule sharply decreases as soon as $\lambda\sim 1$; this sharp decrease is driven by the fall of the Drude weight, which rapidly approaches zero. Note further that even if, for $\lambda>1$, the finite frequency polaronic absorption appears besides the Drude weight, its weight also decreases as t/g as g increases in the strong-coupling regime.

In Fig. 6 we present similar information for the SSH model. The total sum rule monotonically increases with the coupling, which indicates that the increase of the e-ph term overcompensates the decrease of the hopping term. The Drude weight rapidly decreases for this kind of e-ph coupling as is the case for the Holstein model, whereas the polaronic structures increase their total weight as the coupling increases.

We have separately integrated the optical conductivity for the two different optical absorption bands characteristic of the SSH case, obtaining in both cases an increase in total optical weight with coupling. As far as the high-energy, local feature is concerned, this result is consistent with Eq. (22), which predicts an increasing value for the intensity of the optical absorption as a function of the e-ph coupling. The low-energy feature for the SSH model, on the other hand, which we attributed to the same kind of optical excitation that generates the absorption band for the Holstein model, also shows an increase of total weight with increasing g, whereas the Holstein structure has a decreasing weight as the coupling increases. This difference does not undermine the similarity between the two features, but simply underlines the nature of the e-ph coupling term for the SSH model: the dipole moment associated with this type of transition is an increasing function of the coupling, so that quite naturally the absorption is expected to increase with coupling.

A further aspect to be considered is the dependence of the conductivity on the phonon frequency. As we already stated, the independence of the current operator for the Holstein model on the phonon operators is responsible for the ''survival'' of the adiabatic small-polaron excitation process with increasing phonon frequency. For the SSH model this argument does not work, so we expect that the physical picture we have drawn using the adiabatic approximation will not hold for a sufficiently large value of the adiabatic ratio ω_0/t. The dependence of the current operator on the difference of the phonon displacements makes it possible to consider an optical transition that modifies, even strongly, if ω_0/t is sizeable, the lattice configuration. The short bond can be enlarged as the electron is excited to a neighboring bond and the adiabatic picture can break down.

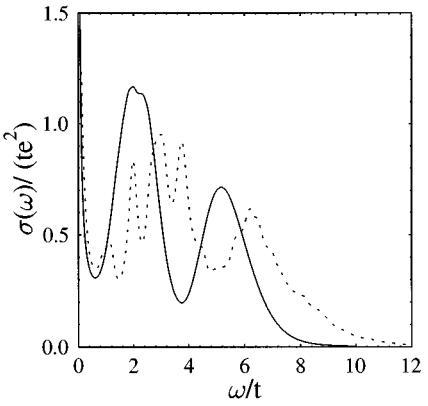

FIG. 7. Finite frequency optical conductivity of the SSH model for a four-site cluster using $\lambda=0.225$. The solid line is for $\omega_0/t=0.2$ and the dashed line is for $\omega_0/t=0.8$.

In Fig. 7 we study the effect of increasing phonon frequency on the optical conductivity for a four-site OBC cluster keeping λ constant. The value of the coupling ($\lambda=0.225$) is large enough to show clear polaronic features in the adiabatic regime. The two optical features are very evident for the smaller of the two frequencies shown $\omega_0/t=0.2$, whereas for the larger phonon frequency $\omega_0/t=0.8$ the absorption bands are broadened and overlap significantly. Larger phonon frequency also results in a more evident phonon structure, which contributes to hide the two features. For an adiabatic ratio $\omega_0/t=1$ there is almost no sign of two distinct optical structures. Note that for larger phonon frequency size effects are also more important: for $\omega_0/t=0.8$ the difference between the high-energy region of the four-site result shown and the two-site case is much larger than is the case for the results for $\omega_0/t=0.2$ in Fig. 4.

IV. CONCLUSIONS

In the present paper we addressed the issue of polaron formation in lattice models with extreme short-range e-ph interactions, the SSH and the Holstein models. Our work was devoted to comparing the properties of the SSH model with the more intensively studied Holstein model. In particular we clarified, both from analytic qualitative arguments and from numerical exact calculations, that λ or α are *not* by themselves independent parameters which determine the free-electron or the polaronic regimes in the e-ph models. Indeed we showed for the Holstein model that both conditions, $\lambda>\lambda_c\approx 1$ and $\alpha>\alpha_c\approx 1$ have to be satisfied in order to realize both the mass enhancement and the energetic advantage to accept the loss in kinetic energy, which characterize the polaronic state. Depending on the adiabatic ratio ω_0/t, the condition for the polaronic regime is determined by $\lambda>\lambda_c$ when $\omega_0<t$ and by $\alpha>\alpha_c$ when $\omega_0>t$.

Comparing our findings with the results of a dynamical mean-field theory calculation, which is exact in the limit of infinite connectivity,[31] we find substantial agreement as far as the value of the parameters ruling the single-polaron formation in the Holstein model is concerned. This clearly indicates that the same physical picture extracted here from the numerical calculation in small (one-dimensional) clusters holds for infinite systems in higher dimensions as well. This ''universal'' behavior is a natural consequence of the local character of the small polarons in the Holstein model.

On the other hand, perturbative and numerical calculations for the SSH model lead to the condition $\lambda>\lambda_c$ irrespective of the adiabatic ratio. This result, apparently contrasting with the corresponding criterion in the Holstein model, may be very naturally understood in terms of a physical argument again based on the kinetic energy reduction and energetic convenience to enhance the electronic mass to gain lattice deformation energy. Therefore, although the final criteria are different, the same physical picture underlies the formation of a single polaron in the two models. In carrying out the investigation of the SSH model we also demonstrated the crucial role played by the phonon dynamics in order to have a polaronic regime within this model, avoiding its pathologies.

The optical absorption of a polaron arising from e-ph coupling of the SSH type has been shown to exhibit marked differences from the well-known Holstein polaron. These differences can be understood in terms of the simple picture of the Holstein small polaron consisting of an electron bound to a single distorted site, whereas the SSH polaron may be described as an electron localized on a shortened bond. The absorption in the Holstein model is due to processes where the electron is excited from the distorted site to a neighboring undistorted site. A feature in the optical conductivity centered at a frequency $\omega=2E_p$, i.e., twice the polaron binding energy, is associated with this kind of process. In the SSH model, corresponding processes exist where the electron is transferred from the distorted bond to a neighboring undistorted bond, leading to a very similar absorption feature. On the other hand, a different channel for the polaron excitation in the SSH model is available. The ground state is an even parity, bonding state localized on a shortened bond. Due to the existence of local excited states of antibonding (odd) symmetry on the ''short'' bond, there is an additional strong absorption feature at twice the energy of the familiar ''Holstein-like'' absorption. The higher energy of this feature may be understood to arise from the antibonding nature of these final states with respect to the shortened bond. This anti-bonding character leads to the raising of the energy of the state by the same amount by which the polaronic ground-state energy is lowered, whereas the ''Holstein-like'' transition occurs from a low-energy state to a zero-energy state as far as the electron-phonon interaction energy is concerned. Although all numerical calculations were performed for one-dimensional systems, due to the local nature of the physics we have described, the dimensionality is not expected to play a crucial role and similar features would be expected also in higher dimensional systems.

ACKNOWLEDGMENTS

We acknowledge fruitful discussions with C. Castellani, S. Ciuchi, C. Di Castro, and D. Feinberg. This work was partly supported by the Istituto Nazionale di Fisica della Materia (INFM).

*Present address: Max-Planck-Institut für Physik komplexer Systeme, Bayreuther Strasse 40 H. 16, D-01187 Dresden, Germany

[1] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. **42**, 1698 (1979).

[2] T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959); **8**, 343 (1959).

[3] For a recent review on polarons, with a particular relation to high-temperature superconductivity, see A. S. Alexandrov and N. Mott, Rep. Prog. Phys. **57**, 1197 (1990).

[4] J. P. Falck *et al.*, Phys. Rev. Lett. **69**, 1109 (1992).

[5] P. Calvani, M. Capizzi, S. Lupi, P. Maselli, A. Paolone, and P. Roy, Phys. Rev. B **53**, 2756 (1996); P. Calvani, M. Capizzi, S. Lupi, and G. Balestrino, Europhys. Lett. **31**, 473 (1995), and references therein.

[6] J. Ranninger, and U. Thibblin, Phys. Rev. B **42**, 2416 (1990).

[7] G. Wellein, H. Röder, and H. Feshke, Phys. Rev. B **53**, 9666 (1996).

[8] A. Greco and A. Dobry, Solid State Commun. **99**, 473 (1996).

[9] H. De Raedt and A. Lagendjick, Phys. Rev. B **27**, 6097 (1983); **30**, 1671 (1984).

[10] H. G. Reik and D. Heese, J. Phys. Chem. Solids **28**, 581 (1967); H. G. Reik and R. Mülstroh, Solid State Commun. **5**, 105 (1967).

[11] D. Emin, Phys. Rev. B **48**, 13 691 (1993).

[12] A. S. Alexandrov, V. V. Kabanov, and D. K. Ray, Physica C **224**, 247 (1994).

[13] For the continuum case accurate results have been obtained using the path-integral formalism; see, e.g., J. T. Devreese, in *Polarons in Ionic Chrystals and Polar Semiconductors*, edited by J. T. Devreese (North-Holland, Amsterdam, 1972), p. 83.

[14] See e.g., Y. Zhao, D. W. Brown, and K. Lindenberg (unpublished), for a discussion of the band structure of this model.

[15] R. Zeyher, Z. Phys. B **80**, 187 (1990).

[16] I. G. Lang and Y. A. Firsov, Zh. Éksp. Teor. Fiz. **43**, 1843 (1962) [Sov. Phys. JETP **16**, 1301 (1963)].

[17] D. Feinberg, S. Ciuchi, and F. de Pasquale, Int. J. Mod. Phys. B **4**, 1317 (1990).

[18] See, e.g., A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Mechanics* (Dover, New York, 1975), Chap. 21.

[19] The trivial result $m^*=m$ is found if one trivially takes the $\omega_0\to\infty$ limit, showing that an infinitely rigid lattice cannot dress the bare electronic mass for any finite (and in particular small) e-ph coupling. Physical effects only arise by taking a large but finite ω_0/t ratio.

[20] F. Marsiglio, Physica C **244**, 21 (1995).

[21] Analogously for the perturbative mass correction in $d=2$ close to a two-dimensional Van Hove singularity one finds $(m^*-m)/m\propto\lambda\ln(t/\omega_0)$ [E. Cappelluti and L. Pietronero, Phys. Rev. B **53**, 932 (1996)]. Also in this case the mass enhancement is proportional to λ with a coefficient stemming from the logarithmically singular density of states.

[22] In order to avoid trivial limiting procedures, the adiabatic limit $\omega_0\to 0$ needs a clear specification. We take the spring constant $k=M\omega_0^2$ finite, while letting the ionic mass $M\to\infty$. To keep finite $\lambda=g^2/(2t\omega_0)$, g has to vanish as $\sqrt{\omega_0}$ giving a divergent α. This leads to a finite value of the lattice displacement $u=2g/(\omega_0\sqrt{2M\omega_0})=g\sqrt{2M\omega_0}/k$.

[23] V. V. Kabanov and O. Yu. Mashtakov, Phys. Rev. B **47**, 6060 (1993).

[24] This argument is only indicative, because once the mass correction grows large the perturbative result is no longer quantitatively reliable.

[25] A single four-site plaquette is a one-dimensional structure. Besides simplicity, this is an additional reason to limit our analytic treatment to the $d=1$ case.

[26] Notice that the numerical value of $\lambda_c\approx 0.2$ is different from the result obtained in the adiabatic regime for the Holstein model $\lambda_c\approx 1$. This is not problematic because the e-ph coupling mechanism in the two models is completely different and no relation between the numerical values of the parameters has to be expected.

[27] This ratio has the same physical meaning of λ in the Holstein model.

[28] W. Kohn, Phys. Rev. **133**, A171 (1964).

[29] B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).

[30] For a review see, e.g., E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994).

[31] S. Ciuchi, F. De Pasquale, and D. Feinberg, Europhys. Lett. **30**, 151 (1995).