Polaronic features in the Su-Schrieffer-Heeger model

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Abstract

A diagrammatic perturbative study of i) effective mass and ii) electron spectral function versus the adiabatic parameter in the Su-Schrieffer-Heeger model is presented. When zone boundary phonons energetically compete with band electrons we observe a sizeable mass enhancement and a spread of the spectral weight associated with an increased relevance of multiphonons contributions at larger e-ph couplings. Accordingly an onset of polaron formation is favoured, particularly in two dimensions.

Key words: Polarons; Effective Mass; Dimensionality;

The Su-Schrieffer-Heeger (SSH) Hamiltonian has been mainly analysed in conjunction with the conducting properties of quasi one dimensional polymers [1]. Recent investigations [2] have revealed the richness of the model also in two dimensions. In momentum space the dimension dependent SSH tight binding Hamiltonian $H = H_0 + H_{int}$ reads

$$H_0 = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} f^{\dagger}_{\mathbf{k}} f_{\mathbf{k}} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}}$$

$$H_{int} = \sum_{\mathbf{k},\mathbf{q}} g(\mathbf{k},\mathbf{q}) \left(b^{\dagger}_{-\mathbf{q}} + b_{\mathbf{q}}\right) f^{\dagger}_{\mathbf{k}+\mathbf{q}} f_{\mathbf{k}}$$

$$g(\mathbf{k},\mathbf{q}) = \frac{i\alpha}{\sqrt{2MN\omega_{\mathbf{q}}}} \left(\sin\left((\mathbf{k}+\mathbf{q})\cdot\mathbf{a}\right) - \sin \mathbf{k}\cdot\mathbf{a}\right) \quad (1)$$

where $\varepsilon_{\mathbf{k}} = -J\cos(\mathbf{k}\cdot\mathbf{a})$, $\omega_{\mathbf{q}} = 2\sqrt{\frac{K}{M}}|\sin\left(\frac{\mathbf{q}\cdot\mathbf{a}}{2}\right)|$, $f^{\dagger}(f)$ are electrons creation (annihilation) operators, $b^{\dagger}(b)$ are phononic operators, N is the total number of lattice sites and $a = |\mathbf{a}|$ is the lattice constant. The model contains three free parameters: the hopping integral J, the zone boundary frequency $\omega_{\pi} = 2\sqrt{K/M}$, the coupling constant $\alpha^2/4K$. Using the Matsubara Green's functions formalism I have computed exactly the self-energy terms due to one phonon and two phonons scattering processes which determine the renormalized electron mass m_{eff}

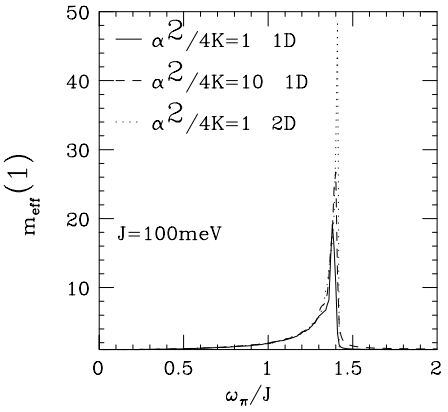

Fig. 1. Renormalized masses (in units of bare band electron mass) versus the adiabaticity parameter in 1D and 2D. $m^{(1)}_{eff}$ is due to the one phonon self-energy. The couplings are in meV.

$$\frac{m_{eff}}{m_0} = \frac{1 - \partial Re\Sigma_{\mathbf{k}}(\epsilon)/\partial\epsilon|_{\mathbf{k}=0;\ \epsilon=-J}}{1 + \partial Re\Sigma_{\mathbf{k}}(\epsilon)/\partial\varepsilon_{\mathbf{k}}|_{\mathbf{k}=0;\ \epsilon=-J}} \quad (2)$$

where, $Re\Sigma_{\mathbf{k}}(\epsilon)$ is the frequency dependent real part of the retarded self-energy. There are three two-phonons diagrams whose effect is however confined to the intermediate regime ($\omega_{\pi} \sim J$) in which the two phonons contributions enhance the effective mass by

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$\sim 15\%$ with respect to the one phonon result. Instead, in the fully adiabatic and antiadiabatic regimes the two phonons corrections are negligible. Figure 1 shows a sizeable mass enhancement at $\omega_\pi \sim J$ with a pronounced spike at $\omega_\pi \sim \sqrt{2}J$. In 2D the effective mass is larger than in 1D but no mass enhancement is obtained in the adiabatic and antiadiabatic limits [3]. The main contribution to both self-energy partial derivatives in eq.(2) comes from the lattice mode vectors connecting two electronic states such that $J + \varepsilon_{\mathbf{q}} - \omega_{\mathbf{q}} \sim 0$. Although for any value $J < \omega_\pi$ a set of singular $\mathbf{q}$-vectors does exist, their divergent contributions to the numerator and denominator in eq.(2) generally cancel out and no substantial effect is seen on the effective mass. Only in the case $\omega_\pi \sim \sqrt{2}J$ something special occurs due to scattering by phonons at the points such that $|q_x + q_y| = \pi/2$. Infact $\partial Re\Sigma_{\mathbf{k}}(\epsilon)/\partial\varepsilon_{\mathbf{k}}$ contains as modulation factor a $cos(\mathbf{q}\cdot\mathbf{a})$ term which is peculiar of the band structure. The vanishing of this term at the same wave vectors which allow for energy conservation finally results in the abrupt increase of the effective mass. In the square lattice the divergent-like behavior is more evident since many points (only one point in 1D) fulfill the simultaneous occurence of the two singular effects. The band bottom spectral function has been computed in a number of representative cases [4]. The sum rule spectral function has to be numerically fulfilled in principle. Here however we approximate the total self-energy by the one-phonon term which linearly depends on the free parameter $\alpha^2/4K$. As the *e-ph* coupling grows multiphonons terms become more relevant and our approximation is less accurate. Accordingly, deviations from the sum rule are expected as a measure of the loss of spectral weight associated with higher order self-energy effects. We present the results for the intermediate regime: electrons are good excitations in the extremely weak coupling and one dimensional case (Fig.2) with one well defined transition at $\epsilon = -100.9meV$ but, at larger couplings (dimensionless effective coupling $\alpha^2/(4KJ) = 0.1$), the sum rule is far from being satisfied and a 40% loss of spectral weight is observed together with a strong reduction of the main peak height. In 2D, the sum rule is fulfilled at very weak couplings (Fig.3) but the appearance of several transitions peaks in the range $[-110, -90]meV$ signals the onset of a polaronic state. At larger couplings the sum rule is strongly violated and the electronic quasiparticle picture breaks down. The absorption spectra broaden (both in 1D and 2D) by enhancing the strength of the *e-ph* coupling as a consequence of the mixing of electronic states and lattice vibrational excitations. In the adiabatic regime, the breakdown of the one phonon approximation is dimension dependent and, by increasing the *e-ph* coupling, 2D systems favour the appearance of multiphononic contributions. On the other hand,

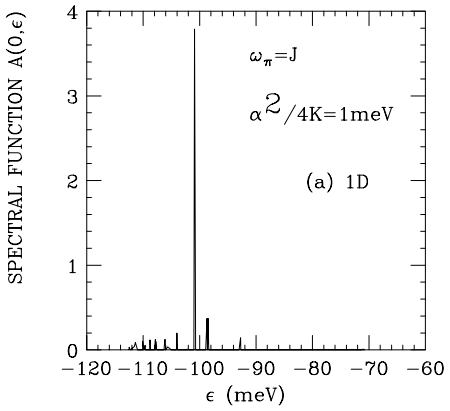

Fig. 2. 1D Electron spectral function in the intermediate regime and weak *e-ph* coupling. $J = 0.1eV$.

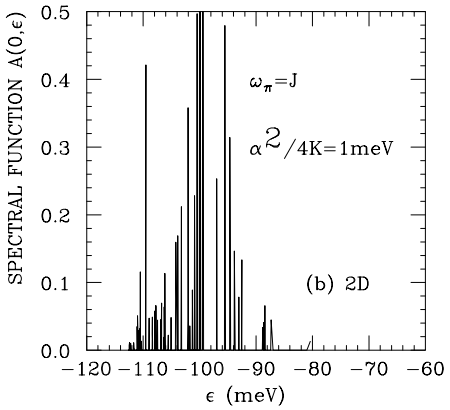

Fig. 3. 2D Electron spectral function in the intermediate regime and weak *e-ph* coupling. $J = 0.1eV$.

electrons behave as good quasiparticles in the fully antiadiabatic regime both in one and two dimensions.

In conclusion, the spectral function analysis shows that the onset of a polaronic state is more likely to occur in 2D than in 1D thus confirming the trend of the effective mass computation and suggesting that the SSH Hamiltonian is rather sensitive to dimensionality effects.

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