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SPECTRAL PROPERTIES OF THE 2D HOLSTEIN t–J MODEL

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Employing the Lanczos algorithm in combination with a kernel polynomial moment expansion (KPM) and the maximum entropy method (MEM), we show a way of calculating charge and spin excitations in the Holstein t–J model, including the full quantum nature of phonons. To analyze polaron band formation we evaluate the hole spectral function for a wide range of electron–phonon coupling strengths. For the first time, we present results for the optical conductivity of the 2D Holstein t–J model.

Polaronic features of dopant–induced charge carriers have been observed in the isostructural copper–based and nickel–based charge–transfer oxides $La_{2-x}Sr_x[Cu,Ni]O_{4+y}$ [1].

Studying (bi)polaron effects in such strongly coupled electron–phonon (EP) systems, the Holstein t–J model (HtJM) has recently attracted much attention [2]. The HtJM Hamiltonian reads

$$\mathcal{H} = \hbar\omega_0 \sum_i \left(b_i^\dagger b_i + \tfrac{1}{2}\right) - \sqrt{\varepsilon_p \hbar\omega_0} \sum_i \left(b_i^\dagger + b_i\right) \tilde{h}_i$$
$$-t \sum_{\langle i,j\rangle\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + J \sum_{\langle ij\rangle} \left(\vec{S}_i \vec{S}_j - \frac{\tilde{n}_i \tilde{n}_j}{4}\right). \quad (1)$$

The first two terms take into account the phonon part and the EP interaction, respectively, whereas the last two terms represent the standard t–J model acting in a Hilbert space without double occupancy. In (1), doped holes ($\tilde{h}_i = 1 - \tilde{n}_i$) are coupled locally to a dispersionsless optical phonon mode (ε_p - EP coupling constant, ω_0 – bare phonon frequency).

In this contribution, we investigate the HtJM by performing exact diagonalizations on a square ten–site lattice, where the phonon degrees of freedom are treated within a well–controlled Hilbert space truncation procedure [3]. To obtain information about dynamical properties of the model under consideration, we combine the Lanczos algorithm with the KPM and MEM approaches [4].

In order to address the problem of polaron formation in an antiferromagnetic correlated spin background, we have calculated the $\vec{K}$–resolved spectral function $A_{\vec{K}}(E)$ for a single dynamical hole at $J = 0.4$ (energies in units of t) [5]. The positions of the two lowest peaks of $A_{\vec{K}}(E)$, denoted by $E_{0/1}(\vec{K})$, are displayed as a function

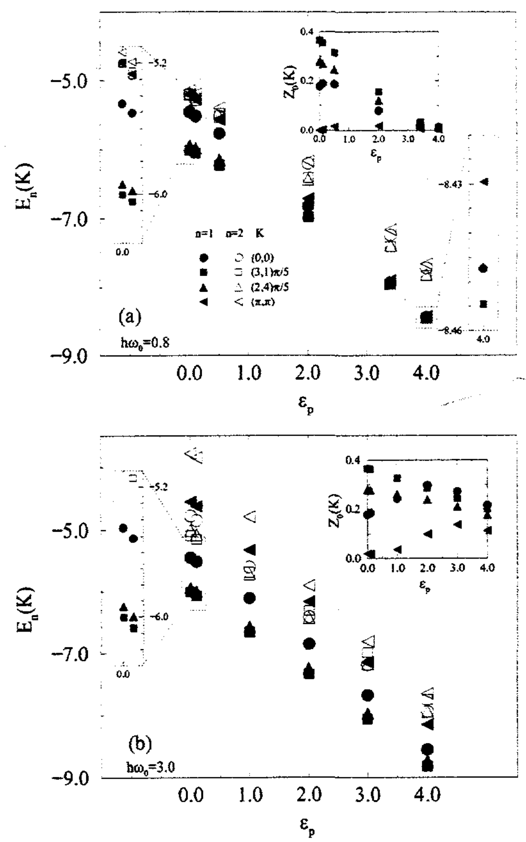

Fig. 1: Polaron band formation in the 2D HtJM. The wave function renormalization factors, $Z_0(\vec{K}) \propto \sum_\sigma |\langle \Psi_0^{(N-1)}(\vec{K})|\tilde{c}_{-\vec{K},\sigma}|\Psi_0^{(N)}(\vec{0})\rangle|^2$, are given as a function of ε_p in the insets.

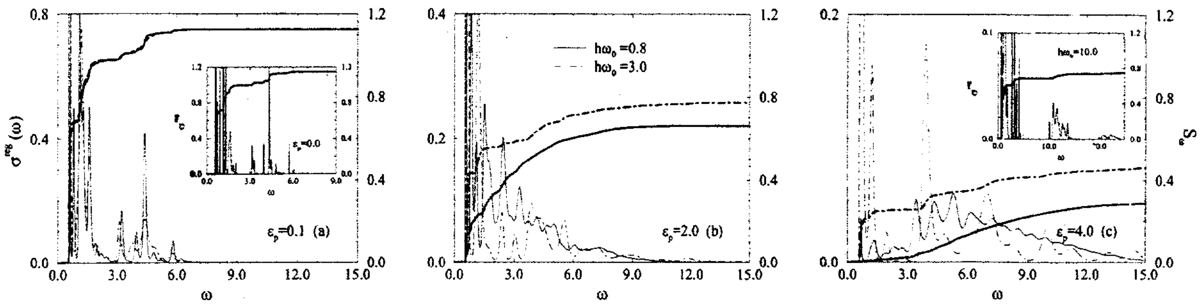

Fig. 2: Optical conductivity $\sigma_{xx}^{reg}(\omega)$ and ω–integrated spectral weight in the dissipative part of σ^{reg}, $S_\omega = \int_0^\omega d\omega' \sigma_{xx}^{reg}(\omega')$, for the 2D single–hole HtJM with 12 phonons (periodic boundary conditions).

of EP coupling strength in Fig. 1 for the allowed $\vec{K}$ vectors at $\hbar\omega_0 = 0.8$ and 3.0. As expected, in the very weak EP coupling limit the low–lying excitations are t–J hole–quasiparticles weakly dressed by phonons. For low and intermediate phonon frequencies, the energy to excite one phonon lies inside the quasiparticle band of the pure t–J model. Thus at arbitrarily small ε_p, predominantly phononic states with a small admixture of electronic character enter the low–energy spectrum in *all* $\vec{K}$–sectors [cf. the region about $E_n \simeq -5.2$ in the inset of (a)]. With increasing ε_p a strong mixing of holes and phonons takes place, whereby both quantum objects completely loose their own identity, and finally an extremely narrow well–separated *polaron* band is formed at large ε_p. This scenario is corroborated by the behavior of the $\vec{K}$–dependent renormalization factor $Z_0(\vec{K})$ shown in the upper insets, which can be taken as a measure of the "electronic" contribution to the polaronic quasiparticle (see insets). As can be seen from Fig. 1 (b), the phonon induced band renormalization is weakened in the non–adiabatic regime, where retardation and multi–phonon effects are of minor importantance.

To discuss the influence of the EP coupling on the optical response of the system, let us evaluate the regular part of the optical conductivity at finite energy transfer ω,

$$\sigma_{xx}^{reg}(\omega) = \frac{e^2\pi}{N} \sum_{n\neq 0} \frac{|\langle \Psi_n | \hat{j}_x | \Psi_0 \rangle|^2}{E_n - E_0}\, \delta[\omega - (E_n - E_0)]\,. \tag{2}$$

Results for $\sigma_{xx}^{reg}(\omega)$ are presented in Fig. 2 for $\varepsilon_p = 0.1$ (a), 2 (b), and 4 (c). In the weak EP coupling region, we recover the main features of the optical conductivity of the t–J model (inset Fig 2. (a)), i.e., (i) an "anomalous" broad mid–infrared absorption band $[J \lesssim \omega \lesssim 2t]$, separated from the Drude peak $[D\,\delta(\omega)$; not shown] by a "pseudo-gap" $\sim J$, and (ii) an "incoherent" tail up to $\omega \sim 7t$. At larger ε_p, we observe a redistribution of spectral weight to higher energies (cf. ΔS_ω), which is much more pronounced in the *adiabatic* regime. In particular, the transition to the (hole) polaron state is accompanied by the development of a broad maximum in $\sigma_{xx}^{reg}(\omega)$ at $\omega \lesssim 2\varepsilon_p$, whereas the optical response becomes strongly suppressed at low ω. Most notably, $\sigma_{xx}^{reg}(\omega)$ has an highly *asymmetric* lineshape at intermediate frequencies and coupling strengths as observed, e.g., for $La_{0.9}Sr_{0.1}NiO_4$ [1]. This effect can be traced back to a rather broad ground–state phonon distribution function obtained for $\varepsilon_p = 2, 4$ and $\hbar\omega_0 = 0.8$ [5]. Contrary, in the anti–adiabatic limit, the "electronic" lineshape is much less affected, but $\sigma_{xx}^{reg}(\omega)$ shows additional superstructures corresponding to "interband" transitions between t–J–like absorption bands with different number of phonons [see Fig 2 (c), inset].

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