SPECTRAL PROPERTIES OF THE 2D HOLSTEIN t–J MODEL

H. Fehske1, G. Wellein1, B. Bäuml1 and R. N. Silver2,

1Physikalisches Institut, Universität Bayreuth, D–95440 Bayreuth, Germany
2MS B262 Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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

$H = \hbar \omega_0 \sum_i (b_i^\dagger b_i + \frac{1}{2}) - \sqrt{\varepsilon_p} \hbar \omega_0 \sum_i (b_i^\dagger + b_i) \tilde{b}_i$

$- t \sum_{\langle i,j \rangle \sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + J \sum_{\langle ij \rangle} (\tilde{S}_i \cdot \tilde{S}_j - \tilde{n}_i \tilde{n}_j / 4). \quad (1)$

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 ($\tilde{n}_i = 1 - \tilde{n}_i$) are coupled locally to a dispersionless optical phonon mode ($\varepsilon_p$ - EP coupling constant, $\omega_0$ – 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, $Z_0(\vec{K}) \propto \sum_{\sigma} |\langle \tilde{c}_{-\vec{K},\sigma}\tilde{c}_{0,\sigma} |\tilde{c}_0^{(N)}(\vec{0})\tilde{c}_0^{(N)}(\vec{0})\rangle|^2$, are given as a function of $\varepsilon_p$ in the insets.
The behavior of the electronic character enters the low-energy spectrum in all $\vec{K}$-sectors [cf. the region about $E_n \sim -5.2$ in the inset of (a)]. With increasing $\varepsilon_p$, a strong mixing of holes and phonons takes place, whereby both quantum objects completely lose their own identity, and finally an extremely narrow well-separated polaron band is formed at large $\varepsilon_p$. 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 nonadiabatic regime, where retardation and multi-phonon effects are of minor importance.

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, $\omega$,

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

(2)

Results for $\sigma_{xx}^{\text{reg}}(\omega)$ 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 $[D \delta(\omega)]$ but not shown by a “pseudo-gap” $\sim J$, and (ii) an “incoherent” tail up to $\omega \sim 7t$. At larger $\varepsilon_p$, we observe a redistribution of spectral weight to higher energies (cf. $\Delta S_\omega$), which is 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 $\sigma_{xx}^{\text{reg}}(\omega)$ at $\omega \lesssim 2\varepsilon_p$, whereas the optical response becomes strongly suppressed at low $\omega$. Most notably, $\sigma_{xx}^{\text{reg}}(\omega)$ has an highly asymmetric lineshape at intermediate frequencies and coupling strengths as observed, e.g., for La$_{1.8}$Sr$_{0.2}$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 antiadiabatic limit, the “electronic” lineshape is much less affected, but $\sigma_{xx}^{\text{reg}}(\omega)$ shows additional superstructures corresponding to “interband” transitions between t–J-like absorption bands with different number of phonons [see Fig 2 (c), inset]. These results clearly demonstrate the complex interplay of electron and EP correlation effects.

REFERENCES

1. X.-X. Bi and P. C. Eklund, Phys. Rev. Lett. 70, 2625 (1993).
2. H. Fehske et al., Phys. Rev. B 51, 16582 (1995); A. Dobry et al., Phys. Rev. B 52, 13722 (1995).
3. G. Wellein, H. Röder, and H. Fehske, Phys. Rev. B 53, 9666 (1996).
4. R. N. Silver, et al., J. of Comp. Phys. 124, 115 (1996).
5. H. Fehske et al., Physica B, to appear (1997).

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