DYNAMICAL PAIRING CORRELATIONS IN THE t–J MODEL WITH NON–ADIABATIC HOLE–PHONON COUPLING

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We examine the effects of hole–phonon interaction on the formation of hole pairs in the 2D Holstein t–J model. Using finite–lattice diagonalization techniques, we present exact results for the two–hole binding energy and the s– and d–wave pairing susceptibilities.

The interplay of electronic and lattice degrees of freedom in strongly electron–correlated systems is now attracting a lot of attention. This interest is partially due to the prominent role of the electron–phonon (EP) interaction in several transition metal oxides with strong Coulomb correlations, such as the colossal magnetoresistive manganites or the charge–ordered (insulating) nickelates. For the high–T_c superconducting cuprates, very recent experiments demonstrate the relevance of the coupling between the charge carriers and the lattice dynamics as well [1].

For the sake of simplicity, we describe the basic interactions in the latter systems by an effective single–band Hamiltonian, the so–called Holstein t–J model [2]

$$\mathcal{H} = \mathcal{H}_{t-J} - \sqrt{\varepsilon_p \hbar\omega_0} \sum_i \left(b_i^\dagger + b_i\right)\tilde{h}_i + \hbar\omega_0 \sum_i \left(b_i^\dagger b_i + \tfrac{1}{2}\right), \qquad (1)$$

which contains besides nearest–neighbour hole transfer (t) and antiferromagnetic (AFM) spin exchange (J) on a square lattice, the coupling of doped holes ($\tilde{h}_i$) to a dispersionsless optical phonon mode (representing, e.g., local apical–oxygen breathing vibrations). Here ε_p is the hole–phonon coupling strength and $\hbar\omega_0$ denotes the phonon frequency. The single–particle excitations of the model (1) have been studied numerically [3,4]; the main result is that in the presence of strong AFM spin correlations even a moderate EP coupling can cause polaronic effects.

In this contribution, we focus on the two–hole subspace in order to comment on hole–pair formation. Employing the Lanczos algorithm in combination with a well–controlled truncation of the phononic Hilbert space [2,5], we are able to calculate both ground–state and dynamical properties preserving the full dynamics and quantum nature of phonons. It is worth noticing, that our multi–mode treatment of the phonons differs significantly from the one–phonon calculation performed in Ref. 6 for the t–J model coupled to oxygen breathing or buckling modes.

The dynamical pair spectral function can be written as

$$\mathcal{A}_{2h}(\omega) = \sum_n |\langle \Psi_n^{(N-2)} \,|\, \Delta_\alpha \,|\Psi_0^{(N)}\rangle|^2 \;\delta\left[\omega - (E_n^{(N-2)} - E_0^{(N)})\right], \qquad (2)$$

where $\Delta_\alpha = \frac{1}{\sqrt{N}} \sum_{i;\delta=\pm x,\pm y} \mathcal{F}_\alpha(\delta)\tilde{c}_{i\uparrow}\tilde{c}_{i+\delta\downarrow}$, with $\mathcal{F}_\alpha(\pm x) = 1$ and $\mathcal{F}_\alpha(\pm y) = -1$ [+1] for d–wave [s–wave] pairing.

Numerical results for the spectral functions of the pairing operators Δ_α are shown in Fig. 1 for exchange interactions $J = 0.4$ (left column) and $J = 0.1$ (right

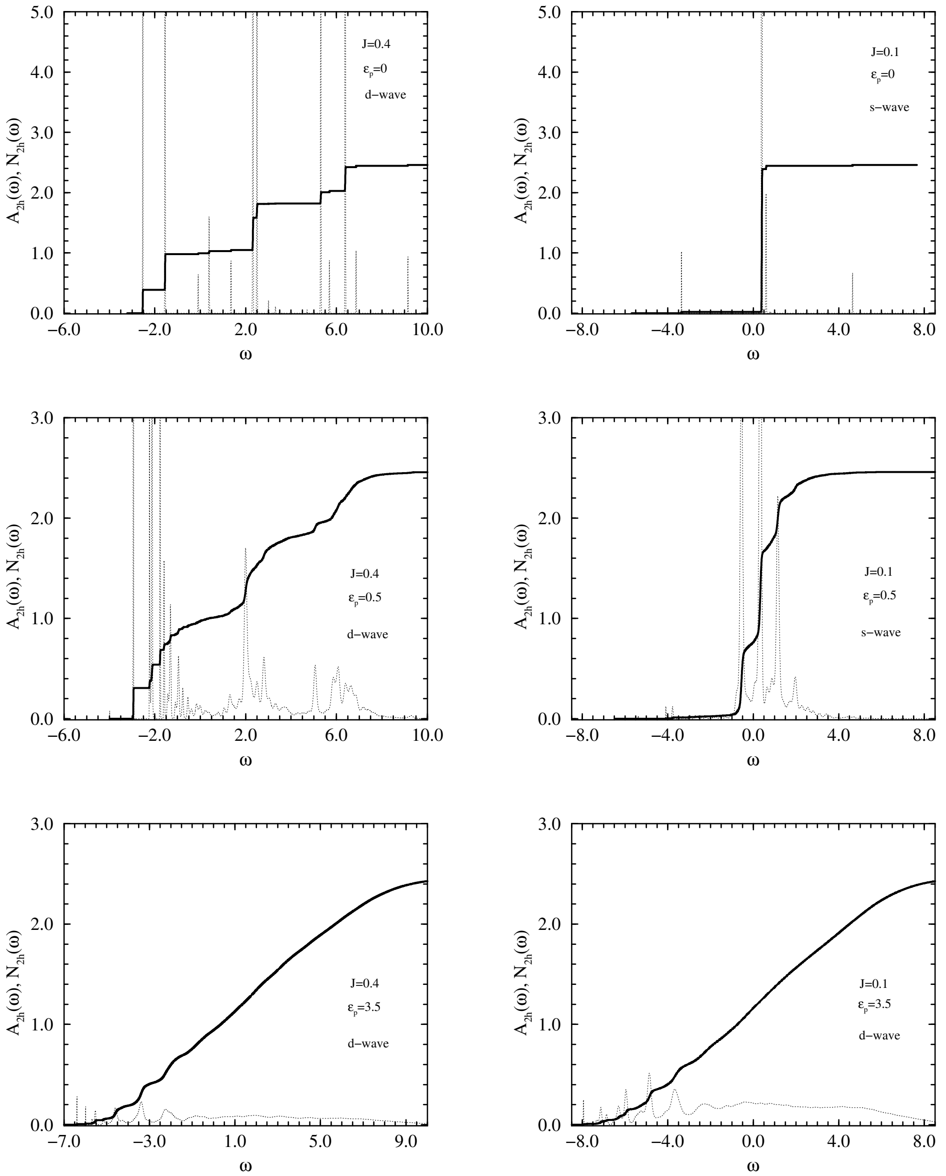

Figure 1: Dynamical pair spectral function $\mathcal{A}_{2h}(\omega)$ (dotted lines) and integrated spectral weight $\mathcal{N}_{2h}(\omega) = \int_{-\infty}^{\omega} d\omega' \mathcal{A}_{2h}(\omega')$ (bold lines) calculated for the 2D Holstein t–J model on a ten–site square lattice with periodic boundary conditions at $\hbar\omega_0 = 0.8$. Depending on the model parameters J and ε_p, results are presented only for those hole–pair wave functions $|\Delta_\alpha \Psi_0^{(N)}\rangle$ which have a finite overlap with $|\Psi_0^{(N-2)}\rangle$. Note that for the the pure t–J model the symmetry of the two–hole ($\vec{K} = 0$) ground state is changed from d–wave (B/C_4) to s–wave (A/C_4) at $J_c = 0.2001$ ($N = 10$). On the other hand, the (symmetry) change in the spectra, observed by comparing the plots for $\varepsilon_p = 0.5$ and 3.5 at $J = 0.1$, is driven by the EP coupling ($\varepsilon_{p,c} \simeq 3.3$). All energies are measured in units of t.

column) corresponding to two different regimes in the pure t–J model (see upper panels). For $J = 0.4$, the d–wave pair spectrum exhibits a well–separated low–energy peak containing an appreciable amount of spectral weight which grows if J is enhanced (cf. the inset of Fig. 2). Since the rest of the spectrum becomes incoherent with increasing lattice size N, the dominant peak at the bottom of the spectrum has been taken as signature of a d-wave quasiparticle bound state [7]. By contrast, the s–wave spectrum shows no such quasiparticle–like excitation. In the weak EP coupling case, the main features of the $\varepsilon_p = 0$ spectra are preserved, although, of course, additional phonon satellite structures appear (cf. the discussion of Fig. 3 below). The situation is drastically different in the strong–coupling regime. Here a strong mixing of electron and phonon degrees of freedom takes place and less mobile (bi)polaronic charge carriers emerge. The polaronic self–trapping transition is accompanied by a dramatic reduction of the coherent band width and, as a result, the AFM spin interaction becomes much more effective. Therefore, at $\varepsilon_p = 3.5$, the spectrum for $J = 0.1$ looks very similar to that for $J = 0.4$.

The relative spectral weight, $\mathcal{Z}_{2h}$, located in the lowest pole of $\mathcal{A}_{2h}$, is plotted in Fig. 2 (left panel). Obviously, we observe a strong suppression of the d–wave quasiparticle residue with increasing EP coupling. However, $\mathcal{Z}_{2h}$ gives only a measure of the “electronic” contribution to the d–wave bound state. In fact, according to previous work [6], composite pair operators $\bar{\Delta}_\alpha$, properly dressed by a phonon cloud, give large quasiparticle weights in $\bar{\mathcal{A}}_{2h}$. That the Holstein EP interaction may stabilize a bound state of two holes is clearly demonstrated by the behaviour of the binding energy E_B^2, which has been calculated for the larger 4×4 lattice in order to reduce finite–size effects (see the right panel of Fig. 2). Whereas the hole attraction ($E_B^2 < 0$) is less affected in the anti–adiabatic limit, the EP coupling promotes the pairing correlations between two holes in the adiabatic regime due to subtle retardation effects. This is to be contrasted with the findings for a coupling of the holes to the in–plane oxygen breathing mode which leads to an hole repulsion for all frequencies and EP interaction strengths [6].

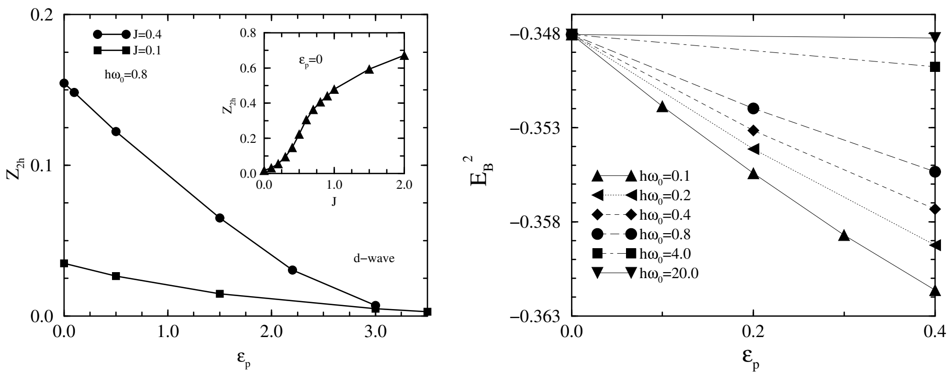

Figure 2: Two–hole “quasiparticle weight” $\mathcal{Z}_{2h} = |\langle \Psi_0^{(N-2)} \,|\, \Delta_\alpha \,|\, \Psi_0^{(N)} \rangle|^2 / |\langle \Psi_0^{(N)} \,|\Delta_\alpha^\dagger \Delta_\alpha|\, \Psi_0^{(N)}\rangle|$ (left panel; $N = 10$) and hole “binding energy” $E_B^2 = E_0^{(N-2)} + E_0^{(N)} - 2E_0^{(N-1)}$ (right panel; $N = 16$) shown as a function of EP coupling strength ε_p at various phonon frequencies $\hbar\omega_0$.

Let us discuss the weak–coupling case in more detail. Fig. 3 presents the spectral decomposition of the d-wave pairing operator at $\hbar\omega_0 = 0.1$ and 3.0. In the high phonon frequency (anti–adiabatic) regime, the pairing susceptibility behaves qualitatively in a similar way as the $\varepsilon_p = 0$ limit, in particular the low–energy part of the spectrum is given by purely electronic resonances. If the phonon frequency is

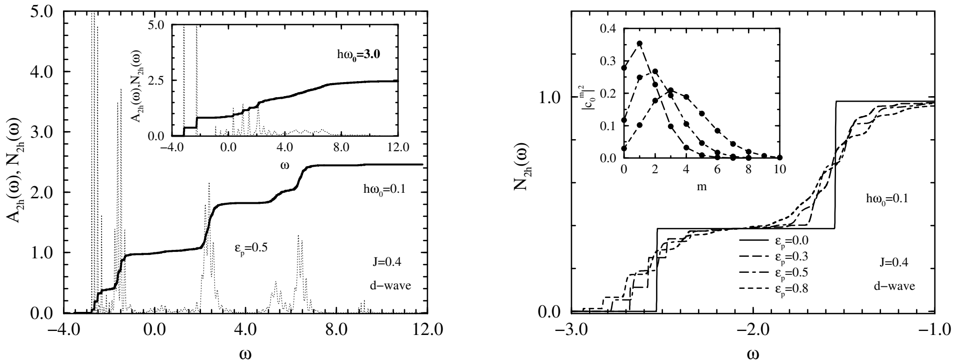

Figure 3: Left panel: d–wave pair spectra $\mathcal{A}_{2h}$ at $\varepsilon_p = 0.5$ and $\hbar\omega = 0.1$ (inset: $\hbar\omega = 3.0$). Right panel: integrated spectral weight $\mathcal{N}_{2h}(\omega)$ in the low–energy part of $\mathcal{A}_{2h}$ for various ε_p (inset: phonon–weight function $|c_0^m|^2$ in the two–hole ground state for the same parameters)

much smaller than the electronic gaps, we found series of predominantly phononic side bands, being separated by $\hbar\omega_0$ and roughly centered around the positions of the electronic excitations. The relative weights of these δ–like peaks can be deduced from the corresponding jumps in $\mathcal{N}_{2h}(\omega)$ depicted for different ε_p in the right panel of Fig. 3. Focusing on the lowest set of phonon sub-bands, it is interesting to note, that the weight of the *zero–phonon state* ($|c_n^0|^2$) in the first *excited states* ($|\Psi_n^{(N-2)}\rangle$, $n = 1, 2, \ldots$), which is measured by $\mathcal{N}_{2h}(\omega)$, is approximately the same as the weight of the *m–phonon states* ($|c_0^m|^2$) in the *ground state* ($|\Psi_0^{(N)}\rangle$). The definition of the coefficients $|c_0^m|^2$ is given in Refs. 4,5. A qualitative understanding of this fact can be obtained from the study of the independent boson model [8], where we can show exactly that $|c_0^m|^2 = |c_m^0|^2$ holds [9].

To summarize, our exact diagonalization studies of the 2D Holstein t–J model give evidence for significant EP coupling effects. Most notably, the hole pairing in the t–J model may be stabilized by a dynamical (Holstein) hole–phonon interaction.

References

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