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Polaronic effects in strongly coupled electron–phonon systems: Exact diagonalization results for the 2D Holstein t–J model

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Abstract

Ground-state and dynamical properties of the 2D Holstein t–J model are examined by means of direct Lanczos diagonalization, using a truncation method of the phononic Hilbert space. The single-hole spectral function shows the formation of a narrow hole–polaron band as the electron–phonon coupling increases, where the polaronic band collapse is favoured by strong Coulomb correlations. In the two-hole sector, the hole–hole correlations unambiguously indicate the existence of inter-site bipolaronic states. At quarter-filling, a polaronic superlattice is formed in the adiabatic strong-coupling regime.

Keywords: Polaron; Holstein t–J model; Exact diagonalization; t–J model

Polaronic features of dopant-induced charge carriers have been detected in the copper-based high-T_c compounds $La_{2-x}Sr_xCuO_{4+y}$, and even more in the isostructural nickel-based charge-transfer oxides $La_{2-x}Sr_xNiO_{4+y}$ [1]. To tackle the problem of (bi)polaron formation in such systems exhibiting besides a substantial electron–phonon (EP) coupling strong Coulomb interactions, it seems, at the moment, that approximation-free numerical quantum Monte Carlo and exact diagonalization (ED) analyses of generic model Hamiltonians yield the most reliable results. Along this line, by use of ED, the ground-state properties of Hubbard and t–J models with an on-site Holstein EP coupling have been studied on finite clusters in 1D and 2D [2–4]. What is missing to date is an application of the powerful ED technique to the calculation of *dynamical* properties of the Holstein t–J model (HtJM), including the full quantum nature of phonons.

In this contribution, we employ the Lanczos algorithm in combination with a kernel polynomial moment expansion and the Maximum Entropy method [5] to investigate the quasiparticle spectrum of a single hole–polaron in the 2D HtJM on a ten-site square lattice. Moreover, we compute different hole–hole/phonon correlation functions at higher doping level in order to comment on hole-binding effects and charge-density-wave (CDW) formation.

The HtJM is described by the Hamiltonian [4]

$$\mathscr{H} = \mathscr{H}_{\mathrm{ph}} + \mathscr{H}_{t-J} - \sqrt{\varepsilon_{\mathrm{p}}\hbar\omega}\sum_i (b_i^\dagger + b_i)\tilde{h}_i, \qquad (1)$$

where $\mathscr{H}_{\mathrm{ph}}$ and $\mathscr{H}_{t-J}$ represent the phonon part and standard t–J model, respectively, and the last term takes into account the interaction of doped holes ($\tilde{h}_i = 1 - \sum_\sigma \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma}$) with a single dispersionless phonon mode (which, e.g., may be thought of as representing a local apical-oxygen coupling; ε_{p} is the EP coupling constant, ω denotes the bare phonon frequency). $\mathscr{H}$ acts in a projected Hilbert space without double occupancy. A general state of (1) can be written as the

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direct product $|\Psi\rangle = \sum_{l,k} c_l^k |l\rangle_{\rm el} \otimes |k\rangle_{\rm ph}$, where l and k label the electronic and bosonic basic states, respectively, and $|k\rangle_{\rm ph} = \prod_{i=1}^{N=10} [\sqrt{n_i^k!}]^{-1} [b_i^\dagger]^{n_i^k} |0\rangle_{\rm ph}$. Since the bosonic part of the Hilbert space is infinite dimensional we use a truncation method [4] restricting ourselves to phononic states with at most M phonons. To control our truncation procedure as a function of M, we calculate the weight of the m-phonon states in the ground state $|\Psi_0\rangle$ of $\mathscr{H}$: $|c^m|^2 = \sum_{l,k} |c_l^k|^2$ with $m = \sum_{i=1}^N n_i^k$. In the numerical work convergence is achieved if the relative error of $E_0(M)$ is less than 10^{-7}.

Fig. 1 shows $|c^m|^2$ for the 2D HtJM with a single hole at weak, intermediate and strong EP couplings [in what follows, we have fixed $J = 0.4$ (all energies are measured in units of t)]. The curves $|c^m|^2(m)$ are bell-shaped and their maxima correspond to the most probable number of phonon quanta in the ground state. These results, as well as the M-dependence of E_0 at $\varepsilon_{\rm p} = 4$ (see inset), confirm the importance of multi-phonon states in the (adiabatic) strong-coupling regime $\varepsilon_{\rm p} \gg 1$, $\hbar\omega$.

In the analysis of the HtJM we start with the study of just a single dynamic hole. Increasing the EP coupling in the adiabatic regime, we notice a continuous but rather sharp crossover from nearly free polaron, described by an effective transfer amplitude that is only weakly reduced from its value in the pure t–J model, to a less mobile (small-size) adiabatic Holstein hole–polaron (AHP). Moreover, we found that the critical EP coupling for the polaron transition is substantially reduced due to prelocalization effects of the hole in the antiferromagnetic spin background [3]. To elucidate the difference between the FP and AHP limits and to demonstrate the formation of a hole–polaron band at large $\varepsilon_{\rm p}$, in Fig. 2 we present the results for

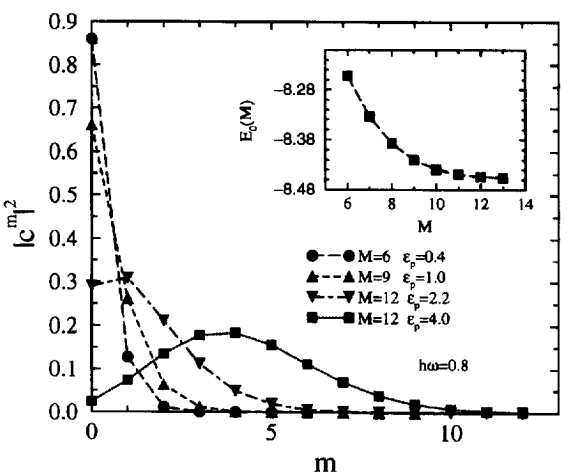

Fig. 1. Phonon-weight function $|c^m|^2$ and ground-state energy $E_0(M)$ for the 2D HtJM.

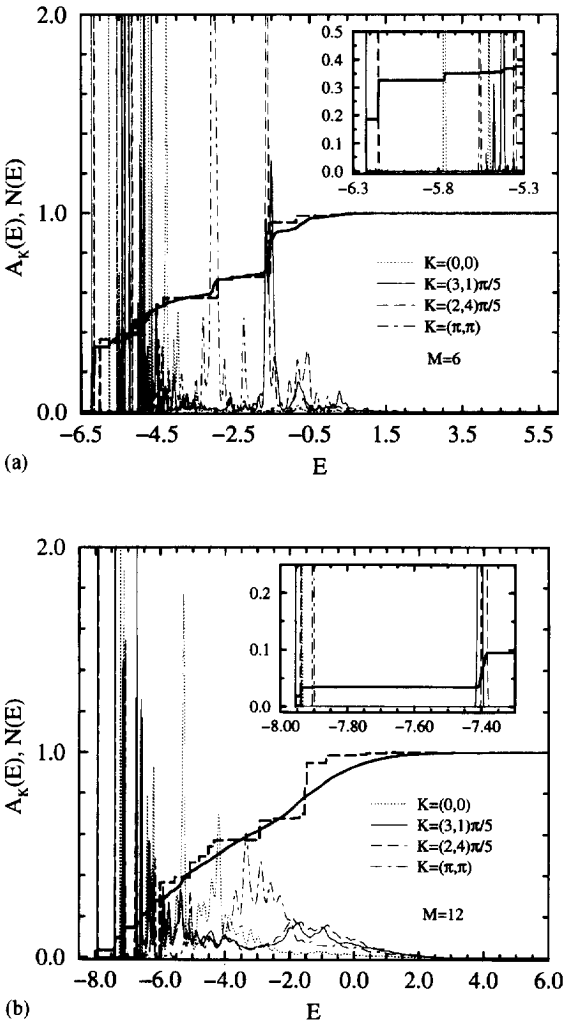

Fig. 2. Single-hole spectral function $A_K(E)$ for the 2D HtJM at $\hbar\omega = 0.8$ and $\varepsilon_{\rm p} = 0.5$ (upper panel) 3.4 (lower panel), where the energy scale is shifted by $E_0^{(N)}$. The insets show the low-energy part of the spectra. The integrated density of states $N(E) = \int_{-\infty}^{E} {\rm d}E' \sum_K A_K(E')$ (bold solid line) is depicted in comparison with the result for the pure t–J model (dashed line).

the $\boldsymbol{K}$-resolved spectral function

$$A_{\boldsymbol{K}}(E) = \sum_{n,\sigma} |\langle \Psi_n^{(N-1)} | \tilde{c}_{\boldsymbol{K}\sigma} | \Psi_0^{(N)} \rangle|^2 \times \delta[E - (E_n^{(N-1)} - E_0^{(N)})]. \quad (2)$$

Of course in the very weak-coupling regime the spectral function is barely changed from that of the pure t–J model. Increasing ε_p, the lowest peaks in each $A_{\boldsymbol{K}}$ separate from the rest of the spectrum. These states become very close in energy and a narrow well-separated energy band evolves in the strong-coupling case, where the gap to the next higher "band" is of the order of the phonon frequency $\hbar\omega$. Note that the transition to the AHP state is accompanied by a strong increase in the on-site hole–phonon correlations which are about one order in magnitude larger than the nearest-neighbour (NN) ones (cf. Fig. 11 in Ref. [4]). This indicates that the AHP quasiparticle comprising a 'quasi-localized' hole and the phonon cloud is mainly confined to a single lattice site. As the phonon frequency is enlarged at fixed ε_p, the hole–phonon correlations are smeared out, and the crossover to the small hole–polaron is shifted to larger values of the EP coupling.

Next we wish to discuss the two-hole problem. To get a feel for hole-binding effects, we have calculated the hole–hole correlation function

$$C_{\mathrm{ho-ho}}(|i-j|) = \langle \Psi_0(\varepsilon_p, J) | \tilde{h}_i \tilde{h}_j | \Psi_0(\varepsilon_p, J) \rangle. \quad (3)$$

Results for $C_{\mathrm{ho-ho}}(|i-j|)$ are given in Fig. 3. In the weak-coupling region, $C_{\mathrm{ho-ho}}(|i-j|)$ becomes maximum at the largest distance of the ten-site lattice, while in the intermediate EP coupling regime the preference is on next NN pairs. As expected, increasing further ε_p, the maximum in $C_{\mathrm{ho-ho}}(|i-j|)$ is shifted to the shortest possible distance, indicating hole–hole attraction. At $\varepsilon_p \gg 1$, the two holes become 'self-trapped' sharing a sizeable common lattice distortion, i.e., a nearly immobile hole–bipolaron is formed. The behaviour of $C_{\mathrm{ho-ho}}$ is found to be qualitatively similar for higher (lower) phonon frequencies (see inset), except that the crossings of different hole–hole correlation functions occur at larger (smaller) values of ε_p, which shows the importance of *both* parameter ratios ε_p/t and $\sqrt{\varepsilon_p/\hbar\omega}$.

Finally, let us consider the quarter-filled band case. Here, we have investigated the more simple spinless

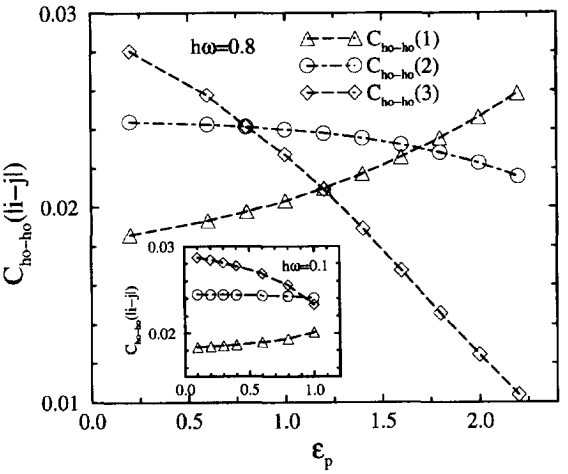

Fig. 3. Non-equivalent hole–hole pair correlation functions $C_{\mathrm{ho-ho}}(|i-j|)$ in the two-hole ground state of the HtJM as a function of ε_p; here 1–3 label NN, next NN, and third NN distances.

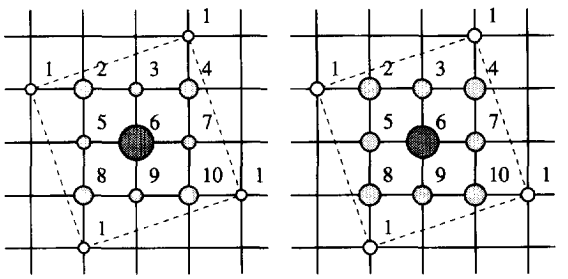

Fig. 4. $C_{\mathrm{ho-ho}}(|6-j|)$ (left) and $C_{\mathrm{ho-ph}}(|6-j|)$ (right) are displayed at $\varepsilon_p = 3$ and $\hbar\omega = 0.8$, where both diameter and gray level of the circles being proportional to the correlation strength.

fermion model (total $S^z = S^z_{\max}$). In accordance with previous approximative treatments based on the inhomogeneous variational Lang–Firsov approach [3], we found, as the EP coupling increases, evidence for a transition from a FP state to a 2D polaronic superlattice, where the holes are self-trapped on every each other site. This cross-over is signaled by a pronounced peak in the charge structure factor at (π, π). To visualize the correlations in this state in more detail, in Fig. 4 we have depicted $C_{\mathrm{ho-ho}}(|i-j|)$ and the corresponding hole–phonon density correlation function $C_{\mathrm{ho-ph}}(|i-j|) = \langle \Psi_0 | \tilde{h}_i b_j^\dagger b_j | \Psi_0 \rangle$ as a function

of $|i-j|$. Our exact results clearly show the phonon-dressing of the holes and the resulting tendency towards CDW formation. A similar polaron ordering was observed in $La_{1.5}Sr_{0.5}NiO_4$.

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