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On the stability of polaronic superlattices in strongly coupled electron–phonon systems

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We investigate the interplay of electron–phonon (EP) coupling and strong electronic correlations in the frame of the two-dimensional (2D) Holstein t–J model (HtJM), focusing on polaronic ordering phenomena for the quarter-filled band case. The use of direct Lanczos diagonalization on finite lattices allows us to include the effects of quantum phonon fluctuations in the calculation of spin/charge structure factors and hole–phonon correlation functions. In the adiabatic strong coupling regime we found evidence for "self-localization" of polaronic carriers in a (π,π) charge-modulated structure, a type of superlattice solidification reminiscent of those observed in the nickel perovskites $La_{2-x}Sr_xNiO_{4+y}$.

Electron diffraction measurements on the nickel oxide analogue of the layered high-T_c 214 copper oxide compound, $La_{2-x}Ni_xCuO_4$, reveal a (π,π)-superstructure spot at *quarter filling*, i.e. for $x = 0.5$, which has been interpreted as sign of a truly 2D polaron ordered phase [1].

To study charge- and spin-ordering phenomena in such systems, exhibiting besides a substantial EP interaction strong Coulomb correlations, let us consider the planar t-J model with an additional on-site Holstein hole-phonon coupling:

$$\mathcal{H}_{H-t-J} = \mathcal{H}_{ph} + \mathcal{H}_{ho-ph} + \mathcal{H}_{t-J}\,, \qquad (1)$$

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

Here $\mathcal{H}_{ph}$ and $\mathcal{H}_{t-J}$ represent the phonon part and standard t–J model, respectively. In (2), ε_p is the local EP coupling constant, ω_0 denotes the bare phonon frequency, $\tilde{h}_i = 1 - \sum_\sigma \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma}$, and $b_i^\dagger$ ($\tilde{c}_{i\sigma}^\dagger$) are the usual phonon (projected fermion) creation operators. Of course the HtJM gives only a very simplified description of the complex hole transport and low-spin high-spin interactions in the nickelates [2].

At quarter-filling and for strong EP interactions, Lanczos studies of the *static* HtJM (frozen-phonon approximation) yield strong indications of a Peierls distorted ground state [3] .

To discuss *non-adiabatic* effects preserving the full dynamics and quantum nature of the phonon degrees of freedom, we perform here a direct exact diagonalization (ED) of the HtJM on a ten-site (N) square lattice with at most M phonons using a well-controlled phononic Hilbert space truncation procedure [4]. Since memory limitations impose severe restrictions on this method, we study an effective polaronic t–J model $\mathcal{H}^{eff}_{H-t-J}(\Delta_i, \gamma, \bar{\gamma}, \tau^2)$ as well, which can be derived from (1) by applying the inhomogeneous modified variational Lang–Firsov (IMVLF) approach outlined in [4]. The N+2 variational parameters take into account *static* displacement field (Δ_i), *dynamic* polaron (γ), finite density ($\bar{\gamma}$) and squeezing (τ^2) effects. We stress that the IMVLF-Lanczos approach correctly reproduces the adiabatic and anti-adiabatic, weak- and strong EP coupling limits [5].

In the numerical analysis of the HtJM, we first consider the case of spinless fermions (total $S^z = S^z_{max}$), i.e., the electronic correlations are neglected. Increasing the EP coupling at fixed phonon frequency ($\hbar\omega_0 = 0.8$), the smooth variation of the charge structure factor $S_c(\pi,\pi)$ in the nearly free polaron state ($\varepsilon_p \lesssim 2$) is followed by a strong enhancement in a "quasi-localized" polaron state indicating the formation of a charge density wave (CDW) [see Fig. 1]. This crossover becomes suppressed in the non-adiabatic regime ($\hbar\omega_0 = 3$). As can be seen from the insets, at $\varepsilon_p = 3$, i.e. in the CDW-like phase, a larger number of phonons is still required to achieve a satisfactory convergence of the ED data. Including more phonons we expect an even more pronounced increase of $S_c(\pi,\pi)$ [cf. the IMVLF curve].

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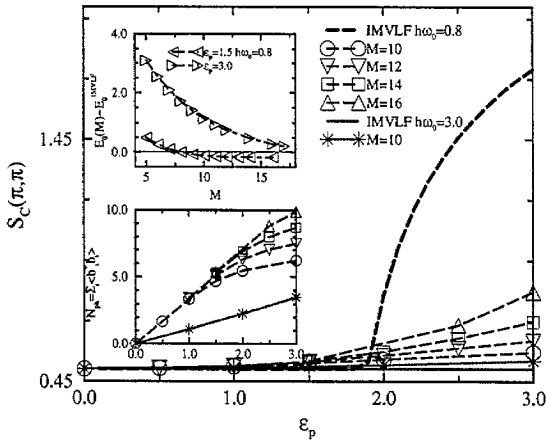

Fig. 1: Charge structure factor $S_c(\vec{q})$ vs ε_p, where ED data with different M are compared with IMVLF results. The insets show the deviation of $E_0(M)$ from the IMVLF–value and the mean number of phonons N_{ph} in the ground state, respectively. All energies are measured in units of t and we adopt $J = 0.4$ throughout.

To visualize the hole–phonon correlations, Fig. 2 displays the variation of $C_{ho-ph}(|i-j|) = \langle\Psi_0|\tilde{h}_i b_j^\dagger b_j|\Psi_0\rangle$ as a function of ε_p for both the spin-1/2 and spinless fermion cases. Our results clearly show the phonon dressing of the holes according to an AB sublattice structure. Due to the possible gain of exchange energy J, the density oscillations are weakened for spin-1/2 particles.

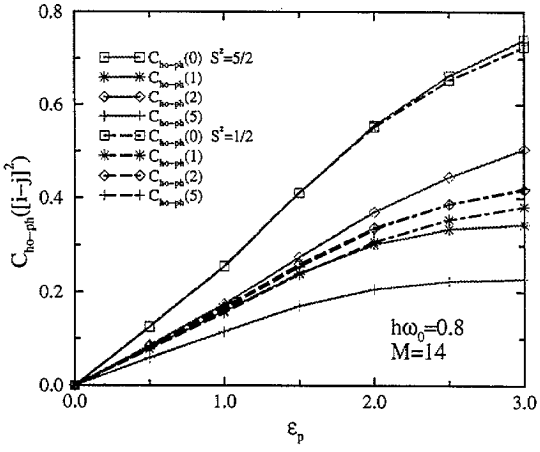

Fig. 2: $C_{ho-ph}(|i-j|)$ vs ε_p at all nonequivalent distances $|\vec{R}_i - \vec{R}_j|/a = 0, 1, \sqrt{2}, \sqrt{5}$. Increasing M for $\varepsilon_p \gtrsim 2$, we expect an upturn of $C_{ho-ph}(0,2)$.

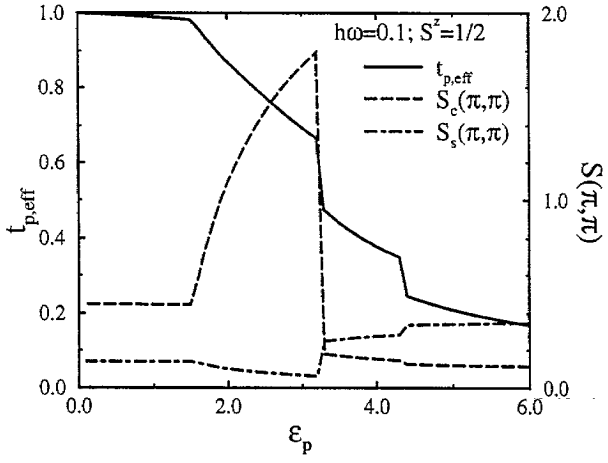

Fig. 3: Magnetic/charge structure factors $S_{c/s}(\vec{q})$ and $t_{p,eff}$ vs ε_p for the 2D HtJM at quarter filling.

Using the IMVLF-Lanczos method to reach the strong–coupling adiabatic regime, we notice, as ε_p increases, a sequence of transitions from nearly free to self–trapped polarons [with less mobility $\propto t_{p,eff} = E_{\rm kin}(\varepsilon_p, J)/E_{\rm kin}(0, J)$] solidifying into a polaronic superlattice and finally to charge–separated (CS) states ($\varepsilon_p \gtrsim 3$). These transitions are accompanied by a change of both charge *and* spin structure factors [see Fig. 3]. Note that the spin correlations are significantly enhanced (weakened) in the CS (CDW) state.

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