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 \((\pi, \pi)\) 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 \((\pi, \pi)\)–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:

\[
H_{H-t-J} = H_{ph} + H_{ho-ph} + H_{t-J}, \tag{1}
\]

\[
H_{ho-ph} = -\sqrt{\varepsilon_p h \omega_0} \sum_i \left( b_i^\dagger \hat{h}_i + b_i \right). \tag{2}
\]

Here \(H_{ph}\) and \(H_{t-J}\) represent the phonon part and standard t–J model, respectively. In (2), \(\varepsilon_p\) is the local EP coupling constant, \(\omega_0\) denotes the bare phonon frequency, \(\hat{h}_i = 1 - \sum_\sigma \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}\), and \(b_i^\dagger (\hat{c}_i^\dagger)\) 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 \(H_{H-t-J}^{eff}(\Delta, \gamma, \tilde{\gamma}, \tilde{\gamma}^2)\) 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 \((\Delta, \gamma)\), dynamic polaron \((\tilde{\gamma})\), finite density \((\tilde{\gamma}^2)\) 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 \(S^z = S_{max}^z\), i.e., the electronic correlations are neglected. Increasing the EP coupling at fixed phonon frequency \((h \omega_0 = 0.8)\), 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 \((h \omega_0 = 3)\). 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 in-
crease of $S_c(\pi, \pi)$ [cf. the IMVLF curve].

To visualize the hole–phonon correlations, Fig. 2 displays the variation of $C_{ho-ph}(|i - j|) = \langle \Psi_0 | h_i b_j^\dagger b_j | \Psi_0 \rangle$ as a function of $\varepsilon_p$ 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.

Using the IMVLF-Lanczos method to reach the strong–coupling adiabatic regime, we notice, as $\varepsilon_p$ increases, a sequence of transitions from nearly free to self–trapped polarons [with less mobility $\propto t_{p,eff} = E_{kin}(\varepsilon_p, J)/E_{kin}(0, J)$ 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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