Interplay between charge-lattice interaction and strong electron correlations in cuprates: Phonon anomaly and spectral kinks

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Abstract – We investigate the interplay between strong electron correlations and charge-lattice interaction in cuprates. The coupling between half-breathing bond-stretching phonons and doped holes in the $t-t'-J$ model is studied by the limited phonon basis exact diagonalization method. Nonadiabatic electron-phonon interaction leads to the splitting of the phonon spectral function at half-way to the zone boundary at $\vec{q}_s = \{ (\pm \pi/2, 0), (0, \pm \pi/2) \}$ and to low-energy kink feature in the electron dispersion, in agreement with experimental observations. Another kink due to strong electron correlation effects is observed at higher energy, depending on the strength of the charge-lattice coupling.

There is a growing confidence that strong electron-phonon interaction (EPI) manifests itself both in vibrational [1] and electronic [2] spectra of cuprates. The most puzzling feature of the cuprate phonon spectra is the anomaly of the half-breathing bond-stretching (HBBS) phonon occurring at half-way to the Brillouin zone (BZ) boundary in the [100]-direction, while the most debating feature of the electronic spectra are the kinks observed in angle-resolved photoemission spectra (ARPES).

It was recently realized in the experimental community that it is highly important to measure both phonons spectra and ARPES on the same sample just to verify possible links between HBBS phonons and ARPES [3]. The results of the above studies support close connection between the HBBS phonon anomaly and the lowest-energy kink in ARPES [3] and, thus, a model describing both anomalies within the same approach is strongly needed.

In the present letter we study the low-density limit (one hole on $4 \times 4$ lattice) of the extended $t-t'-J$ model where holes are coupled to HBBS phonons [4]. In order to calculate the phonon spectral function (PSF) and hole spectral function (HSF), we generalize a recently introduced approach [5], based on limited phonon basis exact diagonalization (LPBED), without adopting self-consistent Born (SCBA) and spin wave approximations [6,7]. This method treats the non-adiabatic effects of the quantum phonon very effectively without approximations for the magnetic degrees of freedom. Because of exponential growth of the basis with size of the system, the $4 \times 4$ lattice has considerably denser quantum states than the smaller $\sqrt{10} \times \sqrt{10}$ system [8], so that it is possible to resolve the fine structure of the PSF and HSF. For the first time we are able to reveal the shape of the PSF while previous studies [9–11] were restricted to at most the second moment of the response.

We show that EPI can lead to the splitting of the PSF at half-way to the BZ boundary in the [100] direction. We demonstrate that the splitting can be easily smeared out by a very small broadening and, thus, the mysterious evasive behavior of double-peak structure can be attributed to tiny variations of chemical composition, crystal quality and/or experimental setup. We argue that the splitting is a rather general phenomenon arising when the phonon branch interacts with a rather soft electronic excitation and we show that the HBBS phonon anomaly is linked to the lowest-energy kink observed in the ARPES.

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Finally we emphasize that the same model supports the spectral kink at higher energy referred to colloquially as the waterfall [12].

McQueeney et al. [13] observed anomalous lineshape of HBBS phonons around $q = (\pi/2, 0, 0)$ and reported its strong temperature dependence. Subsequent studies confirmed that the HBBS phonon anomaly is due to the coupling of the HBBS phonons to the doped carriers. Indeed, the anomaly is absent in undoped compounds [1] and the hardening of the phonon spectra with heating [13,14] excludes such sources of anomaly as anharmonicity or structural inhomogeneity. It is also agreed that HBBS phonon anomaly is located around $q = (\pi/2, 0, 0)$ at any doping [14–16]. On the other hand, there is a controversy on the relation between the HBBS phonon anomaly and the lowest-energy kink in the ARPES. This relation is often denied although the measurements of the phonon spectra and ARPES on the same sample of Bi$_2$Sr$_2$LaO$_{6+\delta}$ suggest that the softening of the HBBS phonon mode matches the energy and momentum of this kink [3]. Another much debated question is the functional theory calculations [21,22] do not predict any HBBS phonon anomaly [23]. Other approaches, especially those associating the anomaly with stripes, have difficulty with the position of the HBBS phonon anomaly. The scenario suggested in ref. [24] relates the HBBS softening to the Kohn anomaly at double Fermi momentum $2k_F$ along the Fermi surface of stripes [24]. Here, in contrast to experiment, the softening must be $\theta$-independent.

In a different theoretical proposal, HBBS anomaly is associated with stripe-mediated collective charge excitations [25] or incommensurate low-energy spin fluctuations [26]. Within these scenarios, in contrast with experiment [14,15,20,27,28], the wave vector of phonon anomaly strongly depends on doping level. Finally we note that phonon softening [9,10], broadening [9], and correct position of the anomaly [11] have already been qualitatively explained by the coupling between phonons and density response of the $t$-$J$ model although none of those studies considered the shape of the phonon spectral function.

The Hamiltonian of the $t$-$t'$-$J$-Holstein model in 2D is the sum of the electronic part and hole-phonon coupling Hamiltonian

$$H' = \omega_0 \sum_{q,\mu} a_{q,\mu}^\dagger a_{q,\mu} + \sum_{i,q,\mu} \left( M_{q,\mu} e^{iq \cdot \vec{R}_i} \right) \left( (1 - n_i) a_{q,\mu} + \text{H.c.} \right).$$

Here $J$ is the exchange interaction constant of the spin-spin interaction, $t$ and $t'$ are hopping amplitudes to nearest and next nearest neighbors. At site $i$ (Cu atoms), $S_i$ is the spin-$1/2$ operator, $c_{i,\sigma}$ is the fermionic operators in the space without double occupancy, and $n_i$ is the number operator. $a_{q,\mu}$ is the phonon annihilation operator with momentum $q$, and $\mu = x$ or $y$ indicates the longitudinal polarization of the oxygen vibrations along the direction of the nearest-neighbor Cu atoms (oxygen atoms are located at $\vec{R}_i + a/2$), $M_{q,\mu}$ is the matrix element of the EPI: $M_{q,\mu} = g_0 \omega_0 / \sqrt{2} \sin(q_\mu/2)$, where $N$ is the number of lattice sites and $\omega_0$ is the frequency of dispersionless optical phonon. The strength of EPI is characterized by the dimensionless coupling constant $\lambda = \sum_{q,\mu} |M_{q,\mu}|^2 / 4 \omega_0 t$. We chose parameters which correspond to hole-doped cuprates: $J = 0.4t$, $t' = -0.25t$, $\omega_0 = 0.15t$, and set $t = a = h = 1$. The PSF is expressed as

$$D(\vec{q}, \omega + i\eta) = \frac{1}{\pi} \frac{1}{D_0^{-1}(\vec{q}, \omega + i\eta)} - \Sigma(\vec{q}, \omega + i\eta),$$

where the self-energy $\Sigma(\vec{q}, \omega + i\eta)$ is given by

$$\Sigma(\vec{q}, \omega + i\eta) = \frac{|M_{q,\mu}|^2 \Pi(\vec{q}, \omega)}{(1 + |M_{q,\mu}|^2 \Pi(\vec{q}, \omega)/D_0^{-1}(\vec{q}, \omega + i\eta))}.$$ 

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Here $D_0(q, \omega + i\eta)$ is the bare phonon Green function and $\Pi(q, \omega) = P(q, \omega + i\eta) + P(q, -\omega - i\eta)$ is the polarization insertion with
\[
P(q, \omega + i\eta) = \left\langle \psi_0 \left| \frac{1}{\omega + i\eta - H + E_0} \right| \psi_0 \right\rangle.
\] (4)

We choose the ground state (GS) $|\psi_0\rangle$ as a linear superposition with equal weights of the 4 degenerate states corresponding to $\vec{k} = (\pm \pi, \pm \pi)$ with energy $E_0$, $\eta$ is a broadening factor that shifts the poles of $D(q, \omega)$ in the complex plane, and $O = \sum e^{i\vec{q}\cdot\vec{R}}(1 - n_i)$. The increase of broadening factor $\eta$ has the physical meaning of phonon damping or limited experimental resolution.

The ground state $|\psi_{GS}\rangle$ and the function $P(q, \omega + i\eta)$ are obtained by the modified [29] and standard Lanczos methods, respectively, within the LPBPD method [5] introduced for the t'-J-Holstein model.

In fig. 1 we plot the PSF $D(q, \omega)$ for different wave vectors along the (1,0) direction in the BZ. For the chosen values of the model parameters the system undergoes, in agreement with [30], a crossover towards the strong EPI regime for $\lambda \approx 0.5$. The anomalous softening of the phonon mode at $q_s = (\pi/2, 0)$ is already observed at moderate values $\lambda < \lambda_c$ of the hole-phonon coupling ($\lambda = 0.3$). We stress that for a large value of the broadening factor $\eta = 0.08$ the phonon peak softens and broadens at $q_s$ (fig. 1(a)), supporting, thus, SBI. On the other hand, reducing the broadening factor to $\eta = 0.03$ the two-peak structure becomes evident (fig. 1(b)), that is in agreement with the experimental observations reported in refs. [15,20].

To clarify the physical nature of the splitting, we study the hole spectral weight function $A(k, \omega)$ at the wave vectors $\vec{k}_f$ that are reached starting from GS wave number at $(\pm \pi/2, \pm \pi/2)$ through phonon momentum $q_s = (\pi/2, 0)$. For example, as shown in fig. 2, by starting from $k = (-\pi/2, \pi/2)$ we get $k_f = (0, \pi/2)$ after absorbing (emitting) a phonon with momentum $-q_s = (\pi/2, 0)$. The lowest energy peak in $D(q, \omega)$ (dotted red curve in fig. 2) is close to the lowest energy peak of $A(k_f, \omega)$ (solid blue curve in fig. 2). Measuring energy from the GS, denoted by the vertical line in fig. 2, one can see that the lowest peaks in the phonon and hole spectral functions are softer than the phonon energy $\omega_0 = 0.15\hbar$. We note that the significant renormalization of the hole spectral weight, with respect to the GS one, indicates strong coupling between phonon at $q_s$ and hole at $k_f$. The high-energy peak in $D(q, \omega)$ is located at energy close to $\omega_0$, and no peak at the same energy is found in $A(k, \omega)$. It is shown below that this is due to the phononic nature of the high-energy resonance of the PSF.

To give a simple explanation of the above scenario, one has to realize that the excited electronic state $|\psi^0_{(0, \pi/2)}\rangle|0\rangle$ with the momentum $(0, \pi/2)$ and without phonons is linked by the matrix elements of EPI with a group of 8 degenerate states $|\psi^0_{(\pm \pi/2, \pm \pi/2)}\rangle|0\rangle$, where the electronic subsystem is in the GS and one phonon is excited. The momentum conservation $(\pm \pi/2, \pm \pi/2) + q_s = (0, \pi/2)$ determines the phonon momenta $q$. The energies of the electronic subsystem at corresponding momenta are $\epsilon^0(0, \pi/2)$ and $\epsilon^0(\pi/2, \pi/2)$, respectively. Then, choosing a set of the model parameters appropriate for cuprates, the resonance relation $\epsilon^0(0, \pi/2) \approx \epsilon^0(\pi/2, \pi/2) + \omega_0$ is satisfied. Hence, even small matrix elements induce strong effects both in electronic and vibrational subsystems. Analytic diagonalization of this degenerate $9 \times 9$ matrix gives 9 levels. The lowest state $L$ has energy below $\omega_0$ and has components on both one-phonon and zero-phonon states. This state corresponds to the peaks of electronic $A(k = (0, \pi/2), \omega)$ and bosonic $D(q = (\pi/2, 0), \omega)$ spectral functions at $\omega < 0.1$ (see the area around letter $L$ in fig. 2). In the highest-energy range, (see the area around letter $H$ in fig. 2), both spectral functions collect contributions at $\omega \gtrsim 0.2$. However, the $H$-state is of predominantly electronic origin with a large peak in the hole spectral function while it generates a weak structure in the PSF, hardly observable in the numerical data. The last 7 degenerate levels with energy $\epsilon^0(\pi/2, \pi/2) + \omega_0$ have no projection.
on the vacuum boson state: this explains why the hole spectral weight function does not show any peak at this energy, at a distance $\omega_0$ from the GS energy. The energies of all levels of the above simple analytic solution are in qualitative agreement with that provided by the numeric LPBED method in fig. 2. So, we conclude that the doubling of the phonon peak is due to coupling between holes and lattice, that lifts a degeneracy and produces one additional state with energy less than $\omega_0$.

Generically, the EPI involving electronic states with energies considerably larger than the phonon frequency does not lead to any splitting since the adiabatic approximation is valid and the electron produces only a renormalization of the adiabatic potential [31]. On the other hand, when the electronic excitation is soft and its energy is comparable with phonon frequency, the nonadiabatic corrections play a crucial role [32] and one can observe exotic spectral functions as is seen in fig. 1(b) and in experiments on cuprates.

The clear connection, established by the above considerations, between phonon at $\vec{q}$, and hole at $\vec{k}_F$ encouraged us to search for an interplay between the HBBS phonon anomaly and the lowest-energy kink in the dispersion of quasiparticles in cuprates [33]. So far we adopted periodic boundary conditions, i.e. the standard approach used in investigating small lattices. In this way only a limited number of wave numbers in the Brillouin zone is allowed and calculations on larger lattices are generally required to obtain a complete picture of the electron structure. To overcome this difficulty one has to go beyond periodic boundary conditions. One way is to introduce twisted boundary conditions. It has been shown [34] that the use of twisted boundary conditions is an effective tool to probe all momenta in the Brillouin zone even in a small lattice. Below we will adopt this approach. In fig. 3(a) we plot hole dispersion derived from momentum distribution curves, i.e. we find the $\vec{k}$ for which the hole Green function $A(\vec{k}, \omega)$ has a maximum at fixed $\omega$ [34]. The energy, measured from the GS, is plotted vs. the wave number $(\vec{k} - \vec{k}_F)$, where $\vec{k}_F$ is the momentum corresponding to the minimum of the hole dispersion relation. We find that, when $E_k - E_{\vec{k}_F}$ is about $\omega_0 = 0.15$, the curve exhibits a slope change related to the coupling between the bare phonon energy and the electronic band in the bare $t$-$t'$-$J$ model. This kink does not appear in the absence of the hole-phonon coupling. A change of slope in the momentum distribution curves is the typical effect of the electron-phonon interaction [2,35]. It takes place for values of the wave number where the bare electron energy becomes equal to the phonon energy. The effect is based on a noncrossing rule and it is present for any small value of the electron-phonon coupling. On the other hand, we obtain another kink at higher energy (see fig. 3(a)) [12]. This distinctive feature is related to the strong electron correlations since it is observed also in the bare $t$-$t'$-$J$ model. At $\lambda = 0$ the kink is located around the exchange interaction energy $J$, in agreement with results by Chakraborty et al. [36] within the Hubbard model. Furthermore, the kink is shifted at higher energy by increasing the hole-phonon coupling. We also investigated the effect of the oxygen isotope substitution [5] on ARPES. The results (fig. 3(b)) show a negligible (below 0.01t) shift upon oxygen isotope exchange, that is in agreement with recent experimental observations by Douglas et al. [37]. A comprehensive study of the hole spectral weight function at all momenta in the Brillouin zone will be addressed in a future work. All these data point out that the scenario based on the interplay between strong electron correlations and hole-phonon interaction is able to capture many physical distinctive features of high-temperature superconductors. In conclusion, we showed that the EPI, in the presence of strong correlations, can lead to the splitting of the phonon spectral function at half-way to the BZ boundary in the [100] direction. We demonstrated that the splitting can be easily smeared out by very small broadening of the eigenstates. The same physical mechanism can explain both the HBBS phonon anomaly and the lowest-energy kink in the ARPES. Finally we found that the isotope effect on ARPES is negligible in accordance with experiment. These results support the claim that strong electron correlations and charge lattice interaction are crucial in understanding cuprate experimental features.

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