Hole pairing and phonon dynamics in generalized 2D \( t - J \)–Holstein models

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The formation of hole pairs in the planar \( t-J \) model is studied in the presence of independent dynamic vibrations of the in-plane oxygen atoms. In-plane (breathing modes) and out-of-plane (buckling modes) displacements are considered. We find strong evidences in favor of a stabilization of the two hole bound pair by out-of-plane vibrations of the in-plane oxygen. On the contrary, the breathing modes weaken the binding energy of the hole pair. These results are discussed in the context of the superconducting cuprates.

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The electron-phonon interaction plays the key role in the conventional BCS theory of superconductivity. It is the source of the effective (retarded) attraction between the electrons and hence of the dynamical effect for pair formation. On the contrary, in unconventional superconductors like the high-\( T_c \) cuprates, the driving force for superconductivity is commonly believed to be the strong electronic correlations. However, it is theoretically known that, in strongly correlated systems, even moderate electron-phonon interactions can have drastic consequences. For example, it can enhance charge density wave (CDW) and spin density wave (SDW) instabilities due to polaronic self-localization effect [1,2]. Experimentally, the observation of some oxygen isotope effect in the high-\( T_c \) cuprates [3] has given evidences for some contribution of the electron-phonon interaction in the superconductivity, even though the dominant pairing mechanism is due to strong antiferromagnetic correlations. The interplay between strong electronic correlations and electron-phonon interaction still remains an open question.

The hamiltonian is a generalization of the \( t-J-Holstein \) Hamiltonian [4],

\[
H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + c_{i,\sigma}^\dagger c_{j,\sigma}) + J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j)
\]

For the sake of simplicity, we describe here the low energy electronic degrees of freedom by a single band \( t-J \) model. We also restrict ourselves to the vibrations of the in-plane oxygen atoms of the \( \text{CuO}_2 \) plane which have been shown to be essential. Two types of displacement have to be considered: (a) in-plane breathing modes and (b) buckling modes, as shown schematically in Fig. 1. When the equilibrium position of the oxygen atom lies away from the \( \text{Cu} \) plane by \( u_0 \) in Fig. 1(b), the electron-phonon interaction becomes linear in the oxygen displacement perpendicular to the plane [4], as it is always the case for the breathing modes. Such a buckling structure is realized in \( \text{YBa}_2\text{Cu}_3\text{O}_7-\delta \). In the antiadiabatic limit the two modes of interaction give an effective nearest-neighbor (NN) hole-hole repulsion (a) and attraction (b) respectively. In a week coupling \( t \)-matrix approximation which included an RPA antiferromagnon spin-fluctuation exchange and a phonon exchange, Bulut and Scalapino [5] found that the buckling mode can enhance \( d_{x^2-y^2} \) pairing. Using an antiferromagnetic induced hole dispersion and treating the electron-phonon interaction at the mean-field level, Nazarenko and Dagotto [6] found that the buckling mode can give rise to a \( d_{x^2-y^2} \) wave superconducting ground state (GS). However, both of these results involve uncontrolled approximations which are inadequate for treating the Hubbard and \( t-J \) models in the absence of phonons. Thus it is of interest to carry out a numerical investigation of this problem. Our results are based on exact diagonalization studies of small \( t-J \)-phonon clusters. In agreement with the approximate results we find that the breathing mode suppresses the two-hole pairing [3], while the buckling mode stabilizes it [3]. However, in addition, we have examined the effect of the phonons on the kinetic energy, antiferromagnetic structure factor and hole-hole correlations, giving a more detailed picture of the role of dynamic lattice vibrations on the hole pairing.

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\]
+ \sum_{i,\delta}(\frac{p^{2}_{i,\delta}}{2m} + \frac{1}{2}m\Omega^{2}u^{2}_{i,\delta}) + g \sum_{i,\delta}(n_{i}^{h} + n_{i+\delta}^{h}) \tag{1}

where $\hat{c}_{i,\sigma}^{\dagger}$ is the usual hole creation operator, $n_{i}$ and $n_{i}^{h}$ are the electron and hole local densities respectively, $m$ is the oxygen ion mass, $\Omega$ is the phonon frequency and $\delta = x, y$ differentiates the bonds along the $x$- and $y$-direction respectively. The sign $- (+)$ in the last term corresponds to the breathing (buckling) mode. Throughout, energies are measured in unit of the hopping integral $t$. The electron-phonon g-term involves the coupling of each copper hole with the displacements of the four neighboring oxygens $u_{i,\delta}$ and $u_{i-\delta,\delta}$. This is clearly different from the on-site Holstein coupling which has been recently used to mimic the coupling with the apical oxygen modes in the framework of the $t$-$J$ model. Note that the displacements $u_{i,\delta}$ are considered throughout as independent variables.

For the purpose of our discussion it is convenient to rewrite the electron-phonon interaction in the boson representation of the phonons,

$$H_{e-ph} = \Omega \sum_{i,\delta}(b_{i,\delta}^{\dagger}b_{i,\delta} + \frac{1}{2})$$ \tag{2}

$$+ \lambda_{0} \sum_{i,\delta}(b_{i,\delta}^{\dagger}b_{i,\delta} + b_{i,\delta}^{\dagger}b_{i,\delta}^{\dagger})(n_{i}^{h} + n_{i+\delta}^{h})$$

where $\lambda_{0} = g \sqrt{\frac{1}{2m\Omega}}$. Since the phononic Hilbert space has an infinite dimension, we truncate it to a finite number of bosonic states i.e. $b_{i,\delta}^{\dagger}b_{i,\delta} \leq n_{ph}$ at each oxygen site. We restrict ourselves to $n_{ph} = 1$. We have tested the validity of the one-phonon approximation on the $2 \times 2$ lattice with $n_{ph}$ up to 5. The behaviors with the coupling constant $\lambda_{0}$ of the various relevant physical quantities are found to be unsensitive to $n_{ph}$. However, $n_{ph} = 1$ generally underestimates the role of the phonons. Clearly the one-phonon calculation is a good approximation in the weak-coupling region ($J = 0.3, \Omega = 0.2, \lambda \leq 0.3$).

This truncation procedure enables us to study $\sqrt{8} \times \sqrt{8}$ cluster with all the phonon modes (16 modes). We investigate the one and two-hole GS of Hamiltonian in a regime ($0.3 \leq J \leq 0.5$) where, in the absence of phonons, the two-hole pairing state is stabilized by the antiferromagnetic correlation, and we take a realistic phonon frequency $\Omega = 0.2$. Since the $\sqrt{8} \times \sqrt{8}$ cluster with periodic boundary conditions has the $C_{4v}$ symmetry, we concentrate on the lowest state with the $d_{x^2-y^2}$ symmetry as the two-hole GS. Although this state is not the GS for small $J (J < 0.43)$ and $\lambda_{0} = 0$ due to finite-size effects, this choice is justified by the fact that the two-hole GS has $d_{x^2-y^2}$ symmetry in the thermodynamic limit.

As a preliminary study, let us first briefly investigate the behavior of a single hole. The absolute values of the kinetic energy ($t$ term in Eq. (1)) per hole $E_{kin}$ are shown as a function of $\lambda_{0}$ in Fig. 3. For the one-hole GS, $E_{kin}$ decreases significantly with increasing $\lambda_{0}$ for the breathing mode, while it does not change significantly for the buckling mode. This is a signature that only the breathing mode leads to a polaronic self-trapping process. The difference between the two modes is also clear from the behavior of the spin structure factor in the one-hole GS

$$S_{s}(\pi, \pi) = \langle (\sum_{i}(-1)^{i_{x}+i_{y}}S_{i}^{z})^{2}\rangle$$ \tag{3}

shown in Fig. 3. A significant increase of $S_{s}(\pi, \pi)$ occurs around $\lambda_{0} = 0.1$ almost independently of $J$ for the
breathing mode. The agreement between the behaviors of $S_n(\pi, \pi)$ and $E_{kin}$ vs $\lambda_0$ suggests that the increase of the effective mass of the hole due to a polaronic self-localization effect leads, for the breathing mode, to an enhancement of the antiferromagnetic spin correlation. Fig. 3 also shows that the buckling mode, on the contrary, does not lead to any crossover characteristic of self-localization.

whether the phonon mediated interaction can be reduced to a static potential. To test this possibility, we consider the expectation value of the hole-hole distance in the two-hole GS

$$d_h = \langle \sum_{i\neq j} n_i^h n_j^h \rangle / \langle \sum_{i\neq j} n_i^h n_j^h \rangle.$$  

Fig. 3 shows that, for the breathing mode, $d_h$ increases monotonously with increasing $\lambda_0$ in agreement with the effective NN hole-hole repulsion derived in the anti-adiabatic limit. However, $d_h$ for the buckling mode does not show the behavior expected for a NN static attraction. On the contrary, it would rather correspond to a small NN static repulsion, at least for small $\lambda_0(<0.2)$. The failure of the anti-adiabatic picture, in this case, suggests that the effective hole-hole interaction stabilizing the hole pairing is controled by an essentially dynamical effect of the electron-phonon interaction and some retardation makes the range of the effective hole-hole attraction longer. In other words, the stabilization of the hole binding cannot be understood simply in terms of a static NN attraction but rather involves more subtle retardation effects.
toward the neighboring hole sites is favored. $D_h$ is essentially a dynamical quantity which should be distinguished from the total lattice deformation $D_{tot}$ given by replacing $(n_i^h ± n_i^{h,i})/N_h$ by unity in the form (3). The static quantity $D_{tot}$ is always zero except where $\Omega = 0$. Fig. 6 shows that, for the buckling mode, the deformation per hole $D_h$ in the two-hole state is larger than the one in the single hole state, in contrast to the case of the breathing mode. Thus, with buckling modes, the pair takes advantage of a larger deformation around the holes. On the contrary, the breathing deformations lead to an energy loss in the pairing state. Thus, the relative change of the lattice contraction around the holes in the paired state ultimately contribute to a decrease or an increase of the binding energy. Particularly for the buckling mode, the energy gain coming from the lattice deformation clearly dominates the behavior of the binding energy, since no significant change appears in the kinetic energy (Fig. 2) or in the antiferromagnetic correlation which can be estimated from the spin structure factor $S_s(\pi, \pi)$ in Fig. 3.

In other words, buckling modes stabilize the hole pairing state dynamically, with little changes in the static features.

In summary, exact diagonalization studies of the generalized 2D $t$-$J$-Holstein model give evidence for a stabilization of the two-hole pairing by out-of-plane buckling vibrations of the in-plane oxygens in the high-$T_c$ cuprates. On the contrary, in-plane breathing modes suppress the pairing. The difference comes from the dynamical effect of the lattice displacements which cannot be reduced to a simple NN static interaction. In addition, we found that the buckling mode does not give rise to any significant polaronic self-localization effect, in contrast to the breathing mode.

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