Numerical diagonalization study on a phonon-assisted hole pairing mechanism of an extended t-J-Holstein model

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Abstract. The phonon effect of the in-plane oxygen breathing vibration in the high-Tc cuprates is investigated by the numerical diagonalization of an extended t-J-Holstein model, including the modulation of t. As a result, it is found that if the modulation of t due to the phonon is sufficiently large, the breathing mode possibly stabilizes the superconductivity.

1. Introduction
The phonon effect on the high-temperature superconductivity is one of interesting problems in the field of strongly correlated electron systems. Particularly it is quite important to clarify whether the phonon can assist the strong correlation mechanism of the superconductivity. In the present paper, we report the results from the numerical exact diagonalization study on the phonon effect in an extended t-J-Holstein model, which is expected to well describe the physical properties of CuO$_2$ plane in the high-Tc cuprates. In our previous studies[1-3] on the t-J-Holstein model including the breathing and buckling vibrations of the in-plane oxygen atoms, the suppression of hole pairing by the breathing mode was indicated, while the buckling mode was revealed to assist it. In the present study, we take the modulation of the hole hopping parameter t due to the phonon effect into account and reconsider the phonon-assisted hole pairing mechanism. As we mention later, it is found that even the breathing vibration of in-plane oxygen can enhance the hole binding for some realistic parameters.

2. Model
In order to investigate the oxygen breathing phonon effect in the CuO$_2$ plane, we consider an extended t-J-Holstein model defined by the Hamiltonian

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

\[ + \sum_{i, \delta} \left( \frac{p_{i,\delta}^2}{2m} + \frac{1}{2} m \Omega^2 u_{i,\delta}^2 \right) + g \sum_{i, \delta} u_{i,\delta} (n_i^h - n_i^h) \]  

(1)
where $\tilde{c}_{j,\sigma}$ and $\tilde{c}_{j,\sigma}^+$ are the hole operators at each Cu site, and the last two terms describe the in-plane breathing vibration of each O atom between the nearest-neighbor Cu sites. The phonon terms can be rewritten in the boson representation

$$H_{\text{e-ph}} = \Omega \sum_{i,\delta} \left( b_{i,\delta}^+ b_{i,\delta} + \frac{1}{2} \right) + \lambda_0 \sum_{i,\delta} \left( b_{i,\delta}^+ + b_{i,\delta}^+ \right) \left( n_i^h - n_i^h \right)$$

(2)

where $\lambda_0 = \sqrt{1/2m\Omega}$.

In our previous work [1] the modulation of the hopping integral $t$ was neglected. The recent analytical work [4], however, indicated that the renormalization effect of the breathing phonon on $t$ would possibly stabilize the d-wave superconductivity. Thus in the present paper, we reconsider the breathing phonon assisted superconductivity, taking the modulation of $t$ due to the phonon into account. For this purpose we change the parameter $t$ in the Hamiltonian (1) to the following form

$$t \rightarrow t\left[1 + \lambda_i \sum_{i,\delta} \left( b_{i,\delta}^+ + b_{i,\delta}^+ \right) \right]$$

(3)

Since the origin of the modulation should be the same as the breathing phonon, we vary the electron-phonon coupling constants $\lambda_0$ and $\lambda_i$ with the ratio $r = \lambda_i / \lambda_0$ fixed to several values.

3. Numerical diagonalization
Using the numerical exact diagonalization of finite-size clusters, we obtain the ground state wave function of the present model (1) including the modulation of the hopping integral $t$. The boson degrees of freedom is in principle infinite and it is difficult to treat by the numerical diagonalization. Thus we approximately truncate the phononic Hilbert space to a finite number of bosonic states up to $n_{ph}$ at each oxygen site. Within the one-phonon approximation ($n_{ph}=1$), we perform the numerical diagonalization based on the Lanczos algorithm to study $\sqrt{8} \times \sqrt{8}$ unit-cell cluster with periodic boundary conditions, with a total of 16 phonon modes, namely a Cu$_8$O$_{16}$ cluster. We fix $J/t=0.4$ as a realistic parameter and take $t$ as a unit of energy.

4. Results
The two-hole binding energy is one of the best parameters to measure the stability of the two-hole pairing state. It is defined by the form

$$\Delta_2 = E_0^{(2)} + E_0^{(1)} - 2E_0^{(1)}$$

(4)

where $E_0^{(0)}$, $E_0^{(1)}$ and $E_0^{(2)}$ are the ground state energies with zero, one and two holes, respectively. The $\lambda_0$ dependence of $\Delta_2$ with $r$ fixed to 0.5, 1.0, 1.5 and 2.0 is shown in Fig. 1. It indicates that $\Delta_2$ decreases with increasing $\lambda_0$ for $r>1$, while increases for $r<1$. It suggests that the electron-phonon interaction would enhance the hole pairing, if $\lambda_i$ is larger than $\lambda_0$. Thus the result implies that even the breathing phonon possibly stabilizes the hole pairing.
Next, in order to investigate the polaronic effect of breathing phonon, we show the $\lambda_0$ dependence of the kinetic energy for the one-hole ground state in Fig. 2. The kinetic energy is defined by the expectation value of the t term in the Hamiltonian (1) and (3). It indicates that the absolute value of the kinetic energy increases with $\lambda_0$ increasing for $r > 1$, while decreases for $r < 1$. Thus it is expected that the breathing phonon does not give rise to the self localization due to the polaronic effect. Namely, even the breathing mode does not suppress the superconductivity for $r > 1$.

Finally, we consider the phonon effect on the static magnetic ordering. The $(\pi, \pi)$ component of the spin structure factor $S_{\pi,\pi}$ is plotted versus $\lambda_0$ for $r=0.5$, 1.0, 1.5 and 2.0 in Fig. 3. It suggests that the breathing phonon suppresses the antiferromagnetic order for $r > 1$, while stabilizes for $r < 1$. 

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**Figure 1.** $\lambda_0$ dependence of the binding energy $\Delta_2$.  

**Figure 2.** $\lambda_0$ dependence of the kinetic energy.
Figure 3. $\lambda_0$ dependence of the antiferromagnetic spin structure factor in the single-hole ground state.

5. Summary
The present numerical study on the in-plane oxygen breathing vibration including the modulation of the hopping integral $t$ suggests that there is some critical value $r_c$ of the ratio $r = \lambda_1 / \lambda_0$ and even this breathing phonon possibly stabilizes the superconductivity for $r > r_c$.

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