Electron-phonon interaction in the $t$-$J$ model

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We derive a $t$-$J$ model with electron-phonon coupling from the three-band model, considering modulation of both hopping and Coulomb integrals by phonons. While the modulation of the hopping integrals dominates, the modulation of the Coulomb integrals cannot be neglected. The model explains the experimentally observed anomalous softening of the half-breathing mode upon doping and a weaker softening of the breathing mode. It is shown that other phonons are not strongly influenced, and, in particular, the coupling to a buckling mode is not strong in this model.

There has been a strong interest in electron-phonon coupling for high-$T_c$ cuprates after the discovery of strong coupling to a mode at 70 meV in many cuprates [1]. The coupling was ascribed to a half-breathing phonon along the (1,0,0) direction, i.e., an in-plane bond-stretching mode, with an electron-phonon coupling $\lambda \sim 1$. This phonon shows an anomalous softening when the cuprates are doped, in particular, towards the zone boundary [2, 3, 4, 5]. While the softening of other phonons upon doping can be understood as a screening of the ions, the softening of the half-breathing mode cannot be described in a shell model with conventional parameters [2]. This suggests a substantial electron-phonon coupling. The phonon has an appreciable broadening [2], also supporting a substantial coupling. Local-density approximation (LDA) calculations, however, show a weak coupling to this phonon, with $\lambda$ at the zone boundary being $\sim 0.01$ [6, 7]. Anomalous behavior of bond-stretching modes has also been observed in other compounds [8, 9, 10]. It is then interesting to study the electron-phonon interaction, taking into account the strong electron-electron interaction [11, 12]. This has been done in the $t$-$J$ model [13] by von Szczepanski and Becker [14], by Khalilullin and Horsch [15] and by Ishihara, Nagaosa and coworkers [16].

The $t$-$J$ model is derived from a three-band model of a CuO$_2$ layer [17], including a Cu $d_{z^2}p^2$ and two O $p$ orbitals. To obtain the electron-phonon coupling, the atoms are displaced. This leads to a change of the hopping integral $t_{pd}$ and the charge transfer energy $\varepsilon_p$ between Cu and O atoms, where the change of $\varepsilon_p$ is assumed to be due to a change of the Coulomb integral $U_{pd}$ between nearest neighbor Cu and O atoms. Transforming to a $t$-$J$ model, this leads to changes of both the on-site energy $E_0$ of the Zhang-Rice singlet and the hopping between the sites (off-site coupling). Two groups [14, 15] assumed the variation of $t_{pd}$ to dominate, while a third group [16] focused on $\varepsilon_p$. The first two groups assumed the off-site coupling in the $t$-$J$ model to be negligible, while the third group emphasized this coupling.

The singlet energy in the $t$-$J$ model is large, $|E_0| \sim 5$ eV. For a rigid lattice and fixed doping, this energy enters only as an uninteresting constant. Because of the strong distance dependence of $t_{pd}$, however, we may expect a strong electron-phonon coupling from this term.

We study modulations of $t_{pd}$ and $\varepsilon_p$ by phonons. The $t_{pd}$ modulation dominates, but destructive interference between the two effects is not negligible. The phonons couple mainly to on-site terms. Phonon spectral functions are obtained from exact diagonalization. The model explains the anomalous softening of the half-breathing mode and correctly gives a weaker softening of the breathing mode. Other phonons are only softed weakly. Experiments suggest a strong coupling of preferentially the anti-nodal electronic state to a phonon at 40 meV, perhaps a $B_{1g}$ buckling mode [18]. We find a weak coupling to the $B_{1g}$ mode in the model studied here.

The derivation of a model with phonons proceeds as for the normal $t$-$J$ model [13], but with displaced atoms. With the atoms in their equilibrium positions, a Cu atom couples only to a given linear combination of $p$-orbitals on the four O neighbors [13]. With displaced atoms there is also coupling to other combinations. This coupling, however, enters to second order in the displacement and is neglected here. Following Zhang and Rice [13], we work to lowest order in $t_{pd}$, although this is not very accurate for realistic parameters. We neglect certain terms where a hole hops $i \to k \to j$ ($k \neq i$, $k \neq j$). We also neglect the electron-phonon interaction via superexchange interaction, since this coupling occurs only via motion of Cu atoms and with a small prefactor [13]. We then obtain a $t$-$J$ model with the linear electron-phonon coupling

$$H_{el-ph} = \sum_{ij\sigma} c_{i\sigma}^\dagger c_{j\sigma} \sum_{q,\nu} g_{ij}(q, \nu) (b_{q,\nu} + b_{-q,\nu}^\dagger),$$

where

$$g_{ij} = i \sqrt{\frac{2\hbar}{N\omega_\nu(q)} \varepsilon_q(R_i + R_j)/2} \left[ A(q, \nu) \delta_{ij} + B^x(q, \nu) \delta_{ij,\pm \hat{x}} + B^y(q, \nu) \delta_{ij,\pm \hat{y}} \right].$$

Here $c_{i\sigma}^\dagger$ creates a $d$-hole on site $i$ if this site previously had no hole, and $b_{q,\nu}$ creates a phonon with wave vector $q$, index $\nu$ and frequency $\omega_\nu(q)$. The system has $N$ sites with coordinates $R_i$, $\delta_{i,j-\hat{x}} = 1$ if site $j$ is one site to the right of $i$ in the $x$-direction. The modulation of $t_{pd}$ gives

$$A = 2t_{pd} \frac{d t_{pd}}{d r} \left( \frac{2\lambda^2 - 1}{\varepsilon_p} + \frac{2\lambda^2}{U - \varepsilon_p} \right) \left[ \frac{\varepsilon_p}{\sqrt{M_O}} s_x + \frac{\varepsilon_p}{\sqrt{M_O}} s_y \right].$$

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and

\[ B^x = \frac{\lambda}{4} t_{pd} \frac{dU_{pd}}{dr} \left( \frac{1}{2} \frac{1}{\varepsilon_p} + \frac{1}{U - \varepsilon_p} \right) \]

\[
\times \left[ \begin{array}{c}
\frac{e^\alpha_{Cus} s_x + 2 \Gamma_1 \frac{e^\alpha_{Cu}}{\sqrt{M_Cu}} s_x c_x + 2 \Gamma_2 \frac{e^\alpha_{Oy}}{\sqrt{M_O}} c_x s_y + 2 \Gamma_3 \frac{e^\alpha_{Oy}}{\sqrt{M_O}} c_x s_y}
\end{array} \right]
\]

(4)

with an analogous form for \( B^y \). Here \( s_i = \sin(q_i a_i/2) \), \( c_i = \cos(q_i a_i/2) \), \( l = x, y \); \( \lambda = \sum \frac{\beta_{k}^{-1}}{N} = \gamma_0 - \gamma_1 = 0.96 \), \( \Gamma_1 = 4(\gamma_2 - \gamma_0) \), \( \Gamma_2 = 8 \gamma_1 - 5 \gamma_0 - 7 \gamma_2 - 2 \gamma_11 \) and \( \Gamma_3 = 8 \gamma_1 - \gamma_0 - \gamma_2 - 6 \gamma_{11} \), with \( \gamma_0 = \gamma(0) = 1.285 \), \( \gamma_1 = \gamma(a \hat{x}) = 0.327 \), \( \gamma_{11} = \gamma(a \hat{x} + a \hat{y}) = 0.209 \) and \( \gamma_2 = \gamma(2a \hat{x}) = 0.164 \), where \( \gamma(R) = \sum_{k} \beta_{k} e^{i k \cdot R}/N \) with \( \beta_{k} = 1/\sqrt{\gamma_x^2 + \gamma_y^2} \) and \( a \) the lattice parameter. \( M_{Cu} \) and \( M_O \) are the masses of the Cu and O atoms, respectively, \( e^\alpha_{Cus} \) is the x-component of the polarization vector for one of the O atoms (O_2) with an analogous meaning of \( e^\alpha_{Cu} \). \( U \) is the hole-hole repulsion on Cu. von Szczepanski and Becker [14] calculated \( q_{ij}(q, \nu) \) for the \( q = (1,1)/\pi/a \) breathing mode and found \( B^x(q, \nu) = 0 \) (since \( e^\alpha_{cu} = 0 \) for this value of \( q \)), as above, and a slightly different result for \( A(q, \nu) \) due to slightly different approximations.

Considering a variation of the charge transfer energy, assuming that it is driven by a nearest neighbor Cu-O Coulomb interaction \( U_{pd} \), we find

\[ A = -8 \alpha t_{pd}^2 \frac{dU_{pd}}{dr} \left( \frac{2 \lambda^2 - 1}{\varepsilon_p^2} - \frac{2 \lambda^2}{U - \varepsilon_p} \right) \]

\[
\times \left[ \begin{array}{c}
\frac{e^\alpha_{O}}{\sqrt{M_O}} s_x + \frac{e^\alpha_{O}}{\sqrt{M_O}} s_y + \frac{1}{2} D
\end{array} \right] - \frac{dU_{pd}}{dr} D,
\]

(5)

here \( D = M_{Cu}^{-1/2} (e^\alpha_{Cus} s_x c_x + e^\alpha_{Cus} s_y c_y) \), and

\[ B^x = -4 \lambda \alpha t_{pd}^2 \frac{dU_{pd}}{dr} \left( \frac{1}{\varepsilon_p^2} - \frac{2}{U - \varepsilon_p} \right) \]

\[
\times \left[ \begin{array}{c}
2 \frac{e^\alpha_{O}}{\sqrt{M_O}} s_x c_x + 2 \frac{e^\alpha_{O}}{\sqrt{M_O}} c_x s_y
\end{array} \right]
\]

\[
+ \frac{1}{4} \frac{e^\alpha_{Cu}}{\sqrt{M_{Cu}} s_x c_x} \frac{3 q_x a}{2} + \frac{1}{4} \frac{e^\alpha_{O}}{\sqrt{M_O}} c_x s_y + \frac{1}{4} \frac{e^\alpha_{Cu}}{\sqrt{M_{Cu}} c_x s_y}
\]

(6)

Here \( \alpha = \sum \frac{\beta_{k}^{-1}}{N} e^{i k \cdot \hat{x}}/N = -0.14 \).

To estimate the relative magnitude of these terms, we use \( t_{pd} = 1.2 \varepsilon, \varepsilon_p = 3 \varepsilon, U = 10 \varepsilon, U_{pd} = 1 \varepsilon, \) and \( a = 3.8 \varepsilon \). We assume the distance dependence \( t_{pd} \sim r^{-n} \) with \( n = 3.5 \), based on LDA calculations [21], and \( U_{pd} \sim r^{-1} \). This gives the hopping integral -0.47 eV in the t-J model, close to values commonly used [22]. For \( q = (q_x, 0) \), \( \omega = 0.07 \varepsilon \), \( e^\alpha_{Ox} = 1 \) and all other polarization vectors zero, we obtain (in eV)

\[
\sqrt{2 \hbar/\omega} A(q) = -0.25 s_x, \quad \sqrt{2 \hbar/\omega} B^x(q) = -0.0032 s_x c_x
\]

(7)

due to modulation of \( t_{pd} \) and

\[
\sqrt{2 \hbar/\omega} A(q) = 0.029 s_x, \quad \sqrt{2 \hbar/\omega} B^x(q) = -0.0049 s_x c_x
\]

(8)

due to modulation of \( U_{pd} \). This shows that the modulation of \( t_{pd} \) dominates over that of \( U_{pd} \). This is mainly due to a stronger power dependence \( (n = 3.5) \) for \( t_{pd} \) than \( U_{pd} \) but also due to a partial cancellation between the terms proportional to \( 1/\varepsilon_p^2 \) and \( 1/(U - \varepsilon_p)^2 \) in the contribution from \( dU_{pd}/dr \). The contribution from \( dU_{pd}/dr \) alone is very small. There is a destructive interference between contributions from \( dt_{pd}/dr \) and \( dU_{pd}/dr \), however, which reduces the phonon softening by about 30%.

The prefactors of the off-diagonal terms are small [Eqs. (7) and (8)], and the diagonal term dominates. We have neglected quadratic terms in the phonon displacement in (11), although some terms may give non-negligible contributions to the doping dependence of phonon energies.

The model (11) describes the softening of phonons due to holes in the doped system, but it does not include other interactions present in both the doped and undoped systems. These interactions are described by a two-spring model, fitted to the phonon frequencies in the (1,0) and (1,1) directions of the undoped system. This spring model provides the eigenvectors \( \epsilon = \) Eqs. (9)–(10).

To study the t-J model with phonons, we use exact diagonalization [22], including all possible electronic states for a finite cluster of size \( M \times N \). To obtain a finite Hilbert space, we allow states containing a maximum of \( K = 5 \) phonons [24], which is sufficient for convergence.

We calculate the phonon spectral function \( \omega > 0 \)

\[ B_{q\nu}^{q}(\omega) = -\frac{1}{\pi} \text{Im} \langle 0 | \phi_{q\nu} \omega - (H - E_0) + i \eta \phi_{q\nu}^\dagger | 0 \rangle \]

(9)

where \( | 0 \rangle \) is the ground-state with the energy \( E_0 \), \( \phi_{q\nu} = b_{q\nu} + b_{q\nu}^\dagger \), and \( \eta \) is infinitesimal. Since the clusters that can be treated are too small to give a quasicontinuous spectrum, we use the center of gravity of the phonon

FIG. 1: Phonon dispersion in the (1,0) and (1,1) directions. Experimental results (dotted line) for \( x = 0 \) and \( x = 0.15 \) are shown. Theoretical results (full curve) for \( x = 0.125 \) show the calculated softening from the experimental \( x = 0 \) results. The average over boundary conditions is shown and the bars show the spread due to different boundary conditions. There is a strong softening in the (1,0) direction, while the softening in the (1,1) direction is weaker.
The softening is about 10% for $x$ is also observed experimentally, e.g. for La$_2$Sr$_2$CuO$_4$ the softening is 10% for $x = 0.01$, 11% for $x = 0.011$, 12% for $x = 0.125$, and 16% for $x = 0.167$. This shows that the softening increases with doping.

The softening is stronger for $x = 0.0167$ than for the half-breathing mode $q = \pi/a$ than would be expected from this argument. The prefactor, however, is a factor $\sqrt{2}$ larger for the breathing mode $q = \pi/a(1,1,0)$ than for the half-breathing mode $q = \pi/a(1,0,0)$, suggesting a softening $\sim \sin^2(q_x a/2)$. This behavior is essentially found in the calculations, although the softening is stronger for $q_x = \pi/(2a)$ than would be expected from this argument. The prefactor, however, is a factor $\sqrt{2}$ larger for the breathing mode $q = \pi/a(1,1,0)$ than for the half-breathing mode $q = \pi/a(1,0,0)$, suggesting twice as large a softening for the breathing mode. Actually, the softening is larger for the half-breathing mode, since it couples to excitations at lower energies.

Figure 2 shows results in a 4 × 4 t-J model for the (1,0) and (1,1) directions. The dotted curves show experimental results, and the full curve shows the softening due to the electron-phonon interaction in the doped system. Because of the small cluster sizes, the results depend on the boundary conditions. We have used periodic, antiperiodic, and mixed boundary conditions, applying periodic boundary conditions in one direction and antiperiodic in the other. Figure 1 shows the average and the bars the spread of the results. Although the results are fairly sensitive to the boundary conditions, the trends are clear. Doping leads to a pronounced softening of different sizes. The corresponding doping is indicated. The calculations have been obtained using analytical treatments [15].

For $x = 0.15$, the softening is 8% for $x = 0.125$, compared with the experimental results 3% for $x = 0.1$ and 8% for $x = 0.15$.

The calculations show that there is a strong coupling to the half-breathing mode, where two O atoms move towards the Cu atom in between. At the zone boundary, the Cu atoms do not move. Towards the zone center, however, there is a substantial movement of Cu. Normalization of the polarization vectors then leads to a reduction of the O polarization vectors. Completeness requires that the missing O weight is transferred to other modes. In a two-spring model the weight goes to an acoustic mode. Because of its small frequency, this mode is then softened far more [almost 50% for $q = \pi/(2a)(1,0)$] than observed experimentally.

To address this, we have used a more realistic shell model for obtaining eigenvectors. This model gives almost exactly the same eigenvectors for the half-breathing mode as our two-spring model. The “missing” O weight transfers to the zone boundary, however, is distributed over several modes, and the softening of a given mode is weaker. For instance, the longitudinal acoustic $q = \pi/(2a)(1,0)$ phonon is softened by about 25%. Although smaller than in the two-spring model, the softening is still too large. It is, however, further reduced by the repulsion from lower-lying modes of the same symmetry.

To study this, we have modified the shell model to
take the electron-phonon interaction into account. The movement of two O atoms towards a Cu atom leads to a lowering of the Zhang-Rice singlet energy. The system can take advantage of this by transferring a singlet to such a site. This is approximately described by introducing a spring with a negative spring constant, \( \kappa = -3 \text{ eV/Å}^2 \), between two O atoms on opposite sides of a Cu atom. A similar term was used to describe La\(_{2-x}\)Sr\(_x\)NiO\(_4\) \[20\]. The present work gives justification for such a spring. Figure 3 compares results of the shell model with and without the additional spring. Apart from the half-breathing mode, no mode is strongly softened by the new spring \[26\]. The \( t-J \) model thus correctly softens the half-breathing mode, without introducing unphysical softening of other modes.

An LDA calculation for the frequency of the half-breathing mode in (doped) YBa\(_2\)Cu\(_3\)O\(_7\) found good agreement with experiment \[7\], although the very small calculated electron-phonon coupling would suggest a weak doping-dependence. Since LDA cannot describe the insulating undoped system, the implications for the doping induced softening are unclear.

The half-breathing and (in particular) breathing modes have unfavorable \( \mathbf{q} \) dependences for \( d \)-wave pairing. The coupling to these modes is not expected to explain superconductivity in Eliashberg-like theories. Recent photoemission experiments suggest strong coupling to a phonon at 40 meV, perhaps a \( B_{1g} \) buckling optical phonon, i.e., a phonon where the in-plane O atoms have c-axis out-of-plane displacements \[18\]. For symmetry reasons, this mode couples only to second order for a single flat CuO\(_2\) plane, due to the hopping between the Cu \( d_{x^2-y^2} \) and O \( p_z \) orbitals. Such terms, however, have a small prefactor, and the coupling constant for the on-site term is more than an order of magnitude smaller than for the half-breathing mode \[27\]. The planes may have local static bucklings, allowing coupling to linear order. Assuming a 0.2 Å (6°) buckling, we find that the coupling constant is still an order of magnitude smaller for the buckling mode. It seems that one would have to go beyond a single layer \( t-J \) model to obtain a strong coupling to the buckling mode.

We have found that the distance dependence of \( t_{pd} \) is substantially more important than that of \( U_{pd} \) for the electron-phonon interaction. Nevertheless, the interference effects cannot be neglected. The \( t-J \) model with phonons describes the strong renormalization of the half-breathing mode, a weaker renormalization of the breathing mode and no anomalies in other modes.

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[1] A. Lanzara et al., Nature 412, 510 (2001).