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

O. Rösch and O. Gunnarsson

Max-Planck-Institut für Festkörperforschung, D-70506 Stuttgart, Germany

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[2–5]. 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[3], also supporting a substantial coupling. LDA calculations, however, show a weak coupling to this phonon, with λ at the zone boundary being ~ 0.01[6, 7]. Anomalous behavior of bond-stretching modes has also been observed in other compounds[8–10]. It is then interesting to study the electron-phonon interaction, taking into account the strong Coulomb interaction. This has been done in the t-J model[11] by von Szczepanski and Becker[12], by Khaliullin and Horsch[13] and by Ishihara, Nagaosa and coworkers[14].

The $t - J$ model is derived from a three-band model of a CuO$_2$ layer[15], including a Cu $d_{x^2-y^2}$ 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 ε_p between Cu and O atoms, where the change of ε_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_s of the Zhang-Rice singlet and the hopping between the sites (off-site coupling). Two groups[12, 13] assumed the variation of t_{pd} to dominate, while a third group[14] focused on ε_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, $|E_s| \sim 5$ eV. For a rigid lattice and fixed doping, this energy only enters as an uninteresting constant. Due to 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 ε_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 softened 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[16]. 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[11], but with displaced atoms. With the atoms in their equilibrium positions, a Cu atom only couples to a given linear combination of p-orbitals on the four O neighbors[11]. 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[11], 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 only occurs via motion of Cu atoms and with a small prefactor[12]. We then obtain a $t - J$ model with the linear electron-phonon coupling

$$H_{el-ph} = \sum_{ij\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} \sum_{\mathbf{q},\nu} g_{ij}(\mathbf{q},\nu)(b_{\mathbf{q},\nu} + b_{-\mathbf{q},\nu}^\dagger), \quad (1)$$

where

$$g_{ij} = i\sqrt{\frac{2\hbar}{N\omega_\nu(\mathbf{q})}} e^{i\mathbf{q}\cdot(\mathbf{R}_i+\mathbf{R}_j)/2}$$
$$\times [A(\mathbf{q},\nu)\delta_{ij} + B^x(\mathbf{q},\nu)\delta_{i,j\pm\hat{x}} + B^y(\mathbf{q},\nu)\delta_{i,j\pm\hat{y}}]. \quad (2)$$

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

$$A = 2t_{pd}\frac{dt_{pd}}{dr}\left(\frac{2\lambda^2-1}{\varepsilon_p} + \frac{2\lambda^2}{U-\varepsilon_p}\right)\left[\frac{\epsilon_{Ox}^x}{\sqrt{M_O}}s_x + \frac{\epsilon_{Oy}^y}{\sqrt{M_O}}s_y\right] \quad (3)$$

and

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

$$\times \left[\Gamma_1 \frac{\epsilon^x_{Cu}}{\sqrt{M_{Cu}}} s_x + 2\Gamma_2 \frac{\epsilon^x_{Ox}}{\sqrt{M_O}} s_x c_x + 2\Gamma_3 \frac{\epsilon^y_{Oy}}{\sqrt{M_O}} c_x s_y \right], (4)$$

with an analogous form for B^y. Here $s_l = \sin(q_l a/2)$, $c_l = \cos(q_l a/2)$, $l = x, y$; $\lambda = \sum \beta_{\mathbf{k}}^{-1}/N = \gamma_0 - \gamma_1 = 0.96$, $\Gamma_1 = 4(\gamma_2 - \gamma_0)$, $\Gamma_2 = 8\gamma_1 - \gamma_0 - 5\gamma_2 - 2\gamma_{11}$ and $\Gamma_3 = 8\gamma_1 - \gamma_0 - \gamma_2 - 6\gamma_{11}$, with $\gamma_0 = \gamma(0) = 1.285$, $\gamma_1 = \gamma(a\hat{\mathbf{x}}) = 0.327$, $\gamma_{11} = \gamma(a\hat{\mathbf{x}} + a\hat{\mathbf{y}}) = 0.209$ and $\gamma_2 = \gamma(2a\hat{\mathbf{x}}) = 0.164$, where $\gamma(\mathbf{R}) = \sum_{\mathbf{k}} \beta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}}/N$ with $\beta_{\mathbf{k}} = 1/\sqrt{s_x^2 + s_y^2}$ and a the lattice parameter. M_{Cu} and M_O are the masses of the Cu and O atoms, respectively, ϵ^x_{Ox} is the x-component of the polarization vector for one of the O atoms (O_x) with an analogous meaning of ϵ^x_{Cu}. U is the hole-hole repulsion on Cu. Von Szczepanski and Becker[12] calculated $g_{ij}(\mathbf{q}, \nu)$ for the $\mathbf{q} = (1,1)\pi/a$ breathing mode, and found $B^x(\mathbf{q}, \nu) = 0$ (since $\epsilon^x_{Cu} = 0$ for this value of $\mathbf{q}$), as above, and a slightly different result for $A(\mathbf{q}, \nu)$ 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

$$A = -8t_{pd}^2 \frac{dU_{pd}}{dr} \left(\frac{2\lambda^2 - 1}{\varepsilon_p^2} - \frac{2\lambda^2}{(U - \varepsilon_p)^2} \right) \quad (5)$$

$$\times \left[\frac{\epsilon^x_{Ox}}{\sqrt{M_O}} s_x + \frac{\epsilon^y_{Oy}}{\sqrt{M_O}} s_y + \frac{1}{2} D \right] - \frac{dU_{pd}}{dr} D,$$

where $D = M_{Cu}^{-1/2}(\epsilon^x_{Cu} s_x c_x + \epsilon^y_{Cu} s_y c_y)$, and

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

$$\times \left[2\frac{\epsilon^x_{Ox}}{\sqrt{M_O}} s_x c_x + 2\frac{\epsilon^y_{Oy}}{\sqrt{M_O}} c_x s_y \right. \quad (6)$$

$$\left. + \frac{1}{4} \frac{\epsilon^x_{Cu}}{\sqrt{M_{Cu}}} \sin\frac{3q_x a}{2} + \frac{1}{2} \frac{\epsilon^y_{Cu}}{\sqrt{M_{Cu}}} c_x s_y + \frac{1}{4} \frac{\epsilon^x_{Cu}}{\sqrt{M_{Cu}}} s_x \right].$$

Here $\alpha = \sum \beta_{\mathbf{k}}^{-1} e^{ia\mathbf{k}\cdot\hat{\mathbf{x}}}/N = -0.14$.

To estimate the relative magnitude of these terms, we use[17, 18] $t_{pd} = 1.2$ eV, $\varepsilon_p = 3$ eV, $U = 10$ eV, $U_{pd} = 1$ eV and $a = 3.8$ Å. We assume the distance dependence $t_{pd} \sim r^{-n}$ with $n = 3.5$, based on LDA calculations[19], and $U_{pd} \sim r^{-1}$. This gives the hopping integral -0.47 eV in the $t - J$ model, close to values commonly used[20]. For $\mathbf{q} = (q_x, 0)$, $\omega = 0.07$ eV, $\epsilon^x_{Ox} = 1$ and all other polarization vectors zero, we obtain (in eV)

$$\sqrt{2\hbar/\omega} A(\mathbf{q}) = -0.25 s_x, \quad \sqrt{2\hbar/\omega} B^x(\mathbf{q}) = -0.0032 s_x c_x \quad (7)$$

due to modulation of t_{pd} and

$$\sqrt{2\hbar/\omega} A(\mathbf{q}) = 0.029 s_x, \quad \sqrt{2\hbar/\omega} B^x(\mathbf{q}) = -0.0049 s_x c_x \quad (8)$$
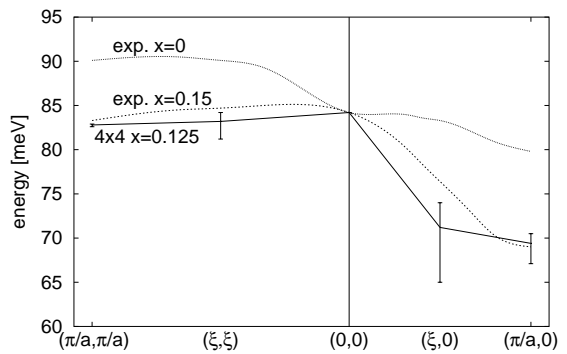

FIG. 1: Phonon dispersion in the (1,0) and (1,1) directions. Experimental results (dotted line) for $x = 0$ and $x = 0.15$ are shown. Theoretical results (full curve) for $x = 0.125$ show the calculated softening from the experimental $x = 0$ results. The average over boundary conditions is shown and 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.

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, and the diagonal term dominates. We have neglected quadratic terms in the phonon displacement in (1), although some terms may give nonnegligible contributions to the doping dependence of phonon energies.

The model (1) 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 ϵ in Eqs. (3)-(6).

To study the $t - J$ model with phonons, we use exact diagonalization[21], 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[22], which is sufficient for convergence. We calculate the phonon spectral function ($\omega > 0$)

$$B_{\mathbf{q}\nu}(\omega) = -\frac{1}{\pi} \text{Im} \langle 0 | \phi_{\mathbf{q}\nu} \frac{1}{\omega - (H - E_0) + i\eta} \phi^\dagger_{\mathbf{q}\nu} | 0 \rangle, \quad (9)$$

where $|0\rangle$ is the ground-state with the energy E_0, $\phi_{\mathbf{q}\nu} = b_{\mathbf{q}\nu} + b^\dagger_{-\mathbf{q}\nu}$ and η is infinitesimal. Since the clusters that can be treated are too small to give a quasi-continuous spectrum, we use the center of gravity of the phonon
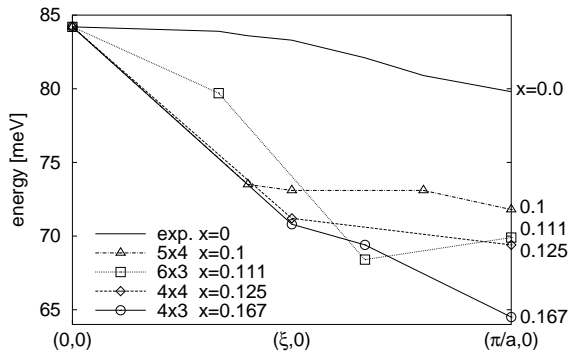
FIG. 2: Phonon dispersion in the (1,0) direction for clusters of different sizes. The corresponding doping is indicated. The figure shows that the softening increases with doping.

spectrum to define the renormalized phonon frequency. This provides the phonon softening in relation to the experimental phonon frequencies of the undoped system. We have used the parameters above and $J/t = 0.3$.

Fig. 1 shows results in a 4×4 $t - J$ model for the (1,0) and (1,1) directions. The dotted curves show experimental results[2], and the full curve shows the softening due to the electron-phonon interaction in the doped system. Due to 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. Fig. 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 the half-breathing mode along the (1,0) direction for $|\mathbf{q}| \gtrsim \pi/(2a)$, while the softening is weaker in the (1,1) direction, in agreement with experiment[2]. Similar conclusions have been obtained using analytical treatments[13].

The prefactor of the dominating diagonal term [Eqs. (3) and (5)] in the coupling for the half-breathing mode is $\sim \sin(q_x a/2)$, 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 [$\mathbf{q} = \pi/a(1,1)$] than for the half-breathing mode [$\mathbf{q} = \pi/a(1,0)$], 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.

Fig. 2 shows results in the (1,0) direction for different cluster sizes. Since all clusters have two holes, the change of cluster size changes the doping. The softening increases with doping x, e.g., at the zone boundary, the softening is 10 % for $x = 0.1$ and 19 % for $x = 0.167$. This is also observed experimentally, e.g, for $La_{2-x}Sr_xCuO_4$ the softening is 10 % for $x = 0.10$[2] and 14 % for $x = 0.15$[3]. For the breathing mode [$\mathbf{q} = \pi/a(1,1)$],
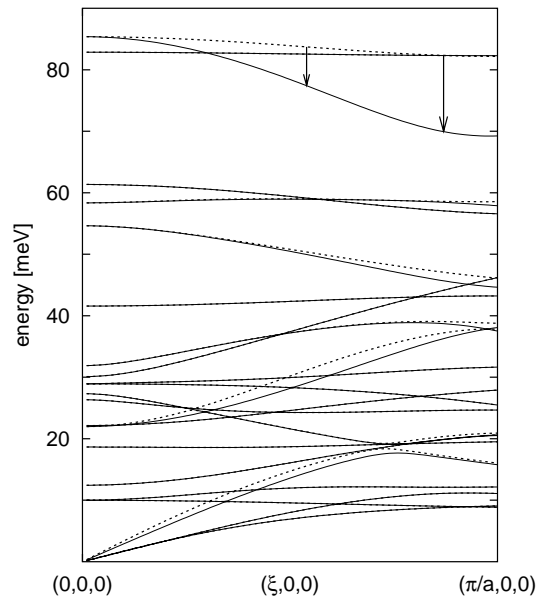

FIG. 3: Phonon dispersion in the (1,0,0) direction for a shell model. The dashed curves show results for the undoped system[2] and the full curves results with the extra O-O spring describing the O atom coupling to the Zhang-Rice singlets. The arrows indicate the strong softening of the half-breathing mode, while other modes are not changed very much.

we obtain 8 % softening ($x = 0.125$), compared with the experimental results 3 %($x = 0.1$) and 8 % ($x = 0.15$)[4].

The calculations show 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 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. Due to its small frequency, this mode is then softened far more (almost 50 % for $\mathbf{q} = \pi/(2a)(1,0)$) than observed experimentally.

To address this, we have used a more realistic shell model[2] 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 towards the zone center, however, is distributed over several modes, and the softening of a given mode is weaker. For instance, the longitudinal acoustic $\mathbf{q} = \pi/(2a)(1,0)$ phonon is softened by about 25 %. This softening is, nevertheless, 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[2] 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 sys-

tem 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, $\kappa = -3$ 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$_4$[8, 23]. The present work gives justification for such a spring. Fig. 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[24]. 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 **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[16]. For symmetry reasons, this mode only couples 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[25]. 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 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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[24] This spring model appropriately softens the breathing mode, but softens a mode with $\epsilon_{Ox}^x = -\epsilon_{Oy}^y = 1/\sqrt{2}$ and $\mathbf{q} = \pi/a(1, 1)$ too strongly. However, Eq. (3) shows that such a mode does not couple strongly in the $t - J$ model.

[25] The buckling (half-breathing) mode has the strongest coupling at the zone center (boundary).