Coupling to optical phonons in the one-dimensional t-J model: Effects on superconducting fluctuations and phase separation

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(March 23, 2022)

The one-dimensional (1D) t-J Holstein model is studied by exact diagonalization of finite rings using a variational approximation for the phonon states. Due to renormalization effects induced by the phonons, for intermediate electron-phonon coupling, the phase separation (PS) boundary, and with it the region of dominating superconducting fluctuations is shifted substantially to smaller values of \( J/t \) as compared to the pure t-J model. Superconducting correlations are weakened through charge density wave interactions mediated by the phonons. Possible consequences for the high-\( T_c \) oxides are discussed.

PACS numbers: 74.20.Mn, 74.25.Kc, 71.27.+a, 71.38.+i

The role of the electron-phonon (e-ph) coupling for the mechanism leading to superconductivity (SC) in the high-\( T_c \) cuprates is still controversial. The importance of electronic correlations suggests itself from the fact that the high-\( T_c \) is achieved upon doping a Mott insulator. Hence, many theoretical approaches neglect the phonons altogether and search for a purely electronic mechanism. An obvious shortcoming of such theories is the fact that they would never lead to an isotope effect.

While the experimental situation concerning the magnitude of the isotope effect and the relevant ions producing it is still not quite settled, it appears to be widely accepted by now that especially for underdoped samples, \( T_c \) is rather susceptible especially to the mass of the oxygen ions. Near optimal doping, however, only a small isotope effect is observed. In addition, anomalous frequency shifts of phonon modes as well as other lattice anomalies have been observed at or slightly above \( T_c \). These findings strongly suggest that the electronic and phonon degrees of freedom should be treated on an equal footing.

The simplest model to describe the electronic low-energy properties of doped \( \text{Cu}_2\text{O}_2 \) sheets is the t-J model. Due to elimination of doubly occupied sites, it describes strongly correlated electrons for all parameters. This explains the extreme difficulties to obtain reliable results by analytical as well as numerical methods. An exception is 1D, where an exact solution exists at \( J/t = 2 \) \[1\]. Numerically, it was possible to extract the full phase diagram with good accuracy \[7\]. In brief, there are three distinct regions: For \( J/t \leq 2.2 \), the physics is dominated by charge density wave (CDW) fluctuations, followed by a small regime \( (2.2 \lesssim J/t \lesssim 3.2) \) where SC fluctuations are strongest, and finally, at large \( J/t \), phase separation sets in. In addition, at low electron density, a spin gap opens in the regime of dominating SC fluctuations.

In this article, we study the influence of the e-ph coupling on the phase diagram of the 1D t-J model. In particular, it is important to know how this affects the SC fluctuations. The e-ph coupling is incorporated by a Holstein term, i.e., a linear coupling of the local electronic charge to the ionic displacement. Together with the free phonon part, we arrive at the t-J Holstein model. Its phase diagram is calculated by exact diagonalization. The phonons are treated by a variational approximation which preserves their dynamics. The main results are: (i) Increasing the e-ph coupling shifts the regime of dominating SC fluctuations to smaller values of \( J/t \). (ii) The PS boundary acquires a non-trivial density dependence due to an enhancement of CDW correlations by the e-ph coupling, and (iii) the spatial extent of SC correlations is shortened.

The formation of a Zhang-Rice (ZR) singlet (representing a \text{Cu}^{III} oxidation state) by holes doped in the insulating half-filled state of the \( \text{Cu}_2\text{O}_2 \) sheets is the central idea underlying the derivation of the t-J model from the more complete three-band model \[3,8\]. We have demonstrated previously in the context of \( \text{Cu}_2\text{O}_3 \) chains \[8\] that the total energy \( E_s \) of this singlet is sensitive to displacements of the planar oxygen towards the Cu atoms (the so-called breathing mode) through the distance dependence of the hopping matrix elements \( t_{pd} \) and \( t_{pp} \). The dependence of \( E_s \) on the displacement is particularly strong for an in-phase motion, since the doped hole is predominantly in a state delocalized with equal probability on the four oxygens surrounding a Cu. A rough estimate of the coupling (as in \[3\]) gives a value of \( g \equiv dE_s/dQ \approx \text{10eV/Å} \) for the displacement.

Experimentally, \( g \) can be estimated from the difference \( \delta Q \) of the Cu-O bond lengths of compounds with pure four-fold oxygen coordinated \text{Cu}^{III} (e.g., \text{Nd}_2\text{CuO}_4, d_{\text{Cu-O}} \approx 1.97\text{Å} \[10\]), versus \text{Cu}^{III} (e.g., \text{KCuO}_2, d_{\text{Cu-O}} \approx 1.83\text{Å} \[11\]). From this, \( g \approx \delta QK \approx \text{10–15eV/Å} \), in good
agreement with the theoretical estimate. \( K = \Omega^2 M \approx 100\text{eV}/a^2 \) is the spring constant obtained from the measured phonon frequencies \( P(\Omega = 4M_{\text{Ox}}, M_{\text{Ox}} \text{ the oxygen atomic mass}) \).

The simplest model which incorporates the dependence \( E_s(\Omega) \) is the \( t-J \) Holstein model \[2\]

\[
H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \mathcal{P}_i c_{i\sigma}^\dagger c_{j\sigma} + J \sum_{\langle i,j \rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) + \hbar \Omega \sum_i a_i^\dagger a_i + \Lambda \sum_i (1 - n_i) \left( a_i + a_i^\dagger \right).
\]

where \( \langle i,j \rangle \) denotes nearest neighbors (nn), the \( c_{i\sigma}, c_{i\sigma}^\dagger \) annihilate (create) an electron with spin \( \sigma \) at site \( i \), \( n_i = \sum_{\sigma} n_{i\sigma} \) is the number, and \( \mathbf{S}_i \) the spin operator. The projection operators \( \mathcal{P}_i = 1 - n_i a_i^\dagger n_i \) eliminate configurations with doubly occupied sites, and the \( a_i, a_i^\dagger \) are usual bosonic phonon annihilation (creation) operators. For simplicity, the phonon spectrum is assumed to be dispersionless, characterized by a single frequency \( \Omega \). The e-ph coupling constant is defined as \( \Lambda = (\hbar g^2/2M\Omega)^{1/2} \).

The total Hamiltonian has four dimensionless parameters: the spin exchange \( J/t \), the phonon frequency \( h\Omega/t \), the e-ph coupling strength \( \Lambda/t \), and the electron density \( 0 \leq n \leq 1 \). The energy scale is fixed by the value of \( t \). Here, we choose \( h\Omega/t = 0.2 \), realistic for the cuprates \( \approx 0.4\text{eV} \), and \( \Omega \approx 60-80\text{meV} \) for the breathing modes \[12\]. We measure the e-ph coupling in terms of the polaron binding energy, \( E_B \equiv g^2/(2K) = \Lambda^2/(\hbar \Omega) \) \( (-E_B \text{ is the energy of a localized polaron}) \), instead of \( \Lambda/t \). Using the above values for \( g, \Omega \), we obtain \( E_B \approx 0.1 - 0.4\text{eV} \), i.e., a sizeable \( E_B/t \approx 0.25 - 1 \). This corresponds to a rather small value \( \lambda \equiv E_B/W \approx 0.1 - 0.2 \) \((W, \text{the bandwidth in 2D}) \).

The model is studied using the Lanczos method on finite rings of length \( L \). To minimize finite-size effects, we chose closed shell boundary conditions (BC), which prevent spurious degeneracies. For single-band 1D models, this corresponds to periodic BC if the number of electrons \( n_e = 4m + 2 \), and antiperiodic BC if \( n_e = 4m \) \((m \text{ a positive integer}) \). Then the ground state is a spin singlet.

The infinite-dimensional phonon Hilbert space (for each mode) requires some further approximation even for arbitrarily small systems. Previous approaches to similar models \[13,14\] treated the phonons in the static limit, i.e., classically. The ground state within this limit is obtained by minimizing the electronic energy with respect to the lattice displacement (Born-Oppenheimer). However, neglecting the phonon dynamics can lead to a rather severe overestimate of the tendency towards small polaron formation, i.e., self-trapping of the carriers, especially for the large optical phonon frequencies found in the cuprates.

An unbiased approximation preserving the phonon dynamics results from a truncation of the Hilbert space to include \( n_p \) phonon states per site. We have shown \[15\], that for the simplest case, \( n_p = 2 \), there is a natural and unique choice for the two states at site \( i \), \( |\phi_1\rangle_i, |\phi_2\rangle_i \) defined in terms of the phonon vacuum \( |0\rangle \), and the coherent (displaced oscillator) state \( |\bar{0}\rangle_i = e^{-\eta^2/2}e^{\eta a_i^\dagger}|0\rangle \).

The non-perturbative character of this ansatz allows for asymptotically exact ground state properties in the weak and strong coupling limit. For intermediate coupling, the approximation was checked by including additional phonon states (see Ref. \[3\]). Apart from an upward renormalization of the coupling constant, we found no changes of ground state properties (electronic properties of the system with additional phonon states at \( E_B \) are identical within an error \( \approx 0.1\% \)) to the properties of the system with only \( |\phi_1\rangle_i, |\phi_2\rangle_i \) at \( E_B \), with \( 0.55 \lesssim E_B/E_B < 1 \) depending on \( E_B \). More details will be published elsewhere. Here, we shall restrict ourselves to \( n_p = 2 \) using \( |\phi_1\rangle_i, |\phi_2\rangle_i \).

The phase diagram of the model is determined by calculating (i) the compressibility \( \kappa \), and (ii) the critical exponent \( K_\rho \) which determines the decay of correlation functions in 1D models belonging to either the Tomonaga-Luttinger liquid (TLL) \[16,18\] or the Luther-Emery liquid (LEL) \[19\] universality class. Both systems are characterized by gapless charge excitations. The spin excitations are gaped in a LEL, while they remain gapless in a TLL.

The transition to a phase separated state is signaled by a divergent \( \kappa \), which we calculate from

\[
\kappa = \frac{L}{n_e^2} E_0(L, n_e + 2) - E_0(L, n_e - 2) - 2E_0(L, n_e),
\]

\( E_0(L, n_e) \) the ground state energy of a ring with \( n_e \) electrons and \( L \) sites. \( K_\rho \) is given by \( K_\rho = (\pi D n_e^2/\rho^3)^{1/2} \) \((n = n_e/L, \text{the electron density}) \), with the Drude weight \[20\]

\[
D = \pi L \left| \frac{\partial^2 E_0(\Phi)}{\partial \Phi^2} \right| _{\Phi = \Phi_0}.
\]

Here, \( E_0(\Phi) \) is the ground state energy for BC with a phase factor \( e^{i\Phi} \), and \( \Phi_0 = 0, \pi \) for periodic and antiperiodic BC respectively. A value of \( K_\rho > 1 \) indicates that SC correlations dominate the long-range fluctuations for both a TLL, and a LEL, while \( K_\rho < 1 \) is characteristic for dominating CDW correlations.
To check the consistency of the assumed TLL scaling, we calculated the central charge $c$ from the finite size corrections of the ground state energy as predicted by conformal field theory, $E(L)/L = \epsilon_{\infty} - \pi c(v_c + v_s)/(6L^2)$ [21]. Here $v_c, v_s$ are the charge and spin velocity which we extract from the dynamical charge and spin structure factor as in Ref. [22]. Using the results for $L = 8, 12$, we found a maximum deviation of 0.07 from the expected value $c = 1$ for the range of parameters studied. Given the finite-size errors in the velocities, this confirms the validity of TLL scaling.

In Fig. 1 we show the calculated phase diagrams for $E_B = 0, 0.25, 0.5, 0.75, L = 10, 12, 16$. Including the phonons, we were restricted to $L \leq 12$, but reliable results can already be obtained for $L = 10$. The main observations are: (i) With increasing e-ph coupling, the PS boundary, as determined from the condition $1/k = 0$, is shifted considerably to lower $J/t$. An independent criterion for PS is the long wavelength divergence of the charge structure factor $S_{\text{ch}}(k) = 1/L \sum_{i,j} e^{ik(i-j)}\langle n_{ij}\rangle$ which gives an error estimate $< 5\%$ for the phase boundary. A similar shift without a significant reduction in area is observed for the region of dominating SC fluctuations occurring below the onset of PS. For $E_B = 0.75$, it extends down to values as low as $J/t \approx 1.0$, compared to $J/t \approx 2.2$ in the pure $t$-$J$ model. Qualitatively, this shift can be explained by an enhancement of the effective mass of the charge carriers due to the e-ph coupling, i.e., a downward renormalization of $t \rightarrow \bar{t} < t$, which results in an enhanced effective $J/\bar{t}$. Note, that $J$ is not expected to be appreciably renormalized, since the phonons couple to the charge. Also, the direct dependence of $J$ on the displacements of the breathing mode is weak, since out of the two Cu-O bonds between a nn Cu pair, they strengthen one, but weaken the other one.

(ii) Especially at large $E_B$, the PS line and the contours of constant $K_\rho$ acquire a strong density dependence. In particular, a dip in the $K_\rho = 0.6$ contour develops for $E_B = 0.75$ at quarter filling. This is due to enhanced CDW correlations from the e-ph coupling. In fact, at $E_B = 0.75$, there is long-range CDW order for $J/t \lesssim 0.4$, as indicated by a saturation in the staggered density-density correlation function

$$D_{\text{ch}}(j) = \frac{1}{L} \sum_i (-1)^i \langle \langle n_{i+} \rangle \rangle - \langle \langle n_{i} \rangle \rangle \rangle,$$ \hspace{1cm} (5)

i.e., $\lim_{j \rightarrow \infty} D_{\text{ch}}(j) \neq 0$. Note, that for the case $J/t = 0$ (equivalent to spinless fermions), it is fairly well established by analytical and numerical results [15][23] that the system undergoes a CDW transition at $n = 0.5$ above a finite critical coupling strength $E_B^c(\Omega)$. In the static limit, $E_B^c = 0$, demonstrating the importance of quantum fluctuations. Previously [15], we estimated $E_B^c/t \approx 0.53$ for $\Omega/t = 0.2, n_F = 2$. Note however, that this value is definitely too low because of the renormalization of the coupling constant by additional phonon states as explained above. An analysis of the charge structure factor $S_{\text{ch}}(k) = 1/L \sum_{i,j} e^{ik(i-j)}\langle n_{ij}\rangle$ strongly indicates that the appearance of a $4k_F$ CDW is not unique to density $n = 0.5$ (which is obvious at the mean-field level). However, we found that for $n \neq 0.5$, the weakened lattice commensurability leads to an enhanced $E_B^c/t$, as estimated from the values at which $S_{\text{ch}}(4k_F)$ appears to diverge as a function of $L$. We conclude that the e-ph coupling in this model mediates an effectively repulsive interaction between the electrons, and hence does not support SC.

![Fig. 2. The phase diagram of the 1D t-J Holstein model in the $E_B, J$ plane at quarter filling for $\Omega/t = 0.2$, and $L = 12$.](image)

Fig. 2 shows the phase diagram in the $E_B, J$ plane at quarter filling. This plot clearly demonstrates that the regime of SC fluctuations is shifted almost rigidly to smaller values of $J/t$ as the e-ph coupling is increased. Note, the small region of CDW order at small $J/t$, large $E_B/t$. Within a strong coupling perturbation expansion for the case of spinless fermions, it was shown [23] that apart from the well known exponential renormalization of the hopping, $t \rightarrow t e^{-E_B/\Omega}$, the Holstein coupling also leads to an effective nn repulsion, which dominates in the limit $E_B \rightarrow \infty$. The competition of this effective

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**Fig. 1.** The phase diagram of the 1D $t$-$J$ Holstein model for $\Omega/t = 0.2$ and various values of the e-ph coupling $E_B$. The phase diagram of the 1D $t$-$J$ Holstein model in the $E_B, J$ plane at quarter filling for $\Omega/t = 0.2$, and $L = 12$.**
phonon-mediated repulsion with the attractive spin exchange term is responsible for the corresponding strong competition between CDW and SC correlations in the $t$-$J$ Holstein model. For $E_B > E_B^c (J = 0)$, a phase transition from a CDW to a metal takes place as $J$ is increased from 0.

Next, we analyze the effect of the e-ph coupling on the superconducting correlations directly, by looking at (i) the singlet SC structure factor defined as

$$S_{\text{pair}}(k) = \frac{1}{L} \sum_{j,l} \langle j \uparrow j \downarrow \rangle \langle P_j^\dagger P_l \rangle,$$

where $P_j^\dagger = (c_{j+1}^\dagger c_j^\dagger - c_j^\dagger c_{j+1}^\dagger)/\sqrt{2}$ creates a nn singlet pair, and (ii) the pair-pair correlation function in real space $D_{\text{pair}}(i) = \langle P_i^\dagger P_i \rangle$. It is important to study $D_{\text{pair}}(i)$ separately to distinguish short and long-range correlations.

In Fig. 3(a), we plot $S_{\text{pair}}(k = 0)$ at quarter filling as a function of $J/t$, $E_B$. We observe an overall suppression of $S_{\text{pair}}(k = 0)$, as $E_B$ increases. This can be traced back to the repulsive CDW correlations introduced by the phonons. In addition, the peak at the onset of PS is increasingly smeared out as $E_B$ grows. Looking at the correlations in real space, Fig. 3(b), we note that this suppression is coming primarily from a reduction of long-range correlations. This underlines our conclusion that the e-ph coupling is detrimental to SC in this model.

![Fig. 3](image-url)

Fig. 3. (a) The singlet SC structure factor $S_{\text{pair}}(k = 0)$ for various $E_B$. The arrows mark the occurrence of PS. (b) The pair-pair correlation function $D_{\text{pair}}(i)$ for various $E_B$ evaluated at the value $J = J_{\text{max}}(E_B)$, where $S_{\text{pair}}(k = 0, J, E_B)$ has a maximum.

Another question concerns the existence of a spin gap $\Delta_s$, defined as the energy difference between the singlet ground state and the lowest triplet excitation for $L \to \infty$. It was shown [24] that the addition of a nn repulsion to the $t$-$J$ model can lead to a large $\Delta_s$ in the region of dominating SC fluctuations. Since the e-ph coupling also induces an effective short-range repulsion, one might expect an analogous appearance of a spin gap. Due to the restriction $L \leq 12$, an accurate finite-size scaling for $\Delta_s$ is not possible. Nevertheless, extrapolating $\Delta_s (1/L)$ for $L = 8, 12$ at $n = 1/4$ to $1/L = 0$, the intercept is negative or very small for all $E_B$. However, at $E_B = 0.75$, we consistently observe a small positive intercept for several $J$ in the region of dominating SC fluctuations, possibly indicating a small spin gap. For the $t$-$J$-$V$ model studied in [24], we found that extrapolating results from $L = 8, 12$ calculations also produces a negative intercept as long as $\Delta_s/t \lesssim 0.1$. This is due to the fact that the scaling function is exponential at small $1/L$ if a spin gap is present [24]. Assuming the same scaling of $\Delta_s$ with $1/L$ for the $t$-$J$-$V$ and the present model, we can give an upper bound $\Delta_s/t \lesssim 0.1$ for all $E_B$ studied.

In the 2D $t$-$J$ model, coherent charge motion is already renormalized by spin-exchange scattering resulting in an effective bandwidth $\sim J/\Omega$ [25]. This should make the e-ph coupling more effective, i.e., probably a smaller coupling (as in 1D) is needed to see appreciable effects. Substantial evidence for a SC ground state of $d_{x^2-y^2}$ symmetry in the 2D $t$-$J$ model has been reported [26,28]. The most reliable estimate for the SC phase boundary predicts a critical value $J/\Omega \approx 0.5$ above which SC appears in the interesting regime of hole doping ($\delta = 1 - n = 0.15 - 0.25$) [28]. Our results suggest that the additional mass enhancement by the e-ph coupling could push down the phase boundary to lower $J$, so that SC might arise in the regime of $J/\Omega \approx 1/4 - 1/3$, relevant for the cuprates [8]. Concerning the isotope effect, our results are ambiguous. A smaller phonon frequency increases the ratio $E_B/\Omega$, i.e., strengthens the effect of the e-ph coupling. However, this has two competing effects on SC: (i) the effective ratio $J/\Omega$ increases through a further mass enhancement, but (ii), the induced repulsive CDW correlations also grow. The identification of the dominating effect requires further calculations in 2D.

The author would like to thank M. R. Norman and T. M. Rice for useful comments, and a careful reading of the manuscript. We acknowledge financial support by the NSF (NSF-DMR-91-20000) through the Science and Technology Center for Superconductivity. Numerical calculations have been performed on the Convex C38, and HP 735 workstations at CSSC Manno, Switzerland, and on the Cray2 at NERSC, Lawrence Livermore Lab., CA.

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