Effect of long-range hoppings on \( T_c \) in a two-dimensional Hubbard-Holstein model of the cuprates

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We study the effect of long-range hoppings on \( T_c \) for the 2D Hubbard model with and without Holstein phonons using parameters evaluated from band structure calculations for cuprates. Employing the dynamical cluster approximation (DCA) with a quantum Monte Carlo (QMC) cluster solver for a 4-site cluster, we observe that without phonons, the long-range hoppings \( t' \) and \( t'' \), generally suppress \( T_c \). We argue that this trend remains valid for larger clusters. In the presence of the Holstein phonons, a finite \( t' \) enhances \( T_c \) in the under-doped region for the hole-doped system, consistent with LDA calculations and experiment. This is interpreted through the suppression of antiferromagnetic correlations and the interplay between polaronic effects and the antiferromagnetism.

**Introduction-** While most theoretical studies of the cuprates are in the framework of the simplest version of the two-dimensional Hubbard model with only nearest neighbor hopping, both band structure calculations and experimental data suggest a richer set of parameters for this model. Angle-resolved photoemission spectroscopy (ARPES) plays an important role in this regard, suggesting different topologies of the Fermi surface for different high-\( T_c \) superconductors. The inclusion of the next nearest neighbor hopping, \( t' \), in the Hubbard model is also necessary to capture the electron-hole asymmetry. Furthermore, \( t' \) is an important parameter in determining the charge orderings and their textures in cuprates. The effect of \( t' \) on \( T_c \) has been studied by different groups. E. Pavarini et al. notice a correlation between the experimental maximum superconducting temperature (\( T_c^{\text{max}} \)) and the value of \( t' \) evaluated from the band structure calculations in different cuprates. However, the mechanism which may govern this relationship in cuprates is not well-understood.

Theoretical investigations employing simple models such as single-band Hubbard and t-J models, do not show strong evidence of a direct relationship between \( T_c \) in different doping regions and the magnitude of the long-range hoppings. Varieties of techniques have been used to study the effect of \( t' \) and \( t'' \) (third nearest neighbor hopping) on superconducting properties of these models. For hole-doped systems, by employing finite size calculations and slave-boson mean field theory, C. T. Shih et al. find a strong enhancement of the superconducting correlations due to \( t' \) and \( t'' \) in the intermediate- and over-doped regions and a slight suppression in the under-doped region. For electron-doped systems, density matrix renormalization group calculations have shown that \( t' \) leads to the enhancement of d-wave pairing correlations. Unlike finite-size calculations where the transition temperature cannot be directly calculated and the superconducting properties are estimated from cluster pairing correlations, the DCA25,27,28 is an approximation for the thermodynamic limit and allows calculation of \( T_c \) and other superconducting properties for all doping regions. The DCA has been successful to derive the phase diagram of the Hubbard model, showing the antiferromagnetic (AF), pseudogap and d-wave superconductivity phases which are in a very good qualitative agreement with experiments.

In this work, we investigate the effect of \( t' \) and \( t'' \) on the superconducting properties of the 2D single-band Hubbard model with and without phonons. We find that without phonons, \( T_c \) is generally suppressed by \( t' \) and \( t'' \). However, with Holstein phonons, \( T_c \) increases with \( t' \) in the under-doped region for hole-doped systems. In other doping regions, phonons reduce the suppression of \( T_c \) due to \( t' \). The interplay between electron-phonon (EP) coupling and \( t' \) plays an essential role in the dependence of \( T_c \) on \( t' \) and is consistent with experimental data showing evidence of strong EP interaction in the cuprates. Previously, we established a synergistic relationship between short ranged AF order and EP coupling in the doped Hubbard model, i.e., we found that AF correlations enhance the polaronic effects (dressing of electrons by phonons) and at the same time, the EP coupling enhances the AF correlations. We also established that local phonons which couple to the electronic density, strongly suppress \( T_c \) due to the renormalization of the single-particle propagator. Here, we show that \( t' \) can strongly affect this synergism and thus the suppression of \( T_c \). A finite \( t' \) in the hole-doped systems suppresses AF correlations and hence reduces the polaronic effects and enhances \( T_c \).

**Model-** We consider a 2D Hubbard-Holstein model

\[
H = -\sum_{i,j} t_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.) + t\sum_{i\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \frac{\hat{n}_i^2}{2M} + \frac{1}{2} M \omega_0^2 u_i^2 + g n_i u_i
\]

where \( t_{ij} \) is the hopping matrix, \( c_{i\sigma}^\dagger (c_{i\sigma}) \) is the creation (annihilation) operator for electrons on site \( i \) with spin \( \sigma \), and \( U \) is the on-site Coulomb repulsion which is taken to be equal to the bandwidth (8\( t \)). We vary the filling,
be exact in the limit of longer range correlations. Therefore, the solution would be feasible if an on-site and proportional to the density of electrons with the coupling strength $g$. We define the dimensionless EP coupling for Holstein phonons as

$$\lambda = \frac{g^2}{(M\omega_0^2)l}$$

which is the ratio of the single-electron lattice deformation energy and half of the electronic bandwidth.$^{30}$

**Formalism.** We employ the dynamical cluster approximation with a quantum Monte Carlo algorithm as the cluster solver. The DCA approximates the self-energy of the system by mapping it into a cluster of size $N_c$ embedded in a self-consistent host. All of the correlations inside the cluster are treated non-perturbatively while a mean-field (MF) approximation is used to deal with longer range correlations. Therefore, the solution would be exact in the limit of $N_c \to \infty$. The Monte Carlo simulation performs the sum over both the discrete field used to decouple the Hubbard repulsion$^{32,33}$, as well as the phonon field, $u$. Details about an efficient Monte Carlo simulation of systems with low energy phonons will be given elsewhere.

The sign problem in QMC limits our calculations to relatively small clusters. Most of the calculations are done for a $2 \times 2$ cluster, the smallest cluster which allows $d$-wave pairing. Note that the length scale associated with $t''$ is not represented for this cluster. Thus, the effect of $t''$ will be similar to that in the dynamical mean field approximation$^{32,33}$; i.e. only through changes in the cluster densities of states.

In order to investigate the effect of $t'$ on the $d$-wave superconductivity, we calculate the eigenvalues of the pairing matrix $\Gamma_0$, where $\chi_0$ is the bare bubble and $\Gamma$ is the particle-particle irreducible vertex function calculated in the QMC process. At $T_c$, the leading eigenvalue (in this case, the one with $d$-wave symmetry) goes to unity and causes a singularity in the two-particle pairing Green’s function $\chi = \chi_0 + \chi_0 \Gamma \chi = \chi_0 (1 - \Gamma \chi_0)$. The value of the $d$-wave pairing interaction can be measured by calculating the $d$-wave projected vertex

$$V_d = -\frac{\langle g(K)\Gamma(K',\pi T)g(K')\rangle_{KK'}}{\langle g(K)^2\rangle_K}$$

for the lowest Matsubara frequency and $g(K) = \cos(K_x) - \cos(K_y)$ where $K$ is the momentum at the center of each of the $N_c$ cells which tile the Brillouin Zone in the DCA. To capture the effect of the dressed electronic propagator on the $d$-wave eigenvalue, we also calculate the $d$-wave projected bare bubble as

$$P_{d0} = \frac{T}{N_c} \frac{\langle g(K)^2 \chi_0(K,\pi T)\rangle_K}{\langle g(K)^2\rangle_K}$$

**Results.** The long-range hoppings, $t'$ and $t''$ can affect the superconducting phase diagram through both the band structure and the interaction vertex. In the electron-doped systems, $t'$ favors hopping in the same sub-lattice and enhances the AF correlations at finite doping while in the hole-doped systems, $t'$ suppresses the AF correlations.$^{34,35}$ Presumably, $t''$ which also introduces hopping in the same sub-lattice, would affect AF correlations as well. However, previous calculations indicate that there is a close relationship between AF and superconductivity in cuprates.$^{36,37,38}$. Therefore, $t'$ and $t''$ can influence pairing by affecting the AF correlations. They also change the bandwidth which alters the density of states at the Fermi energy and thus can influence $T_c$.

We find that $t'$ and $t''$ generally suppress $T_c$ in most doping regions, apart from a slight increase in $T_c$ at small dopings. First, we consider a finite $t'$ and $t'' = 0$. The superconducting phase diagrams for three different values of $t'$ are shown in Fig. 1(a), 1(b) and 1(c). When $t' = -0.3t$, $T_c$ is slightly smaller in comparison with the case of $t' = 0$ from $10\%$ to $25\%$ hole-doping and at large electron-doping ($\geq20\%)$. With a larger $t' = -0.4t$ for the hole-doped system, we find that $T_c$ is strongly suppressed in intermediate- and over-doped regions while in the under-doped region, the overall effect of $t'$ on $T_c$ is negligible. The effect of $t''$ on the superconducting phase diagram is shown in Fig. 1(c) and (d). We see a stronger suppression of $T_c$ in the over-doped region and a slight increase ($\sim 10\%$) in $T_c$ in the under-doped region when both $t'$ and $t''$ are finite. Moreover, a non-zero $t''$ with $t' = 0$, does not have a considerable effect on $T_c$.

We find that the band renormalization effects due to $t'$ are mostly responsible for changes in $T_c$ and the effect of $t'$ on the interaction vertex is less significant. In order to

![Graphical representation of the superconducting phase diagram](image-url)
illustrate this, we plot the \( t' \)-dependence of the d-wave bare bubble, \( P_{d0} \) (Eq. 1), and the d-wave pairing interaction, \( V_d \) (Eq. 3), at 5\% and 15\% hole-doping in Fig. 2 (empty symbols). \( t' \) strongly suppresses \( P_{d0} \) and slightly increases \( V_d \) in both doping regions. The former effect is responsible for the decrease in \( T_c \). The suppression in \( P_{d0} \) is a result of the band renormalization effects of \( t' \) which decrease the density of states at the anti-nodal points.\(^{35,40}\)

The effect of \( t' \) on the d-wave pairing shows a similar trend when larger clusters are considered. The inverse of the d-wave pairing susceptibility for 4-site and 16-site clusters at 15\% hole-doping are shown in Fig. 3. For both clusters and in the temperature range available, \( t' \) suppresses the d-wave pairing susceptibility.

In the presence of phonons, long-range hoppings change the polaronic effects which have a direct influence on \( T_c \). In previous works, we have found that at the intermediate EP coupling, local phonons suppress \( T_c \) due to polaronic effects which reduce the mobility of carriers.\(^{29}\) The polaronic effects are enhanced by the AF correlations.\(^{32}\) Therefore, the effect of \( t' \) on the AF correlations will directly influence them. Using exact diagonalization methods, T. Tohyama et al.\(^{10,35}\) have shown that \( t' \) suppresses the AF correlations in the hole-doped cuprates. As a result, the polaronic effects are reduced by \( t' \) which enhances \( T_c \).

When Holstein phonons are considered, \( T_c \) increases with \( t' \) in the under-doped region and remains almost unchanged in the intermediate-doped region as shown in Fig. 4. Note that without phonons, \( T_c \) decreases with \( t' \) in the intermediate-doped and does not change in the under-doped region. The effect of \( t' \) on \( T_c \) becomes more significant with increasing \( \lambda \). As shown in Fig. 4 (a), for \( \lambda = 0.6 \) at 5\% doping, \( T_c \) is strongly enhanced when \( |t'| \) increases. At 15\% doping, it is difficult to fix the filling due to the large charge fluctuations for the values of \( \lambda \) larger than 0.5. Presumably, \( T_c \) would increase with \( t' \) at 15\% doping for \( \lambda = 0.6 \). Note that phonons do not increase \( T_c \), they only reverse the behavior of \( T_c \) with \( t' \). At fixed \( t' \), their effect is to reduce \( T_c \), but the reduction is less significant when \( |t'| \) is larger.

Phonons change the behavior of \( P_{d0} \) with respect to \( t' \) at low temperatures. As shown in Fig. 2 (b) and (d) with full symbols, \( t' \) has a small effect on suppressing \( P_{d0} \) around \( T_c \) when phonons are present. While the band renormalization effects, caused by \( t' \), tend to suppress \( P_{d0} \), the reduction in the polaronic effects due to \( t' \) enhances \( P_{d0} \). As a result of these two competing effects, \( P_{d0} \) remains almost unchanged near \( T_c \) by changing \( t' \). On the other hand, the \( t' \)-dependence of \( V_d \) is not influenced much by phonons. Therefore, \( T_c \) increases in the under-doped region where \( V_d \) shows a slight increase with
It is known that the $2 \times 2$ cluster overestimates the d-wave superconductivity due to the neglect of phase fluctuations. However, here we focus mainly on investigating the role of AF correlations in enhancing the phase fluctuations. The 16-site cluster results suggest that these trends do not change when larger clusters are considered.

The transition temperature at small doping would be the strongest affected by phase fluctuations. In general, $t'$ should enhance $T_c$ by suppressing the phase fluctuations. In part, this is due to the suppression of AF correlations. The AF correlations reduce the mobility of the carriers and increase the effective mass which leads to the enhancement of phase fluctuations. This effect is enhanced in the presence of phonons. Phonons play a role similar to the AF correlations in enhancing the phase fluctuations by reducing the mobility of electrons. In addition, through polaronic effects, they also enhance the AF correlations. Therefore, the effect of phonons on suppressing $T_c$ is underestimated in the absence of the phase fluctuations. The decrease of the polaronic effects due to $t'$ would increase $T_c$ more significantly in the under-doped region in the presence of phase fluctuations. Hence, the effect of $t'$ on $T_c$ is underestimated by small cluster calculations, suggesting that $t'$ will have a stronger effect on $T_c$ in larger clusters.

**Conclusion**—We find that without phonons, the long-range hoppings generally suppress $T_c$ in the Hubbard model. However, by including Holstein phonons, $T_c$ increases with $t'$ in the under-doped region for the hole-doped system while the suppression in $T_c$ due to $t'$ is reduced in the intermediate-doped region. Phonons do not increase $T_c$, but rather reverse the behavior of $T_c$ with $t'$. We find that the increase in $T_c$ with $t'$ becomes more significant for larger values of the EP coupling. We interpret these by the effect of $t'$ on suppressing the polaronic effects as a result of suppressing the AF correlations and the interplay between AF and EP coupling.

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