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We study the effect of long-range hoppings on T_c for the two-dimensional (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 local-density approximation (LDA) calculations and experiment. This is interpreted through the suppression of antiferromagnetic (AF) correlations and the interplay between polaronic effects and the antiferromagnetism.

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I. 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.[1–8] 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[3,9] which can be reproduced by choosing finite long-range hoppings $(t',t'',\ldots)$.[4–8] The inclusion of the next-nearest-neighbor hopping, t', in the Hubbard model is also necessary to capture the electron-hole asymmetry.[10–12] Furthermore, t' is an important parameter in determining the charge orderings and their textures in cuprates.[13–16]

The effect of t' on T_c has been studied by different groups.[2,3,17] For example, Pavarini *et al.*[2] noticed a correlation between the experimental maximum superconducting temperature ($T_c^{\max}$) 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[12,18–21] do not show strong evidence of a direct relationship between T_c in different doping regions and the magnitude of the long-range hoppings. Variety 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 (MF) theory, Shih *et al.*[18] found 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[14] 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 dynamical cluster approximation (DCA)[22–24] 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 in deriving the phase diagram of the Hubbard model, showing the antiferromagnetic (AF), pseudogap and d-wave superconductivity phases which are in very good qualitative agreement with experiments.[25,26]

In this work, we investigate the effect of t' and t'' on the superconducting properties of the two-dimensional (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.[27,28] Previously, we established a synergistic relationship between short-ranged AF order and EP coupling in the doped Hubbard model,[29] 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.

II. MODEL

We consider a 2D Hubbard-Holstein model,

$$H = -\sum_{ij\sigma} t_{ij}(c_{i\sigma}^{\dagger}c_{j\sigma} + \mathrm{H.c.}) + \epsilon\sum_{i\sigma} n_{i\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + \sum_{i}\frac{p_i^2}{2M} + \frac{1}{2}M\omega_0^2u_i^2 + gn_iu_i, \quad (1)$$

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 σ, and U is the on-site Coulomb repulsion which is taken to be equal to the bandwidth ($8t$). We vary the filling, $\langle n\rangle$, from values less than one to values larger than one to cover the hole-doped to the electron-doped regions, respectively. ω_0 is the frequency of phonons and $\{u_i,p_i\}$ are canonical conjugate coordinates for the phonon on site i. The EP coupling is on-site and proportional to the density of electrons with the coupling strength g. We define the dimensionless EP coupling for Holstein phonons as

$$\lambda = g^2/(M\omega_0^2 8t) \tag{2}$$

which is the ratio of the single-electron lattice deformation energy and half of the electronic bandwidth.[30]

III. 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 nonperturbatively while a MF approximation is used to deal with longer range correlations. Therefore, the solution would be exact in the limit of $N_c\rightarrow\infty$. The Monte Carlo simulation performs the sum over both the discrete field used to decouple the Hubbard repulsion,[31] 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 quantum Monte Carlo (QMC) limits our calculations to relatively small clusters. Most of the calculations are done for a 2×2 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 $\Gamma\chi_0$, where χ_0 is the bare bubble and Γ 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[34,35]

$$V_d = -\frac{\langle g(\mathbf{K})\Gamma(\mathbf{K},\pi T|\mathbf{K}',\pi T)g(\mathbf{K}')\rangle_{\mathbf{K}\mathbf{K}'}}{\langle g(\mathbf{K})^2\rangle_{\mathbf{K}}} \tag{3}$$

for the lowest Matsubara frequency and $g(\mathbf{K})=\cos(\mathbf{K}_x)-\cos(\mathbf{K}_y)$, where $\mathbf{K}$ 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

$$P_{d0} = \frac{T}{N_c}\frac{\langle g(\mathbf{K})^2\chi_0(\mathbf{K},\pi T)\rangle_{\mathbf{K}}}{\langle g(\mathbf{K})^2\rangle_{\mathbf{K}}}. \tag{4}$$

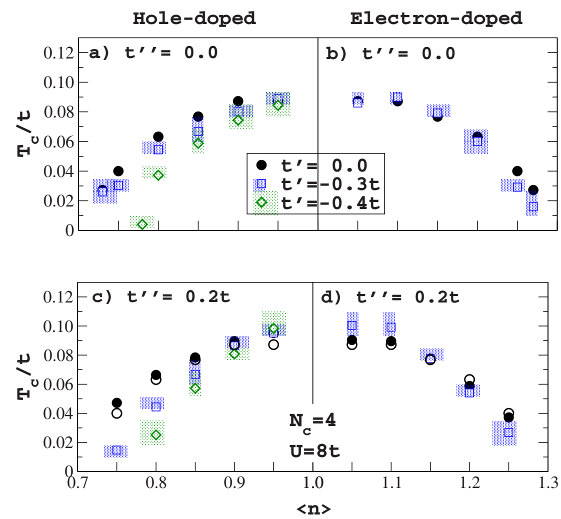

FIG. 1. (Color online) The superconducting phase diagram of the hole-doped (left panels) and the electron-doped (right panels) system for different values of t'. The upper (lower) panels correspond to $t''=0$ ($t''=0.2t$). The open circles in (c) and (d) correspond to $t'=t''=0$ and are plotted for comparison.

IV. 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 sublattice and enhances the AF correlations at finite doping while in the hole-doped systems, t' suppresses the AF correlations.[10,36] Presumably, t'', which also introduces hopping in the same sublattice, would affect AF correlations as well. However, previous calculations indicate that there is a close relationship between AF and superconductivity in cuprates.[35,37,38] Therefore, t' and t'' can influence pairing by affecting the AF correlations. They also change the band structure 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 Figs. 1(a) and 1(b). When $t'=-0.3t$, T_c is slightly smaller in comparison to the case of $t'=0$ from 10% to 25% hole doping and at large electron doping ($\gtrsim$20%). 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 Figs. 1(c) and 1(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 nonzero t'' with $t'=0$ does not have a considerable effect on T_c.[39]

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 illustrate this, we plot the t'-dependence of the d-wave bare bubble, P_{d0} [Eq. (4)], and the d-wave pairing interaction, V_d [Eq.

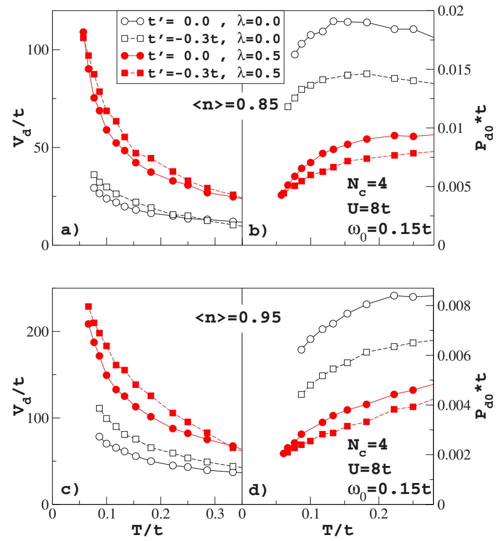

FIG. 2. (Color online) d-wave pairing interaction, V_d [Eq. (3)], and the d-wave projected bare bubble, P_{d0} [Eq. (4)], versus temperature in the under-doped and intermediate-doped regions. The empty (filled) symbols correspond to the Hubbard model without (with) Holstein phonons. The circles (squares) correspond to $t'=0.0$ ($t'=-0.3t$).

(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 antinodal points.[36,40]

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.[26] The polaronic effects are enhanced by the AF correlations.[41] Therefore, the effect of t' on the AF correlations will directly influence them. Using exact diagonalization methods, Tohyama *et al.*[10,36] have shown that t' suppresses the AF correlations in the

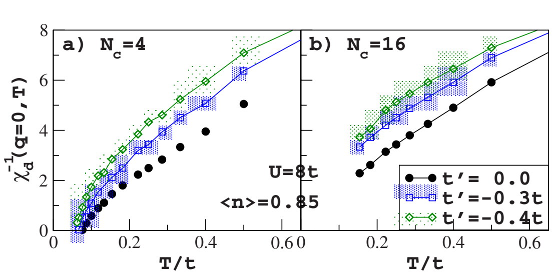

FIG. 3. (Color online) Inverse of the d-wave pairing susceptibility for (a) 4-site and (b) 16-site cluster at 15% doping for different next-nearest hoppings.

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 region and does not change in the under-doped region. The effect of t' on T_c becomes more significant with increasing . As shown in Fig. 4(a), for =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 larger than 0.5. Presumably, T_c would increase with t' at 15% doping for =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 Figs. 2(b) and 2(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 t'.

It is known that the 2×2 cluster overestimates the d-wave superconductivity due to the neglect of phase fluctuations.[42] However, here we focus mainly on investigating the relative dependence of T_c on different parameters such as EP coupling and long-range hoppings and not on calculating the exact value of T_c. The 16-site cluster results (shown in Fig. 3) suggest that these trends do not change when larger clusters are considered.

The transition temperature at small doping would be the most strongly affected by phase fluctuations.[43] 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.[43] 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

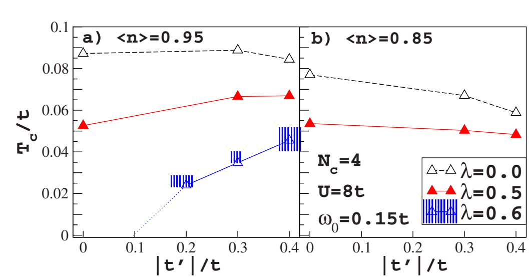

FIG. 4. (Color online) t'-dependence of T_c at (a) 5% and (b) 15% dopings for different values of the dimensionless EP coupling, [Eq. (2)]. A finite t' increases T_c in the under-doped region when EP coupling is present. For =0.6 in (a), the $t'=0$ point has been extrapolated from the data at temperatures larger than T_c.

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.

V. 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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