Interplay between the Pseudogap and Superconductivity in Doped Mott Insulators: a Cluster Dynamical Mean-Field Theory Study

Jinbin Liu(刘晋斌), Dao-Xin Yao(姚道新)*, and Wei Wu(吴为)*

Guangdong Provincial Key Laboratory of Magnetoelectric Physics and Devices, State Key Laboratory of Optoelectronic Materials and Technologies, Center for Neutron Science and Technology, School of Physics, Sun Yat-sen University, Guangzhou 510275, China

(Received 17 April 2025; accepted manuscript online 7 July 2025)

We investigate the interplay between the pseudogap state and d-wave superconductivity in the two-dimensional doped Hubbard model by employing an eight-site cluster dynamical mean-field theory method. By tuning electron hopping parameters, the strong-coupling pseudogap in the two-dimensional Hubbard model can be either enhanced or suppressed in the doped Mott insulator regime. We find that in underdoped cases, the closing of pseudogap leads to a significant enhancement of superconductivity, indicating competition between the two in the underdoped regime. In contrast, at large dopings, suppressing the pseudogap is accompanied by a concurrent decrease in the superconducting transition temperature T_c, which can be attributed to a reduction in antiferromagnetic correlations behind both the pseudogap and superconductivity. We elucidate this evolving relationship between pseudogap and superconductivity across different doping regimes.

DOI: 10.1088/0256-307X/42/8/080711 CSTR: 32039.14.0256-307X.42.8.080711

1. Introduction. The emergence of unconventional superconductivity (SC) from the normal state of cuprates, which exhibits various abnormal phenomena of electrons,[1–6] has posed persistent challenges in the field of condensed matter physics. One prominent issue is the relationship between the occurrence of pseudogap (PG) state[7–9] and the d-wave SC.[10–14] In underdoped cuprates, PG appears as a partial energy gap at the Fermi level,[7] which usually sets in at a temperature T^* well above the superconducting transition temperature T_c. Despite extensive studies from experiments,[5,7,15–18] theories,[19–23] or numerical computations,[12,14,21,24–31] the nature of PG and its connections to SC are still open to debate.[4,16,32]

Inspired by the Uemura relation[10] that relates T_c to the superfluid density ρ_s, phase fluctuation theories[33,34] were proposed to explain the remarkable difference between the PG temperature T^* and superconducting T_c in underdoped cuprates. In these theories, PG can generally be seen as stemming from the precursor effects of electron pairing. For example, in the slave-boson mean-field theory[34–36] or the renormalized mean-field theory,[37] the spin degrees of freedom of electrons can form resonating spin-singlet pairs, causing a PG in the single-particle spectra below a relatively high T^*. The long-range phase coherence of pairing is, however, essentially determined by the Bose–Einstein condensation of the charge degrees of freedom of electrons, which can only happen at a much lower T_c in the underdoped regime.[34] Hence, at small dopings, the appearance of PG signals preformed Cooper pairs,[38,39] which is recognized as the parent state of d-wave SC in these theories. It is notable that both the slave-boson mean-field and renormalized mean-field methods essentially implement Anderson's resonating valence bond conception of unconventional SC.[40,41]

In experiments, nevertheless, the measurements of the Nernst effect[42,43] suggest that preformed Cooper pairs are likely to occur only at temperatures much lower than the PG temperature T^*. This observation renders a possible multiple-origin scenario for PG,[43] where the phase fluctuations of Cooper pairs would represent only a secondary contribution in depleting low-energy electrons in PG. Hence, accordingly, the PG state should rather be seen as a distinct state of matter that may essentially compete with SC.[44,45] We note that there is mounting evidence from both experiments and numerical computations suggesting that short-ranged antiferromagnetic (AFM) spin fluctuations play a dominant role in opening up the PG.[22,27,46–50] On the other hand, spin fluctuations have also been demonstrated to be the main source of d-wave pairing as well,[51–56] from both numerical computations[57–59] and experiments.[11,60,61] This disagrees with resonating valence bond theory which suggests an "instantaneous pairing glue"[62] in electron pairing. Up to date, however, the question of how the roles played by the spin fluctuations differ in generating both PG and SC is still far from clear.

Recently, it has been proposed that the strong-coupling PG can be continuously tuned by changing certain noninteracting hopping parameters[30] of electrons. This opens up the possibility of manipulating PG while retaining strong Coulomb interactions between electrons in a

*Corresponding authors. Email: yaodaox@mail.sysu.edu.cn; wuwei69@mail.sysu.edu.cn

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model system, hence disentangling PG from other strong-coupling physics. For example, one can switch on/off PG by varying hopping parameters in doped Mott insulators which possess d-wave superconducting instability at low temperatures. In such a way, one can thus tackle the relation between PG and SC in a controlled manner, which is the main goal of this work.

Here, we use the dynamical cluster approximation,[63] which is a cluster extension of the dynamical mean-field theory (DMFT),[64] to solve the two dimensional doped Hubbard model.[13] Following Ref. [30], we adjust the next-nearest-neighbour hopping t' and other hopping terms to tune the strength of PG effects. We systematically study the correlation between PG and d-wave SC. We find that in the underdoped regime, suppressing PG leads to a significant enhancement of SC. PG acts as a competing factor to SC. At large dopings, this trend is, however, reverted: suppressing PG is accompanied by a concurrent decrease in superconducting T_c. We explain that this is because at small dopings, PG severely depletes the low-energy density of states (DOS) available for condensation into Cooper pairs, hence detrimentally affecting SC. At large dopings, where the suppression of DOS by PG becomes insignificant, the strength of AFM correlations play a primary role in determining both PG and SC temperatures. Therefore, when certain hopping terms are tuned to reduce AFM correlations to suppress PG, SC would also be suppressed in the overdoped regime.

2. Model and Method. To tackle the strong correlation effects underlying the PG and SC in cuprates, we consider the Hubbard model Hamiltonian on the two-dimensional square lattice,[65]

$$H = -\sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}, \qquad (1)$$

where $c^{\dagger}_{i\sigma}$ are electronic creation operators on site i with spin $\sigma = \uparrow, \downarrow$, $n_{i\sigma} = c^{\dagger}_{i\sigma} c^{\dagger}_{i\sigma}$, and μ denotes the chemical potential that is varied in the hole-dope system in this work. The hopping amplitude t_{ij} is nonzero for nearest-neighbor hopping t, and for next-nearest-neighbour hopping t' such that the dispersion relation reads $\epsilon_{\boldsymbol{k}} = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x)\cos(k_y)$. It has long been noted that the t' term can significantly affect PG and SC.[47,66,67] Recently, it was found[30] that at large Hubbard U, the strength of the PG effects can be remarkably sensitive to the value of the so-called "renormalized energy" $\epsilon^{*}_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu + \langle n \rangle U/2$ of the van Hove singularities (vHS) in the system. It is observed that when $\epsilon^{*}_{\boldsymbol{k}}$ of vHS approaches zero, PG effects can be greatly enhanced. When the absolute value $|\epsilon^{*}_{\boldsymbol{k}}|$ of vHS becomes large, the strong electron scattering will essentially be quenched and the system forms a good metal with quasiparticle peaks spiking at the Fermi level, despite the presence of a large Hubbard U.[30] This finding tentatively explains the t'-dependence of PG found in literature.[47] In this work, we will first use t' to adjust $\epsilon^{*}_{\boldsymbol{k}}$ of the vHS [$\boldsymbol{k} = (0, \pi)$ and $\boldsymbol{k} = (\pi, 0)$] to alter PG. In addition, an asymmetric next-next-nearest-neighbor hopping t_3 will also be adopted to change PG without introducing geometric frustrations (see Fig. 1 and also below for details). The value of t defines the energy unit throughout this paper, which is taken as $t \equiv 1$. The strength of Hubbard repulsion U is chosen to be always larger than Mott transition U_c, ensuring our study resides in doped Mott insulator regime.

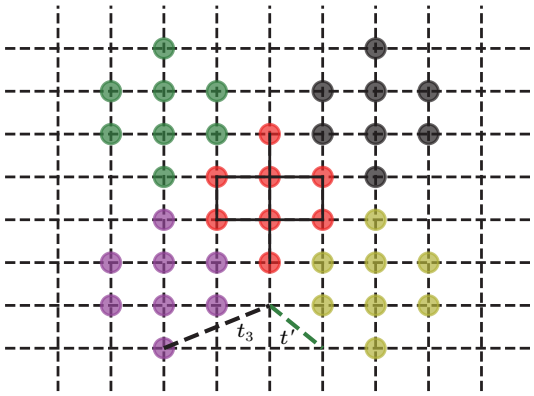

Fig. 1. Illustration of the eight-site DCA clusters tiling the two-dimensional square lattice. The next-nearest-neighbour hopping t' and asymmetric next-next-nearest-neighbor hopping t_3 are depicted by dashed lines.

To solve the above Hamiltonian, we employ the dynamical cluster approximation (DCA),[63] a cluster extension of single-site DMFT,[64] which can capture exactly the temporal correlations as well as the short-ranged spatial correlations inside the cluster, while longer range correlations beyond the cluster are treated in a dynamical mean-field way. This approximation is embodied by mapping the original lattice problem onto a small quantum cluster model embedded in an effective medium.[64] The eight-site DCA cluster we use in this work is illustrated in Fig. 1. Here we use the Hirsch–Fye quantum Monte Carlo[68,69] as an impurity solver with a time discretization $\Delta\tau = 0.071$.

3. DCA Results. In order to study the relation between PG and d-wave SC, we compute two energy scales here: the PG temperature T^{*}, and SC transition temperature T_c, for different hopping t'. In this work T^{*} is defined as the temperature where the antinodal spectral function $A(\boldsymbol{k}, \omega) \equiv -(1/\pi)\mathrm{Im}G(\boldsymbol{k}, \omega)$, $\boldsymbol{k} = (0, \pi)$ starts to decease with temperature T at the Fermi level $\omega = 0$. Here $\mathrm{Im}G(\boldsymbol{k}, \omega = 0)$ is obtained by a linear extrapolation of the Green's function in Matsubara frequency space $G(\boldsymbol{k}, \mathrm{i}\omega_n)$,[26] as shown in Fig. 2. To obtain the superconducting T_c, we apply a small uniform inducing d-wave pairing field to the Hamiltonian of Eq. (1), and calculate the pairing response to get the d-wave pairing susceptibility $\chi_{\mathrm{d-SC}} = (1/N)\sum_{i,j} \int_0^{\beta} \langle T_\tau P^{\dagger}_j(\tau) P_i(0) \rangle \mathrm{d}\tau$, where $P_i = (1/\sqrt{2}) f(r)(c_{i\uparrow} c_{i+r,\downarrow} - c_{i\downarrow} c_{i+r,\uparrow})$ is the d-wave spin singlet pairing operator, $f(r)$ represents the d-wave form factor associated with pairing on bond $(i, i+r)$ that follows $\sum_r f(r) \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = \cos(k_x) - \cos(k_y)$. In our calculations, we are careful to make sure that the inducing fields are small enough such that the pairing resides in the linear response regime. As displayed in Fig. 2, for a typical computation

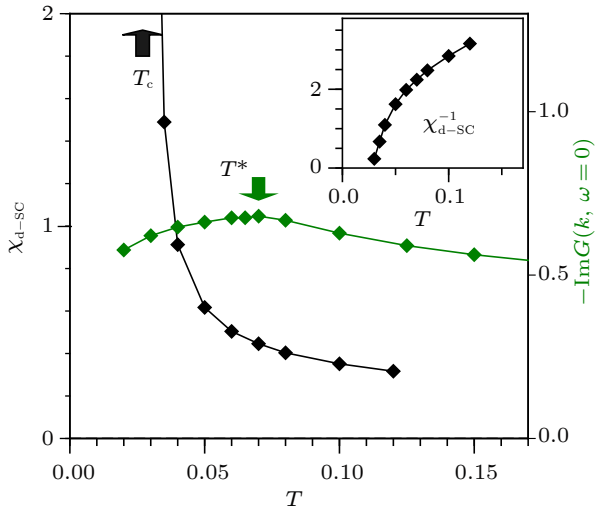

Fig. 2. The d-wave pairing susceptibility $\chi_{\mathrm{d-SC}}$, and the imaginary part of the antinodal Green's function at zero frequency $-\mathrm{Im}G(\boldsymbol{k}, \omega = 0)$ as functions of temperature at $U = 7$, $t' = 0$, and $p = 0.08$. Here $\boldsymbol{k} = (0, \pi)$. Insert shows the inverse of $\chi_{\mathrm{d-SC}}$ as a function of temperature T, which becomes vanishingly small as approaching the superconducting T_c. The black and green arrows indicates T_c and PG temperature T^* respectively.

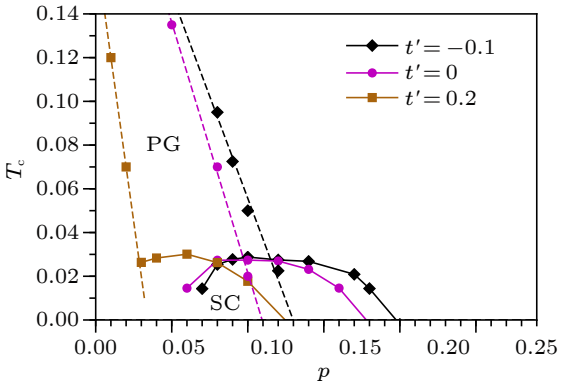

Fig. 3. Phase diagram of the doped Hubbard model for different nearest-neighbor hopping t'. Dashed lines and solid lines show respectively the pseudogap temperature T^* and superconducting T_c as functions of doping level p at $U = 7$. Here, the calculation of T^* is carried out always in the normal state.

at $U = 7$, $t' = 0$, and $p = 0.08$, $\chi_{\mathrm{d-SC}}$ increases slowly as temperature T decreases, and it starts to spike when T approaches the superconducting T_c that indicated by the black arrow. Here, T_c is determined by assuming a mean-field criticial exponent of $\chi_{\mathrm{d-SC}}$ [12] in vicinity of phase transition. In other words, T_c is obtained by extrapolating linearly data points of $\chi^{-1}_{\mathrm{d-SC}}$ at two lowest temperatures to $\chi^{-1}_{\mathrm{d-SC}} \to 0$. To summarize, in Fig. 2 we find that T_c and T^* at $U = 7$, $t' = 0$, $p = 0.08$ are respectively about $T_c \sim 0.027$ and $T^* \sim 0.07$.

Carrying out calculations on T_c and T^* for different dopings p and different t', we obtained a phase diagram shown in Fig. 3. Note that here $U = 7$ is larger than all the Mott transition critical values of U_c for the three different t' values,[70] namely for $t' = 0.2$ ($U_c = 6.7$), $t' = 0$ ($U_c = 6.2$), and $t' = -0.1$ ($U_c = 6.4$). Therefore, at half-filling, all these cases are in the Mott insulator phase.[35,71] At low temperatures ($T < T^*$), upon finite doping, the insulating states transit to PG phases. As shown by the dashed lines in Fig. 3, one can see that as t' becomes more positive, the PG phase shrinks to a smaller doping regime in parameter space. This phenomenon was systematically studied and documented before,[30] which can be explained by noting that here the positive case of $t' = 0.2$ has a large $|\epsilon^*_{\boldsymbol{k}}|$ for vHS at $\boldsymbol{k} = (0, \pi)/(\pi, 0)$ that inactivates electron scatterings related to vHS. We note that it was also observed in earlier DCA studies that strong particle–hole asymmetry occurs in PG state.[47] Namely, for negative t', the electron-doped case (which translates to hole-doping with positive t' via particle–hole transformation) is much less correlated than the hole-doped case, which agrees with our observation here.

Now we discuss how the changing of PG affects SC. The solid curves in Fig. 3 denote the dome-like SC phase for different t'. One can see that as the PG regime shrinks (t' becomes more positive), the SC dome as a whole moves to the underdoped side. Namely, in the small doping regime ($p < 0.08$), superconducting T_c increases as t' becomes more positive. We note that at small dopings, the opening of the PG strongly suppresses the low-energy spectral function in the antinodal direction.[26] This is clearly demonstrated in Figs. 4(a) and 4(b), which display respectivley the antinodal and nodal spectural function $A(\boldsymbol{k}, \omega)$ for three different t' at $p = 0.06$ and $= 0.05$. As can be seen at this doping, the case of $t' = -0.1$ has a vanishing $A(\boldsymbol{k}, \omega)$ around $\omega = 0$ at antinode since $T = 0.05$ is much smaller than its PG temperature $T^* \sim 0.15$. On the other hand, at $p = 0.06$ and $t' = -0.1$, superconducting T_c becomes vanishingly small (see Fig. 3). This is in contrast to the case of $t' = 0.2$ at the same doping, which does not have a finite T^* and pronounced peaks remain in both nodal and antinodal spectra. Here a finite superconducting $T_c \sim 0.03$ can be found for $t' = 0.2$ (Fig. 3). The comparison between the cases of $t' = -0.1$ and $t' = 0.2$ strongly suggests that at small dopings, PG competes with SC due to the depletion of the low-energy antinodal electrons.

In the phase fluctuation theory, PG is caused by strong phase fluctuations of pairing at small dopings. Hence, suppressing PG would meanwhile lead to the suppression of SC at a given doping. This is obviously not the case in our DCA study. As exemplified by the case of $t' = 0.2$ at small dopings ($p = 0.06$, for example), where SC can be greatly enhanced as long as PG is suppressed. Therefore, in our calculations, phase fluctuations should not play a significant role in the opening of PG.

At large dopings ($p > 0.08$), figure 3 displays that the superconducting T_c decreases as t' becomes more positive, contrasting the underdoped situation. To further understand this difference, we examine the case of $p = 0.15$ in Fig. 3 as an example. At this doping level, PG disappears in the $T \to 0$ limit for all three values of t'. Therefore, the t'-dependence of T_c, shown in Fig. 3, cannot be attributed directly to the changing of DOS at Fermi level or

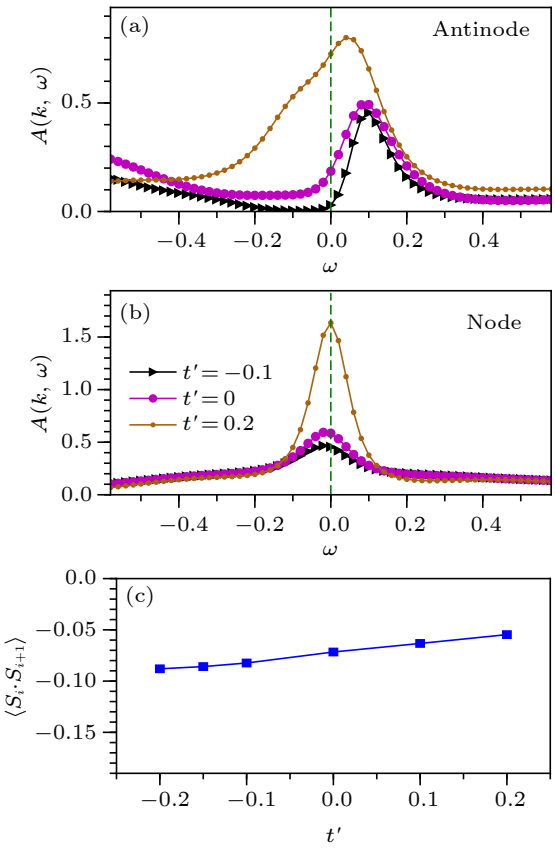

Fig. 4. Spectral functions and nearest-neighbor magnetic correlations of the doped Hubbard model. (a) Spectral function $A(\boldsymbol{k},\omega)$ at the antinode $\boldsymbol{k}=(0,\pi)$ for three different t' at $U=7$, $p=0.06$, and $T=0.05$. (b) Spectral function $A(\boldsymbol{k},\omega)$ at the node $\boldsymbol{k}=(\pi/2,\pi/2)$ with the same parameters as those for the antinodal case. (c) Magnetic correlations $\langle S_i\cdot S_{i+1}\rangle$ between a pair of nearest-neighboring sites in the DCA cluster as a function of t' in the overdoped regime, namely, at $U=7$, $p=0.15$, and $T=0.05$.

to the physics of PG. As a matter fact, as many-body effects weaken upon overdoping, electrons tend to restore Fermi liquid behavior that dominates in weak-coupling limits.[72] The crucial point in determining T_c then is no longer the amplitude of low-energy DOS but whether correlation effects suffice to drive SC instability in less correlated electrons. To understand this point, we note that cluster DMFT studies have revealed intrinsic connections between SC and AFM fluctuations.[57,58] In particular, a recent DCA study explicitly indicates that d-wave SC is rooted in short-ranged AFM fluctuations.[73] To gain insight into the evolution of AFM fluctuations in our study, we plot the spin correlator $\langle S_i\cdot S_{i+1}\rangle$ as a function of t' at $p=0.15$ in Fig. 4(c). Indeed, as one can see, the AFM correlation between two neighbouring sites $(i,i+1)$ diminishes as t' increases, signaling the decreasing in AFM fluctuations with increasing t'.

Hence, the decrease of both superconducting T_c and PG T^* with increasing t' in the overdoped regime can be explained: AFM correlations serve as both the "pairing glue" of SC and the driving force of PG. A more positive t' leads to weaker AFM correlations, resulting in both smaller SC T_c and weaker PG effects.

Above, we have studied the relation between SC and PG via changing the value of t'. To make our argument more concrete, below we tune PG in a different approach, which involves the introduction of an asymmetric next-next-nearest neighbour hopping t_3 term such that $\epsilon_{\boldsymbol{k}}=-2t[\cos(k_x)+\cos(k_y)]-4t_3\cos(2k_x)\cos(k_y)$ (see also Fig. 1). Unlike t', the t_3 term does not introduce any magnetic frustrations, allowing us to study the problem without the potential interference of frustration effects. Figure 5(a) illustrates $\epsilon_{\boldsymbol{k}}$ with $t_3=-0.3$ where vHS are shown pushed away from the Fermi level. Indeed, as shown in Fig. 5(b), $-\mathrm{Im}G(\boldsymbol{k},\omega=0)$ increases monotonically as T decreases for doping values of $p=0.02$ and 0.04 (solid lines), indicating the absence of PG at $t_3=-0.3$ in the temperature range accessible to our study for $p\gtrsim 0.02$. The immediate impact of closing PG on SC can be seen from Fig. 6(a), where $\chi^{-1}_{\mathrm{d-SC}}$ continuously decreases as $|t_3|$ increases at a given temperature T for $p=0.04$, suggesting a growing SC instability as PG is suppressed.

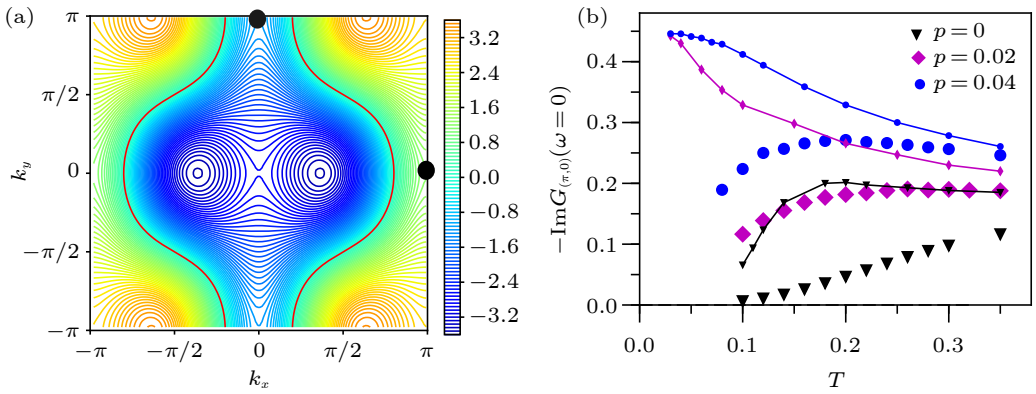

Fig. 5. Vanishing PG in the doped Hubbard model with t_3 hopping term at finite doping p. (a) Bare band dispersion $\epsilon_{\boldsymbol{k}}=-2t[\cos(k_x)+\cos(k_y)]-4t_3\cos(2k_x)\cos(k_y)$ at $t_3=-0.3$, where the red curve shows the Fermi surface at half-filling. (b) $-\mathrm{Im}G(\boldsymbol{k},\omega=0)$ as a function of temperature T at three different doping levels for the antinode at $t_3=-0.3$ (lines), which suggests no obvious PG behavior for finite doping $p\gtrsim 0.02$. The comparison result at $t_3=0.0$ (ordinary Hubbard model) is shown in dots, where PG behavior can be found as $-\mathrm{Im}G(\boldsymbol{k},\omega=0)$ decreases with lowering T. Here, $U=8.5$.

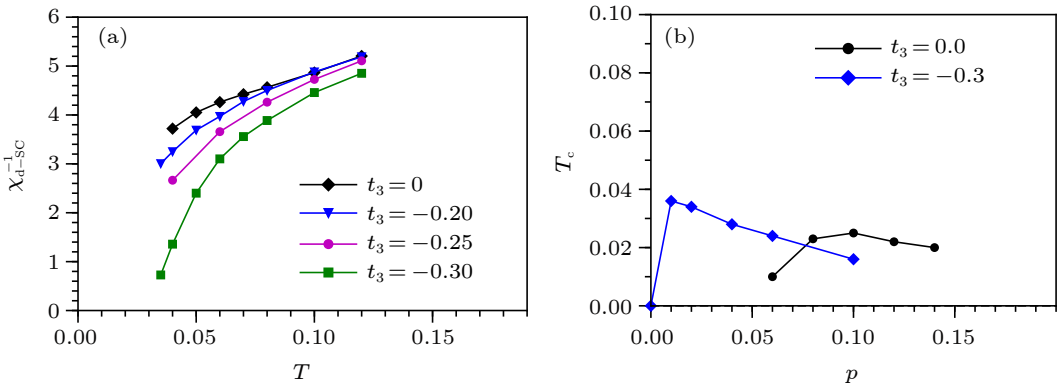

Fig. 6. d-wave SC in the doped Hubbard model with t_3 hopping term. (a) $\chi^{-1}_{\mathrm{d-SC}}$ as a function of temperature T for different values of t_3. (b) Superconducting phase diagram at $t_3 = 0$ and $t_3 = -0.3$. Here, $U = 8.5$.

Figure 6(b) compares the superconducting T_c as a function of doping p for $t_3 = -0.3$ and $t_3 = 0$, resembling the phase diagram shown in Fig. 3 for different values of t': as hopping parameters t' or t_3 are increased to suppress PG, the superconducting dome moves to the underdoped side in the phase diagram. This result emphasizes again that for both PG and SC, the competition between them occurs at small dopings while concurrent reliance on AFM correlations prevails at large dopings.

4. Discussion and Conclusion. A recent systematic 2×2 cluster DMFT study of the 2D Hubbard model has shown that in the intermediate U regime $[U \in (6.2t, 12t)]$, the superconducting transition temperature T_c increases with increasing U at large dopings, while exhibiting a slight decrease with increasing U at small dopings.[14] This trend is broadly consistent with our findings in the overdoped and underdoped regimes upon decreasing t'. However, in our study U remains unchanged, which minimizes potential side effects associated with modifications of Mott physics. In particular, in our t_3 model, the adjustment of PG strength does not introduce any magnetic frustrations.

To summarize, in this work we have systematically analyzed the interplay between PG and SC by tuning tight-binding hopping terms in the two-dimensional Hubbard model in the doped Mott insulator regime. We found that at underdoping, the closing of PG leads to an enhancement of SC, whereas in the overdoped regime, the suppression of PG is accompanied by a weakening of SC. We conclude that PG competes with SC in the underdoped regime, while on the overdoped side, PG and SC share the same physical origin: short-ranged antiferromagnetic correlations.

Acknowledgements. This work was supported by the National Natural Science Foundation of China (Grant Nos. 12274472, 12494594, 12494591, and 92165204), National Key Research and Development Program of China (Grant No. 2022YFA1402802), Guangdong Provincial Key Laboratory of Magnetoelectric Physics and Devices (Grant No. 2022B1212010008), Guangdong Fundamental Research Center for Magnetoelectric Physics (Grant No. 2024B0303390001), and Guangdong Provincial Quantum Science Strategic Initiative (Grant No. GDZX2401010).

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