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Emergent Superconductivity and Competing Charge Orders in Hole-Doped Square-Lattice t-J Model

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The square-lattice Hubbard and closely related t-J models are considered as basic paradigms for understanding strong correlation effects and unconventional superconductivity (SC). Recent large-scale density matrix renormalization group (DMRG) simulations on the extended t-J model have identified d-wave SC on the electron-doped side (with the next-nearest-neighbor hopping $t_2 > 0$) but a dominant charge density wave (CDW) order on the hole-doped side ($t_2 < 0$), which is inconsistent with the SC of hole-doped cuprate compounds. We re-examine the ground-state phase diagram of the extended t-J model by employing the state-of-the-art DMRG calculations with much enhanced bond dimensions, allowing more accurate determination of the ground state. On 6-leg cylinders, while different CDW phases are identified on the hole-doped side for the doping range $\delta = 1/16 - 1/8$, a SC phase emerges at a lower doping regime, with algebraically decaying pairing correlations and d-wave symmetry. On the wider 8-leg systems, the d-wave SC also emerges on the hole-doped side at the optimal $1/8$ doping, demonstrating the winning of SC over CDW by increasing the system width. Our results not only suggest a new path to SC in general t-J model through weakening the competing charge orders, but also provide a unified understanding on the SC of both hole- and electron-doped cuprate superconductors.

Introduction.— Understanding the mechanism of unconventional superconductivity (SC) in cuprates is a major challenge of condensed matter physics [1, 2]. Soon after the discovery of cuprate superconductors, the resonating valence bond (RVB) theory [3] was proposed to describe unconventional SC. The square Hubbard (with large U) and closely related t-J models are considered as the minimum models [1–8] to realize unconventional SC, which have attracted intense explorations [6–14]. However, it remains illusive if these models can describe the SC of cuprates. In the presence of strong correlations, analytical solutions are not controlled, while numerical studies in the relevant regime [15–48] are also extremely difficult in determining the ground state due to the extensive entanglement and low-energy excitations associated with competing spin and charge degrees of freedom. In recent years, numerical simulations have reached a possible consensus on the ground states of the pure large-U Hubbard and t-J models near the optimal doping, which is the stripe phase [15–28] characterized by a charge density wave (CDW) order coexisting with π-phase shifted antiferromagnetic domains, accompanied by exponentially decaying SC correlation.

On the other hand, the Fermi surface topology identified experimentally for cuprates indicates the importance of a small next-nearest-neighbor (NNN) hopping t_2 [49], with the sign of t_2 modeling the hole- ($t_2 < 0$) and electron-doped ($t_2 > 0$) cuprates, respectively [50]. Numerical studies on 4-leg Hubbard and t-J models find that introducing either positive or negative t_2 can lead to the coexistence of quasi-long-range SC and CDW orders [37–40]. To improve our understanding of how these orders evolve towards two dimensions (2D), recent density matrix renormalization group (DMRG) studies on 6- and 8-leg t-J model (with the nearest-neighbor (NN) hopping $t_1 > 0$) have identified a robust d-wave SC with suppressed CDW at $t_2 > 0$ [41–43], giving insights into the SC of electron-doped cuprates. For $t_2 < 0$, the stripe order appears to win over SC near the optimal doping [41, 44, 51], in sharp contrast with hole-doped cuprates [52]. However, while accurate DMRG simulations have been applied to 6-leg ladders [42, 43, 51], large-bond-dimension simulations are absent for 8-leg systems, which leaves the true nature of the ground state of the hole-doped t-J model an open question.

In this Letter, we study the phase diagram of the hole-doped t-J model and examine the interplay between SC and CDW through accurate DMRG calculations. By tuning the doping level δ and hopping ratio t_2/t_1 on 6-leg system, we identify the dominance of CDW phases at $\delta = 1/16 - 1/8$. However, the SC and weak CDW can coexist at lower doping region $\delta = 1/24 - 1/36$ [Fig. 1(a)], where pairing correlations show the d-wave symmetry and slow power-law decay with the exponent $K_{\rm sc} \lesssim 1$. Importantly, we observe dominant quasi-long-range SC order at the optimal doping ($\delta = 1/8$) on 8-leg cylinder [Fig. 1(b)]. On the electron-doped side ($t_2 > 0$), we confirm the existence of a robust uniform d-wave SC in agreement with previous studies [41, 44]. On the hole-doped side ($t_2 < 0$), we observe the remarkable emergence of SC with weak or vanishing CDW order in our large-bond-dimension simulation, with power-law decaying pairing correlations ($K_{\rm sc} < 2$). Furthermore, we confirm the robustness of these SC phases at different model parameters. Our work suggests that the t-J model may offer a unified framework for understanding the unconventional SC for both electron- and hole-doped cuprates.

Model and method.— The Hamiltonian of the extended t-J model is defined as

$$H = -\sum_{\{ij\},\sigma} t_{ij}(\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma} + \mathrm{H.c.}) + \sum_{\{ij\}} J_{ij}(\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{1}{4}\hat{n}_i\hat{n}_j),$$

where $\hat{c}^\dagger_{i\sigma}$ ($\hat{c}_{i\sigma}$) is the creation (annihilation) operator of the electron with spin σ ($\sigma = \pm 1/2$) on site $i = (x_i, y_i)$, $\hat{\mathbf{S}}_i$ is the spin-1/2 operator, and $\hat{n}_i = \sum_\sigma \hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$ is the electron number operator. The Hilbert space for each site is constrained by no double occupancy. We consider the NN and NNN hoppings (t_1 and t_2) and spin interactions (J_1 and J_2). We choose $J_1 = 1.0$ and set $t_1/J_1 = 3.0$ to make a connection to the corresponding Hubbard model with $U/t = 12$ [53]. The length and width of the lattice are denoted as L_x and L_y, giving total site number $N = L_x \times L_y$. The doping ratio δ is defined as $\delta = N_h/N$ (N_h is the number of doped holes). We focus on the doping regime $1/36 \leq \delta \leq 1/8$ on 6-leg cylinders and $\delta = 1/8$ on 8-leg cylinders, and tune t_2/t_1 with fixed relation $(t_2/t_1)^2 = J_2/J_1$ [42, 43]. We also examine the SC phases in the t_1-t_2-J_1 model with $t_1/J_1 = 2.5, 3.0$, as shown in Fig. 5.

We solve the ground state of the system by DMRG [54] calculations with $\mathrm{SU}(2) \otimes \mathrm{U}(1)$ symmetry implemented [55]. We study cylindrical systems with open and periodic boundary conditions along the axial (x) and circumferential (y) directions respectively, and keep the bond dimensions of $\mathrm{SU}(2)$ multiplets up to $D = 15000$ for 6-leg and 28000 for 8-leg systems, equivalent to about 45000 and 84000 U(1) states respectively, which ensure accurate results with the truncation error less than 1.2×10^{-6} for 6-leg and 2.5×10^{-5} for 8-leg systems (see Supplemental Materials (SM) for more details [56]).

Quantum phase diagram.— Our results are summarised in the phase diagram Fig. 1 as a function of hopping ratio t_2/t_1 and doping level δ. For 6-leg system with $-0.22 \leq t_2/t_1 \leq 0$ [Fig. 1(a)], we identify two charge ordered phases: a stripe phase with wavevector $Q = (3\pi\delta, 0)$ and a $\mathrm{W_y3}$ CDW phase with $Q = (6\pi\delta, 2\pi/3)$ (see SM for the results of the $\mathrm{W_y3}$ state [56]), which shares a similar charge density distribution with the W3 phase found in the t_1-t_2-J_1 model [41]. Strikingly, below $\delta = 1/18$, we find a quasi-long-range SC order ($K_{\mathrm{sc}} \lesssim 1$) coexisting with a weak CDW.

For the 8-leg system with $-0.2 \leq t_2/t_1 \leq 0.3$ at $\delta = 1/8$ [Fig. 1(b)], a robust d-wave SC order emerges for $t_2/t_1 \gtrsim 0.12$ with a uniform charge density distribution, which is similar to the uniform SC phase found on 6-leg cylinder [43]. This uniform SC phase may extend to larger t_2/t_1 regime [42, 57] and persist in 2D limit. Remarkably, the quasi-long-range SC order is also observed on the hole-doped side for $t_2/t_1 \lesssim -0.05$, which exhibits a very weak or vanishing charge order. The SC power exponent $K_{\mathrm{sc}} < 2$ indicates a divergent SC susceptibility at zero-temperature limit. This result contradicts a previous work studying a similar t_1-t_2-J_1 model that claims the absence of SC at $t_2 < 0$ [41], which may be attributed to the existence of competing charge ordered states in low-energy regime. In our calculation, extremely large bond dimensions are used for reaching convergence and identifying

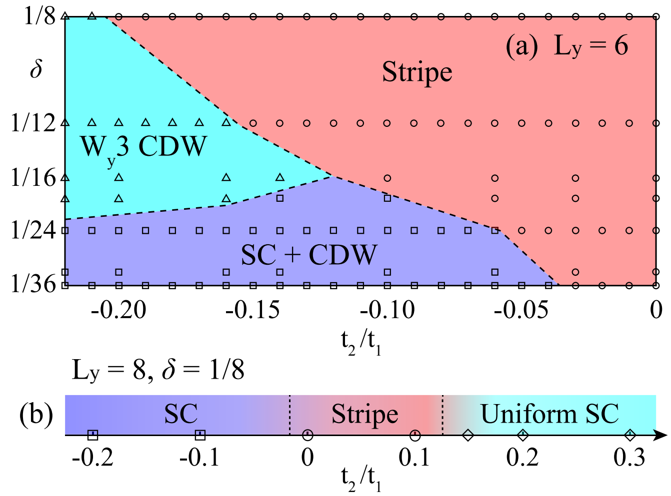

FIG. 1. Quantum phase diagrams of the t_1-t_2-J_1-J_2 model at different system widths. (a) $L_y = 6$ cylinder with $-0.22 \leq t_2/t_1 \leq 0$ and $1/36 \leq \delta \leq 1/8$. We identify a stripe phase, a $\mathrm{W_y3}$ CDW phase, and a SC + CDW phase with coexisted d-wave SC and a weak CDW. (b) $L_y = 8$ cylinder with $-0.2 \leq t_2/t_1 \leq 0.3$ at $\delta = 1/8$. We identify two SC phases and a stripe phase. The hole-doped SC phase at $t_2/t_1 < 0$ has a weak or vanishing CDW order. Pairing correlations in the $L_y = 8$ stripe phase show a slow increase with bond dimension, but its tendency to develop a quasi-long-range SC order cannot be pinned down within our currently accessible bond dimensions. The symbols denote the parameter points that we have calculated. The same SC phases on both 6- and 8-leg systems are obtained in our model with $(t_2/t_1)^2 = J_2/J_1$ and the t_1-t_2-J_1 model with $t_1/J_1 = 2.5$ and 3.0 (see Fig. 5 and SM [56]).

the emergence of SC. For both 6- and 8-leg systems at hole doping, SC emerges through suppressing charge order.

SC pairing correlation.— We examine SC by the dominant spin-singlet pairing correlations $P_{\alpha,\beta}(\mathbf{r}) = \langle \hat{\Delta}^\dagger_\alpha(\mathbf{r}_0)\hat{\Delta}_\beta(\mathbf{r}_0 + \mathbf{r})\rangle$, where the pairing operator is defined as $\hat{\Delta}_\alpha(\mathbf{r}) = (\hat{c}_{\mathbf{r}\uparrow}\hat{c}_{\mathbf{r}+\mathbf{e}_\alpha\downarrow} - \hat{c}_{\mathbf{r}\downarrow}\hat{c}_{\mathbf{r}+\mathbf{e}_\alpha\uparrow})/\sqrt{2}$ and $\mathbf{e}_{\alpha=x,y}$ denote the unit vectors along the x and y directions. Since the wave function in DMRG calculation is represented as a matrix product state, correlation functions usually decay exponentially at finite bond dimensions [59]. We make the bond dimension scaling to demonstrate the true nature of correlations at $D \to \infty$ (see Fig. 2 and SM [56]).

We first examine pairing correlations on 6-leg systems. In the stripe phase represented by $t_2/t_1 = -0.06$ and $\delta = 1/12$ [Fig. 2(a)], the pairing correlation $P_{yy}(r)$ follows an exponential decay $P_{yy}(r) \sim \exp(-r/\xi_{\mathrm{sc}})$ with $\xi_{\mathrm{sc}} \simeq 3.69$ after the extrapolation to $D \to \infty$. In the SC + CDW phase, as shown in Fig. 2(b) for $t_2/t_1 = -0.08$, $\delta = 1/24$, $P_{yy}(r)$ increases drastically compared with that in the stripe phase and exhibits an algebraic decay $P_{yy}(r) \sim r^{-K_{\mathrm{sc}}}$ with $K_{\mathrm{sc}} \simeq 0.82$, characterizing a quasi-long-range SC order. We also confirm that other pairing correlations satisfy $P_{yy}(r) \simeq -P_{yx}(r) \simeq P_{xx}(r)$, in accordance with the d-wave symmetry illustrated in the inset of Fig. 2(b) rather than the plaquette d-wave symmetry found in the 4-leg Hubbard model at $t_2 < 0$ [39].

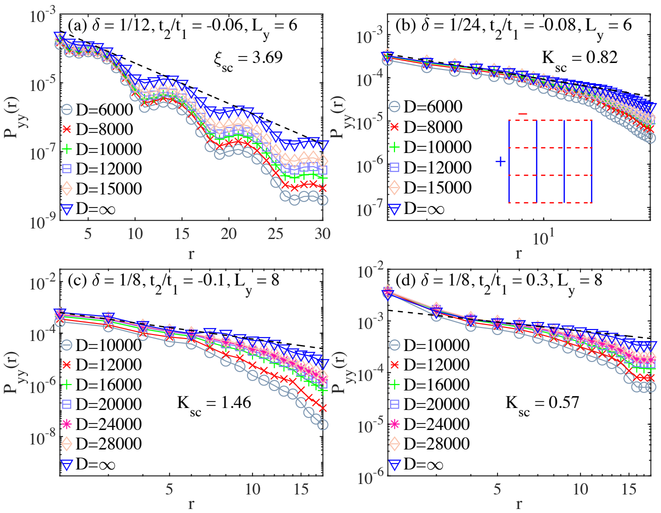

FIG. 2. SC pairing correlation functions. (a) Semi-logarithmic plot of the pairing correlations $P_{yy}(r)$ at different bond dimensions in the stripe phase at $L_y = 6$. The correlation length $\xi_{\rm sc}$ is obtained by exponential fitting. (b) Double-logarithmic plot of $P_{yy}(r)$ in the SC + CDW phase on 6-leg cylinder. The dash line represents the algebraic fitting of the data extrapolated to $D \to \infty$. The power exponent $K_{\rm sc} \simeq 0.82$ characterizes a quasi-long-range SC order. The inset shows the d-wave pairing symmetry. (c) and (d) are similar plots in the hole-doped SC ($t_2 < 0$) and electron-doped uniform d-wave SC phases ($t_2 > 0$) on 8-leg cylinders, both with $K_{\rm sc} < 2$ indicating the divergence of SC susceptibilities [58].

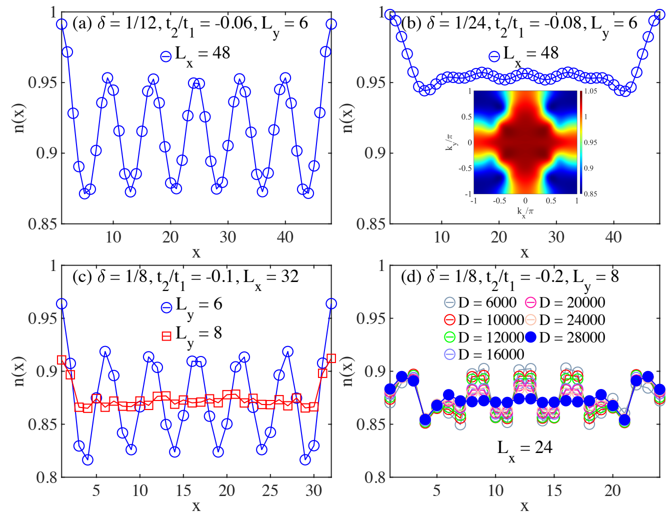

FIG. 3. Charge density profiles $n(x)$ in the (a) stripe phase and (b) SC + CDW phase on 6-leg cylinders with $L_x = 48$. The inset of (b) shows the corresponding electron momentum distribution $n(\mathbf{k})$. (c) Comparing $n(x)$ in the SC phase on $L_y = 8$ and stripe phase on $L_y = 6$ at $t_2/t_1 = -0.1$ and $\delta = 1/8$, obtained with $D = 24000$ and 15000, respectively. (d) $n(x)$ in the SC phase of 8-leg cylinder at $t_2/t_1 = -0.2$, $\delta = 1/8$ obtained by different bond dimensions.

To further investigate whether SC can emerge on wider systems, we extensively simulate the 8-leg cylinder at $\delta = 1/8$, which is more relevant to the experiments of cuprates. For $t_2/t_1 = -0.1$ [Fig. 2(c)], the pairing correlations at long distance grow rapidly with bond dimension. The extrapolated results at $D \to \infty$ can be fitted by a power-law decay with $K_{\rm sc} \simeq 1.46$, demonstrating an emergent quasi-long-range SC order. In the uniform SC phase at $t_2 > 0$ [Fig. 2(d)], pairing correlation exhibits a slow algebraic decay with a small exponent $K_{\rm sc} \simeq 0.57$ characterizing a robust SC phase. We have also checked the triplet pairing correlations in both SC phases on 8-leg systems. While the p-wave symmetry can appear at $t_2 > 0$, the corresponding pairing correlations always decay very fast, indicating the absence of triplet SC order [56].

Charge density distribution.— Except in the $\mathrm{W_y}3$ phase, the converged charge density distributions are uniform along the y direction, and we show the averaged charge density for each column as $n(x) = \sum_{y=1}^{L_y} \langle \hat{n}_{x,y} \rangle / L_y$ in Fig. 3. For 6-leg systems, we find the CDW wavelength $\lambda \simeq 4/(L_y\delta)$ in the stripe phase [Fig. 3(a)], corresponding to four holes on average for each CDW unit. In the SC + CDW phase, $\lambda \simeq 2/(L_y\delta)$ indicates two holes per CDW unit [Fig. 3(b)]. Significantly, the oscillation amplitude of $n(x)$ (i.e. charge order) is much weaker than that in the stripe phase shown in Fig. 3(a). The momentum distribution $n(\mathbf{k}) = (1/N)\sum_{i,j,\sigma} \langle \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} \rangle e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)}$ in the SC + CDW phase [the inset of Fig. 3(b)] exhibits the unenclosed Fermi surface topology around $\mathbf{k} = (\pm\pi, 0)$ and $(0, \pm\pi)$ in consistent with that observed in the ARPES measurement of hole-doped cuprates [49, 60, 61], which is distinctly different from the topology for electron doping at $t_2 > 0$ [41, 43], where the Fermi surface forms a closed pocket around $\mathbf{k} = (0, 0)$.

A natural question is how the charge order evolves towards 2D limit. Crucially, we find that the strong CDW in the stripe phase for $L_y = 6$ can be significantly suppressed on wider system, as shown in Fig. 3(c). The quite weak charge density oscillation for $L_y = 8$ is similar to that of the SC + CDW phase on 6-leg cylinders [Fig. 3(b)], which is accompanied with the emergent quasi-long-range SC order [Fig. 2(c)]. In Fig. 3(d) for $t_2/t_1 = -0.2$, one can find the charge distribution is gradually transformed from a CDW-like pattern to a nearly uniform one with growing bond dimension, demonstrating an extremely weak or vanishing charge order in the hole-doped SC phase and the importance of a large bond dimension for reaching the true ground state (see SM [56]).

Correlation functions.— In Fig. 4, we further compare correlation functions in each phase. While all the correlations are presented in the semi-logarithmic scale, the exponents K and correlation lengths ξ are obtained by power-law and exponential fittings, respectively [56]. For the stripe phase on 6-leg cylinders [Fig. 4(a)], while the single-particle Green's function $G(r) = \langle \sum_\sigma \hat{c}^\dagger_{x,y,\sigma} \hat{c}_{x+r,y,\sigma} \rangle$ and pairing correlation appear to decay exponentially [56], the intertwined density correlation $D(r) = \langle \hat{n}_{x,y}\hat{n}_{x+r,y} \rangle - \langle \hat{n}_{x,y} \rangle \langle \hat{n}_{x+r,y} \rangle$ and spin correlation $F(r) = \langle \mathbf{S}_{x,y} \cdot \mathbf{S}_{x+r,y} \rangle$ are more dominant at long distance. In contrast, in the SC + CDW [Fig. 4(b)], hole-doped SC [Fig. 4(c)], and uniform d-wave SC phases [Fig. 4(d)], pairing correlations are dominant over other cor-

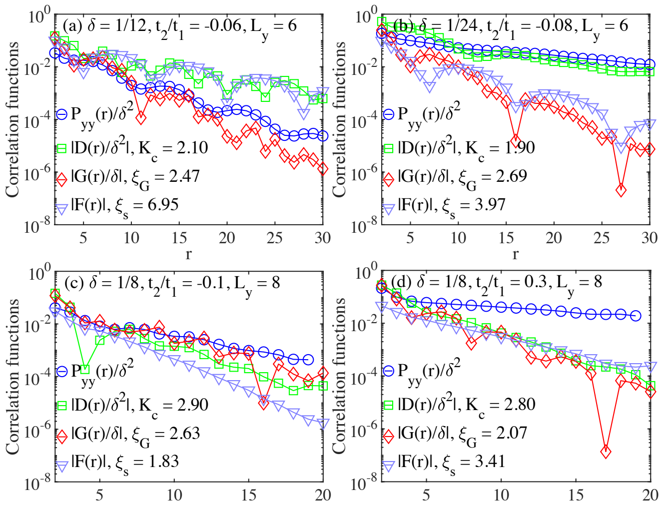

FIG. 4. Correlations in different phases. The data are those extrapolated to $D \to \infty$. Comparison of pairing correlation $P_{yy}(r)$, charge density correlation $D(r)$, single-particle Green's function $G(r)$, and spin correlation $F(r)$ for (a) stripe phase at $L_y = 6$, (b) SC + CDW phase at $L_y = 6$, (c) hole-doped SC phase at $L_y = 8, \delta = 1/8$, and (d) uniform d-wave SC phase at $L_y = 8, \delta = 1/8$. The correlations are rescaled by δ to make a direct comparison. The power exponent K and correlation length ξ are obtained by algebraic and exponential fittings, respectively (see the details in SM [56]).

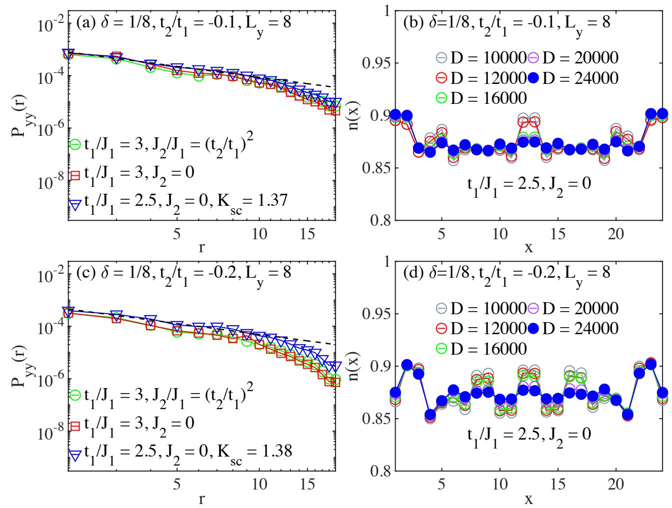

FIG. 5. Robust SC states at different model parameters on the 8-leg cylinders at $\delta = 1/8$. (a) Pairing correlations $P_{yy}(r)$ for $t_1/J_1 = 3$, $J_2/J_1 = (t_2/t_1)^2$; $t_1/J_1 = 3$, $J_2 = 0$; and $t_1/J_1 = 2.5$, $J_2 = 0$. We fix $t_2/t_1 = -0.1$. The data are those extrapolated to $D \to \infty$. The algebraic fitting of the results at $t_1/J_1 = 2.5$, $J_2 = 0$ gives $K_{\rm sc} = 1.37$. (b) Charge density distributions $n(x)$ obtained under different bond dimensions for $t_2/t_1 = -0.1$, $t_1/J_1 = 2.5$, $J_2 = 0$. (c) and (d) are similar plots for $t_2/t_1 = -0.2$.

relations at long distance. Furthermore, on 8-leg systems, $G(r)$ and $F(r)$ show exponential decay with short correlation lengths at $t_2/t_1 = 0.3$, which is consistent with the DMRG results of the same model at $t_2/t_1 \approx 0.5$ corresponding to doping either the J_1-J_2 spin liquid or valence bond solid [57].

Robust SC phases at different model parameters.— In the study of extended t-J models, the t_1-t_2-J_1 model with $t_1/J_1 = 2.5$ has also been widely considered [19, 41, 62]. To confirm the discovered SC phases at hole doping for different model parameters, we further examine the t_1-t_2-J_1 model with $t_1/J_1 = 2.5$ and 3.0 ($J_2 = 0$). By comparing the pairing correlation and charge density distribution on 6- and 8-leg systems (see Fig. 5 and SM [56]), we confirm that the identified SC phases are robust against both a small change of t_1/J_1 and the absence of J_2 interaction.

Summary and Discussion.— We have presented a global picture for both the electron-doped ($t_2 > 0$) and hole-doped ($t_2 < 0$) t-J models by DMRG calculations. While we confirm the d-wave SC for electron doping [41] on wider cylinders, we find that the ground states of the hole-doped case can also be superconducting, at both the low doping regime $\delta = 1/36 - 1/24$ for $L_y = 6$ and optimal doping $\delta = 1/8$ for $L_y = 8$ with d-wave symmetry. For $\delta = 1/8$ at hole doping, SC turns out to be favored on wider system, where the enhanced phase coherence of paired holes [51] helps to destabilize CDW and thus allows superconductivity to develop.

Despite the strong competition between stripe and SC orders under hole doping [41], the SC phases we obtain on both 6- and 8-leg systems are stable against a small tuning of t_1/J_1, and therefore are established as a common phase for different extended t-J models. Thus, we conclude that the single-band t-J model has some generic features including the uniform SC at electron doping, and the dominant SC with near vanishing or coexisting CDW order at hole doping, which may provide a basic description of the cuprate superconductors.

At last we discuss some open questions. For the hole doped t-J model, the charge order with suppressed SC is commonly observed as the ground states of narrower systems ($L_y = 6$) with hole binding [41, 51], which may have some connection with the pseudogap physics [63, 64] of cuprate systems. The d-wave SC on the electron-doped side turns out to be robust on wider cylinders, however the nature of its magnetic order is still under debate [41, 43]. While our analyses of spin correlation lengths suggest a magnetic order at small doping $\delta \simeq 1/24$, we find the magnetic order is suppressed for $\delta = 1/8$ as the ratio of $\xi_{\rm s}/L_y$ reduces with increased L_y [56]. For the stripe phase at $L_y = 8$ (see SM [56]), the CDW order appears to be stable with improved bond dimension, but the pairing correlations keep growing slowly, showing a possible tendency to develop a weak quasi-long-range SC. We believe our work will stimulate more future studies to address these challenging issues.

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Note added.— At the final stage of preparing this work, we have become aware of an independent and related work focusing on the larger positive $t_2/t_1 \simeq 0.7$ regime of the same t-J model on 8-leg cylinder [57], as well as two other works focusing on the Hubbard model [65, 66]. The results in Ref. [57] are consistent with our findings at $t_2/t_1 = 0.3$.

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