

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 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 density matrix renormalization group calculations with much enhanced bond dimensions, allowing more accurate determination of the ground state. On six-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 eight-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.

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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 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 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 four-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 toward two dimensions (2D), recent density matrix renormalization group (DMRG) studies on six- and eight-leg t - J model (with the nearest-neighbor 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

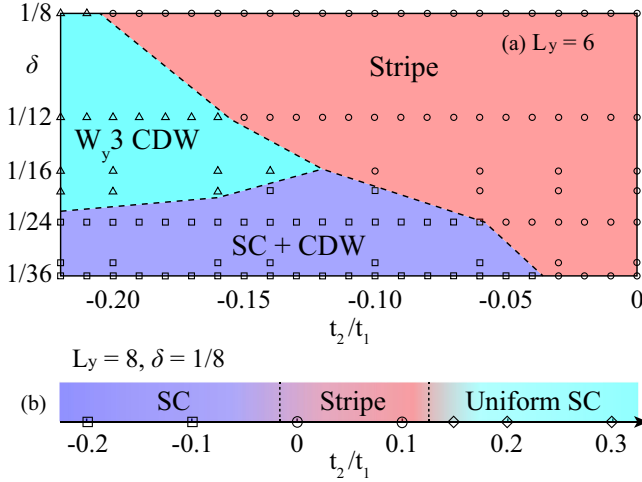


FIG. 1. Quantum phase diagrams of the t_1 - t_2 - J_1 - J_2 model at different system widths. (a) $L_y = 6$ cylinder with $-0.22 \leq t_2/t_1 \leq 0$ and $1/36 \leq \delta \leq 1/8$. We identify a stripe phase, a W_3 CDW phase, and a SC + CDW phase with coexisting d -wave SC and a weak CDW. (b) $L_y = 8$ 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 six- and eight-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 [53]).

simulations have been applied to six-leg ladders [42,43,51], large-bond-dimension simulations are absent for eight-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 six-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 $K_{sc} \lesssim 1$. Importantly, we observe dominant quasi-long-range SC order at the optimal doping ($\delta = 1/8$) on eight-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 ($K_{sc} < 2$). 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

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

where $\hat{c}_{i\sigma}^\dagger$ ($\hat{c}_{i\sigma}$) 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 $\hat{n}_i = \sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ is the electron number operator. The Hilbert space for each site is constrained by no double occupancy. We consider the nearest-neighbor and next-nearest-neighbor 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 $U/t = 12$ [54]. 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 six-leg cylinders and $\delta = 1/8$ on eight-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 [55] calculations with $SU(2) \otimes U(1)$ symmetry implemented [56]. 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 $SU(2)$ multiplets up to $D = 15000$ for six-leg and 28000 for eight-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 six-leg and 2.5×10^{-5} for eight-leg systems [see Supplemental Material (SM) for more details [53]].

Quantum phase diagram.—Our results are summarized in the phase diagram Fig. 1 as a function of hopping ratio t_2/t_1 and doping level δ . For six-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 wave vector $\mathbf{Q} = (3\pi\delta, 0)$ and a W_3 CDW phase with $\mathbf{Q} = (6\pi\delta, 2\pi/3)$ (see SM for the results of the W_3 state [53]), which shares a similar charge density distribution with the W_3 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 ($K_{sc} \lesssim 1$) coexisting with a weak CDW.

For the eight-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 six-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 $K_{\text{sc}} < 2$ 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 the emergence of SC. For both six- and eight-leg systems at hole doping, SC emerges through suppressing charge order.

SC pairing correlation.—We examine SC by the dominant spin-singlet pairing correlations $P_{\alpha,\beta}(\mathbf{r}) = \langle \hat{\Delta}_{\alpha}^{\dagger}(\mathbf{r}_0) \hat{\Delta}_{\beta}(\mathbf{r}_0 + \mathbf{r}) \rangle$, 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 [58]. We make the bond dimension scaling to demonstrate the true nature of correlations at $D \rightarrow \infty$ (see Fig. 2 and SM [53]).

We first examine pairing correlations on six-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 $P_{yy}(r) \sim \exp(-r/\xi_{\text{sc}})$ with $\xi_{\text{sc}} \simeq 3.69$ after the extrapolation to $D \rightarrow \infty$. In the SC + CDW phase,

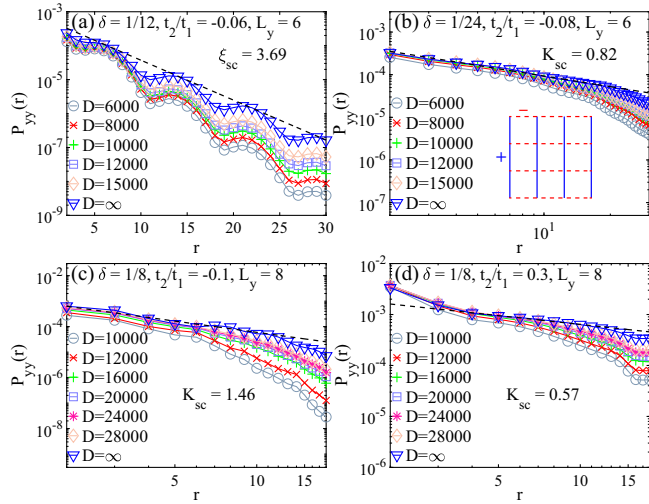


FIG. 2. SC pairing correlation functions. (a) Semilogarithmic plot of the pairing correlations $P_{yy}(r)$ at different bond dimensions in the stripe phase at $L_y = 6$. The correlation length ξ_{sc} is obtained by exponential fitting. (b) Double-logarithmic plot of $P_{yy}(r)$ in the SC + CDW phase on six-leg cylinder. The dash line represents the algebraic fitting of the data extrapolated to $D \rightarrow \infty$. The power exponent $K_{\text{sc}} \simeq 0.82$ 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 eight-leg cylinders, both with $K_{\text{sc}} < 2$ indicating the divergence of SC susceptibilities [59].

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 $P_{yy}(r) \sim r^{-K_{\text{sc}}}$ with $K_{\text{sc}} \simeq 0.82$, 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 four-leg Hubbard model at $t_2 < 0$ [39].

To further investigate whether SC can emerge on wider systems, we extensively simulate the eight-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 $D \rightarrow \infty$ can be fitted by a power-law decay with $K_{\text{sc}} \simeq 1.46$, 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 $K_{\text{sc}} \simeq 0.57$ characterizing a robust SC phase. We have also checked the triplet pairing correlations in both SC phases on eight-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 [53].

Charge density distribution.—Except in the W_y3 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 six-leg systems, we find the CDW wavelength $\lambda \simeq 4/(L_y \delta)$ in the stripe phase [Fig. 3(a)], corresponding to

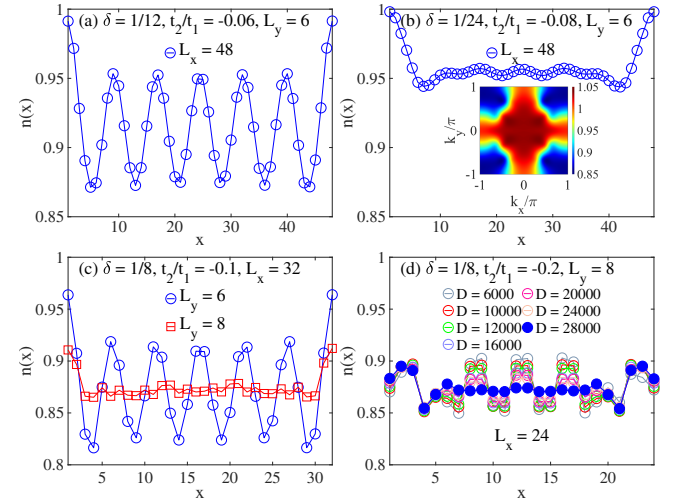


FIG. 3. Charge density profiles $n(x)$ in the (a) stripe phase and (b) SC + CDW phase on six-leg cylinders with $L_x = 48$. The inset of (b) shows the corresponding electron momentum distribution $n(\mathbf{k})$. (c) Comparing $n(x)$ in the SC phase on $L_y = 8$ and stripe phase on $L_y = 6$ at $t_2/t_1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

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 $n(\mathbf{k}) = (1/N) \sum_{i,j,\sigma} \langle \hat{c}_{i,\sigma}^\dagger \hat{c}_{j,\sigma} \rangle e^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$ 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 agreement 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 toward 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 six-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 [53]).

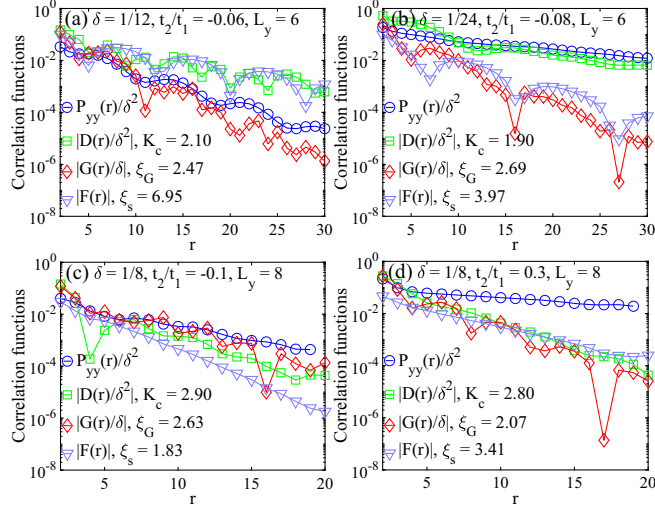


FIG. 4. Correlations in different phases. The data are those extrapolated to $D \rightarrow \infty$. Comparison of pairing correlation $P_{yy}(r)$, charge density correlation $D(r)$, single-particle Green's function $G(r)$, and spin correlation $F(r)$ for (a) stripe phase at $L_y = 6$, (b) SC + CDW phase 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 [53]).

Correlation functions.—In Fig. 4, we further compare correlation functions in each phase. While all the correlations are presented in the semilogarithmic scale, the exponents K and correlation lengths ξ are obtained by power-law and exponential fittings, respectively [53]. For the stripe phase on six-leg cylinders [Fig. 4(a)], while the single-particle Green's function $G(r) = \langle \sum_{\sigma} \hat{c}_{x,y,\sigma}^\dagger \hat{c}_{x+r,y,\sigma} \rangle$ and pairing correlation appear to decay exponentially [53], 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 $F(r) = \langle \hat{\mathbf{S}}_{x,y} \cdot \hat{\mathbf{S}}_{x+r,y} \rangle$ 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 correlations at long distance. Furthermore, on eight-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 six- and eight-leg systems (see Fig. 5 and SM [53]), 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.

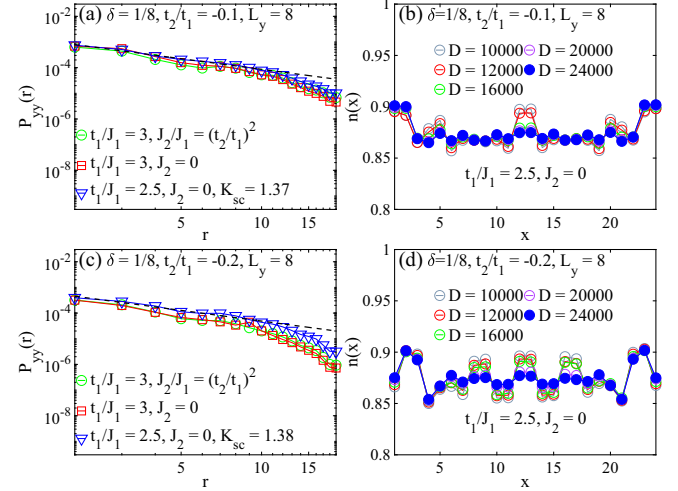


FIG. 5. Robust SC states at different model parameters on the eight-leg cylinders at $\delta = 1/8$. (a) Pairing correlations $P_{yy}(r)$ for $t_1/J_1 = 3, J_2/J_1 = (t_2/t_1)^2$; $t_1/J_1 = 3, J_2 = 0$; and $t_1/J_1 = 2.5, J_2 = 0$. We fix $t_2/t_1 = -0.1$. The data are those extrapolated to $D \rightarrow \infty$. The algebraic fitting of the results at $t_1/J_1 = 2.5, J_2 = 0$ gives $K_{sc} = 1.37$. (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 $t_2/t_1 = -0.2$.

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 six- and eight-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.

Finally, 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 ξ_s/L_y reduces with increased L_y [53]. For the stripe phase at $L_y = 8$ (see SM [53]), 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.

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 eight-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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