Doping-driven Antiferromagnetic Insulator - Superconductor Transition: a Quantum Monte-Carlo Study

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How superconductivity emerges in the vicinity of an antiferromagnetic insulating state is a longstanding issue of strong correlation physics. We study the transition from an antiferromagnetic insulator to a superconductor by hole-doping based on a bilayer generalization of a Hubbard-like model. The projector quantum Monte-Carlo simulations are employed, which are sign-problem-free both at and away from half-filling. An anisotropic Ising antiferromagnetic Mott insulating phase occurs at half-filling, which is weakened by hole-doping. Below a critical doping value, antiferromagnetism coexists with singlet superconductivity, which is a pairing across each rung with an extended $s$-wave symmetry. As further increasing doping, the antiferromagnetic order vanishes, leaving only a superconducting phase. These results provide important information on how superconductivity appears upon doping the parent Mott-insulating state.

Introduction The study on strongly correlated electron systems is a central topic of condensed matter physics for exploring novel states of matter. In the vicinity of the antiferromagnetic (AF) insulating phase, unconventional superconducting (SC) states appear by doping, or, applying pressure to systems of heavy-fermion materials [1], high $T_c$ cuprates [2], iron pnictides [3], and organic superconductors [4]. In the past several decades, the doped Mott insulators and the consequential competitions among antiferromagnetism, superconductivity, and charge orderings have been extensively studied with significant efforts from various different perspectives [5–13].

How superconductivity arises by doping Mott-insulators is an outstanding problem of condensed matter physics. Due to its non-perturbative nature, sufficiently accurate numerical methods are essential to resolve small energy differences among competing orders [11–14]. Nevertheless, exact diagonalizations are limited to small system sizes due to the exponential growth of the many-body Hilbert space [15]. The density-matrix-renormalization group [16] and tensor-network methods [17] have been successfully applied to two-dimensional (2D) spin models [18] and quasi-one-dimensional fermionic ladder systems [19, 20]. However, their applications to 2D fermionic systems are just beginning [13, 21]. The results of the variational Monte Carlo method depend on the input trial wavefunctions [22]. The auxiliary field quantum Monte-Carlo (QMC) method [23, 24] is unbiased, but it suffers from the notorious sign-problem when doping away from half-filling [25]. Once the sign-problem occurs, the numeric errors grow exponentially as enlarging the system size and lowering the temperature, which usually plagues simulations, corresponding to a regime of maximal numerical difficulty in computational science for decades [11].

Recently, a progress has appeared to employ the auxiliary field QMC method to study a spin-fermion model [26], which describes the low energy hot-spot fermionic excitations and yields the $d$-wave like pairing symmetry [27]. This model is designed to be sign-problem free based on the previously proved Kramers-invariant decomposition by one of the authors and Zhang [28]. In such a decomposition, the Hubbard-Stratonovich (HS) transformation to fermion interactions is formulated in a Kramers invariant way, i.e., the fermion matrix in any HS field configuration satisfying the Kramers symmetry. Its determinant, working as the statistical weight, is a product of complex-conjugate pairs, and thus positive-definite. Developments along this line mainly follow the hot-spot dominated pairing mechanism [29–31]. However, these models begin with a metallic normal state far away from the Mott physics. For microscopic models such as the Hubbard-like ones exhibiting Mott-physics at half-filling, QMC simulations contribute significantly to the study of pairing mechanisms [32, 33], nevertheless, they often suffer from the notorious sign-problem upon doping. It is desired to simulate the emergence of superconductivity by doping Mott insulators through QMC simulations in a sign-problem free way.

In this article, we investigate the competition between antiferromagnetism and superconductivity by doping the parent 2D Mott-insulators. We employ the Scalapino-Zhang-Hanke (SZH) model by generalizing it to a bilayer version. It is a Hubbard-like model augmented by charge and spin-exchange interactions across each rung consisting of two sites. In a wide range of interaction parameters, it satisfies the criterion of the Kramers invariant decomposition for QMC simulations [28], hence, is sign-problem free at arbitrary electron fillings. This enables the possibility to study the transition from the AF insulating state to the SC state in a numerically exact manner, that is, any accuracy can be achieved within a polynomial time. At half-filling, the ground
state is either an AF insulator in the case with the Ising anisotropy, or, a rung-singlet Mott phase with the SU(2) invariance. Upon hole doping, the AF ordering is weakened and finally suppressed when the doping level \( x > x_c \approx 0.11 \). Meanwhile, the extended s-wave SC order grows up away from half-filling and coexists with the AF order at \( 0 < x < x_c \).

Model and QMC Simulations. The SZH model [34], originally defined for a two-leg ladder, is an extended Hubbard model for studying competing orders in strongly correlated systems. We further generalize it to a bilayer square lattice as sketched in Fig. 1. The Hamiltonian reads,

\[
H = -t_\parallel \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + d_{i\sigma}^\dagger d_{j\sigma}) + H.c.
\]

\[
- t_\perp \sum_{i\sigma} (c_{i\sigma}^\dagger d_{i\sigma} + H.c. - \mu \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i\sigma} + d_{i\sigma}^\dagger d_{i\sigma})
\]

\[
+ \frac{J_\perp}{2} \sum_i (S_{i\uparrow}^x S_{i\downarrow}^x + h.c.) + J_z \sum_i S_{i\uparrow}^z S_{i\downarrow}^z
\]

\[
+ U \sum_i [(n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) + (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})]
\]

\[
+ V \sum_i (n_{i\uparrow} - 1)(n_{i\downarrow} - 1),
\]

where the electron annihilation operators in the upper and lower layers are denoted as \( c \) and \( d \), respectively. The Hamiltonian Eq. 1 consists of the intra- and inter-layer nearest-neighbor hopping terms of \( t_\parallel \) and \( t_\perp \), respectively, and \( t_\parallel \) is the energy unit set as 1 throughout this article. The interaction terms include the onsite Hubbard interaction \( U \), and the interactions between two sites along each vertical rung: \( V \) is the charge channel interaction; \( J_\perp \) and \( J_z \) are the transverse and longitudinal spin exchanges, respectively. The in-plane AF correlation is intermediated through the 2nd order perturbation theory. For the isotropic case with \( J_\perp = J_z \), the system enters the rung singlet phase at half-filling when the super-exchange interaction across each rung is larger than the in-plane one which is perturbatively small. We first consider the case with the Ising anisotropy by setting \( J_z > J_\perp \) which stabilizes the AF long-range-order along the \( z \)-direction at half-filling. The AF parent insulating state is then doped for achieving the SC phase.

We will use Eq. 1 for studying a hard-core strong correlation problem in 2D that how superconductivity emerges by doping Mott insulators. The major advantage is that such a model will be later shown to be QMC sign-problem free in a large parameter region, hence, it can be studied in a numerically exact way. Furthermore, it can be mapped to a monolayer two-orbital model [35, 36] with the two orbitals equivalent to the upper and lower layers, respectively. Multi-orbital models have been widely studied in strongly correlated systems such as iron-based superconductors [37]. It can also be mapped to a spin-\( \frac{3}{2} \) fermionic Hubbard model [28, 38–40] in a compact way by defining \( \psi_i = [c_{i\uparrow}, c_{i\downarrow}, d_{i\uparrow}, d_{i\downarrow}]^\dagger \),

\[
H = -t_\parallel \sum_{\langle ij \rangle} (\psi_i^\dagger \psi_j + h.c.) - t_\perp \sum_i \psi_i^\dagger \Gamma^5 \psi_i - \mu \sum_i n_i
\]

\[
- \sum_i \frac{g_c}{2} (n_i - 1)^2 - \sum_{i,\alpha=1,5} \frac{g_a}{2} (n_i^\alpha)^2,
\]

(2)

where \( n_i = \psi_i^\dagger \psi_i \), \( n_i^\alpha = \frac{1}{2} \psi_i^\dagger \Gamma^\alpha \psi_i \), and the five \( \Gamma \)-matrices are the rank-2 Clifford algebra, satisfying \( \{ \Gamma^a, \Gamma^b \} = 2\delta_{ab} \) with \( 1 \leq a < b \leq 5 \), as defined in the Supplemental Material (S.M.) I following the convention in Ref. [38]. The interaction parameters in the two different representations of Eq. 1 and Eq. 2 are related by

\[
4g_c = \frac{J_\perp}{2} + \frac{J_z}{4} - U - 3V,
\]

\[
g_{1,5} = \frac{J_\perp}{2} + \frac{J_z}{4} - U + V,
\]

\[
g_{2,3} = \frac{J_\perp}{2} - \frac{J_z}{4} + U - V,
\]

\[
g_4 = \frac{J_\perp}{2} + \frac{3J_z}{4} + U - V.
\]

In Eq. 2, all the interaction terms are expressed in Kramers invariant operators \( n_i \) and \( n_i^\alpha \), which satisfy

\[
\mathcal{T} n_i \mathcal{T}^{-1} = n_i, \quad \mathcal{T} n_i^\alpha \mathcal{T}^{-1} = n_i^\alpha,
\]

(5)

and the Kramers transformation is defined as \( \mathcal{T} = \Gamma^1 \Gamma^3 \mathcal{C} \) (\( \mathcal{C} \) means complex conjugate). \( \mathcal{T} \) is the usual time-reversal transformation followed by switching the upper and lower layers. When all the coupling constants \( g_c \) and \( g_a \) (\( 1 \leq a \leq 5 \)) are non-negative, the HS decomposition can be performed in a Kramers invariant way, such that the auxiliary field QMC is free of the sign problem [28, 38–40]. The discrete HS decomposition for the 4-fermion interaction is performed in an exact way as shown in S. M. II. Roughly speaking, \( g_c \) favors the charge-density-wave (CDW) order, and \( g_{1,5} \) favors the rung current, or,
FIG. 2. QMC simulation results for the structure factors of (a) AFz, (b) AFx(y), (c) SC, and (d) tPDW versus the doping x as varying L. In the disordered phase for each order parameter, each structure factor shows very small size-dependence when \( L \gg \xi \) and converges to a value proportional to the square of correlation length \( \xi^2 \), while in the ordered phase, it grows as \( L \to \infty \). The interacting parameter values are \( U = 3/2, J_\perp = 1, J_z = 8, V = t_\perp = 0 \).

bond-wave order, respectively [39], while \( g_{2,3,4} \) favors the AF order. For simplicity, we set \( g_c = g_1 = g_5 = 0 \) for studying the antiferromagnetism-superconductivity transition. In practice, we have chosen \( U = 3/2, J_\perp = 1, J_z = 8, V = t_\perp = 0 \), corresponding to \( g_4 = 8g_2 = 8g_3 = 8 \). Our QMC simulations employ the projector scheme working at zero temperature with the projection time \( \beta = 4L \) and the discrete imaginary time slice \( \Delta \tau = 0.1 \). The results show convergences with respect to \( \beta \) and \( \Delta \tau \) as shown in the S. M. III, respectively [41]. These simulations are performed on 20 cores for each group of parameters with 500 warm-up steps and more than 1000 steps of measurements.

QMC Results We have performed QMC calculations on \( 2 \times L \times L \) lattices with \( L \) up to 12. A larger size with \( L > 12 \) is technically difficult because of the complicated matrix structures for the general interaction parameters, which significantly reduces the efficiency of the fast update algorithm [42]. Even though, our results show clearly a transition from the half-filled AF insulating phase to the singlet SC phase upon doping.

We first present the QMC simulation results of the structure factors, defined as the equal-time correlations, \( F(\mathcal{O}) = L^2\langle \mathcal{O} | \mathcal{O} \rangle \) where \( \mathcal{O} \) represents a physical observable. In the magnetic channels, \( \mathcal{O} \) is chosen as

\[
N_z = \frac{1}{L^2} \sum_i n_i^z(-1)^i, \quad N_{x(y)} = \frac{1}{L^2} \sum_i n_i^{2(3)}(-1)^i, \quad (6)
\]

for the AF order along the z-direction (AFz), and that along the x(y)-direction (AFx(y)), respectively. Their structure factors \( F_{AFz} \) and \( F_{AFx(y)} \) are shown in Fig. 2 (a) and (b), respectively. The structure factors of AFz increase significantly versus \( L \) at \( x < x_c \approx 0.11 \) indicating the tendency for ordering. In contrast, those of AFx(y) nearly exhibit no size-dependence, showing the absence of long-range order. For the superconducting channel, we have examined the extended s-wave singlet pairing order defined as \( \Delta(i) = \frac{1}{\sqrt{2L^2}} \sum_i (c_{i\uparrow}d_{i\downarrow} - c_{i\downarrow}d_{i\uparrow}) \), i.e., the pairing across each rung. Its structure factor \( F_{SC} \) increases with enlarging the sample size as shown in Fig. 2 (c). If expressed with the bonding and anti-bonding band operators, \( f_{\alpha \sigma}^{(e/o)}(i) = \frac{1}{\sqrt{2}} (c_{\alpha}(i) \pm d_{\alpha}(i)) \), this pairing order parameter exhibits opposite signs on the \( f_{e,o} \)-bases as

\[
\Delta(i) = \frac{1}{\sqrt{2}} (f_{\uparrow}^{(e)}(i)f_{\uparrow}^{(o)}(i) - f_{\uparrow}^{(o)}(i)f_{\uparrow}^{(e)}(i)), \quad (7)
\]

hence, it is an extended s-wave pairing order parameter. We have also measured the superconducting correlations within the layers, but it is much (several orders) smaller than the inter-layer one. Hence, in the following, only the pairing across each rung will be considered. The extended s-wave pairing symmetry is among the promising candidates for the iron-based superconductors [43]. In addition, a triplet pair-density wave (tPDW) correlation is found, whose order parameter is defined as

\[
O_{tPDW} = \frac{1}{\sqrt{2L^2}} \sum_i (c_{i\uparrow}d_{i\downarrow} + c_{i\downarrow}d_{i\uparrow})(-1)^i. \quad (8)
\]

It tends to develop ordering at \( 0 < x < x_c \) even though its magnitudes are small, as shown in Fig. 2 (d).

Next we perform the finite-size scaling for these structure factors to extract the values of orderings in the thermodynamic limit as shown in Fig. 3. It is based on the scaling hypothesis \( F(L)/L^2 = a + b/L + c\xi^2/L^2 \), [44] where \( a \) is the thermodynamic expectation value (square of the order parameter), the \( b \)-term is the contribution from the gapless excitations (e.g. the Goldstone modes), and the \( c \)-term represents the short-range correlations, or, the gapped excitations. For the AFz order, since there is no Goldstone mode, the \( b \)-term is not needed. However, for the superconductivity, all the three terms should be kept since there is no Anderson-Higgs mechanism to “eat” the gapless phase mode in our calculations.

At half-filling (\( x = 0 \)), only the AFz order exhibits a long-range ordering, while the SC order extrapolates to zero. At a small doping level with \( x = \frac{1}{16} \), the AFz order still survives but its value is suppressed accompanied by the emerging of the SC order. As the doping level
In the coexistence regime, where both the AF\textsubscript{z} and SC states to the SC state can be unified by a hidden SO(3) theory \cite{9}, the transition from the AF\textsubscript{z} ordering to induce the tPDW order although its magnitude is too weak for an accurate identification. Similarly to the AF\textsubscript{z} region, which is also plotted in Fig. 4 (b) the single particle gap $\Delta_{1p}$ at all doping levels and the spin gap $\Delta_{AFz}$ at $x > x_c$.

An interesting observation is that the tPDW tends to develop within $0 < x < x_c$ with $x_c \approx 0.11$, and the SC order appears immediately upon doping starting from zero.

![Fig. 3](image-url)  
**Fig. 3.** The structure factors $F/L^2$ vs $1/L$ for both the AF\textsubscript{z} and SC orders. They are plotted at doping levels of (a) $x = 0$, (b) $x = 1/16$, (c) $x = 1/8$, and (d) $x = 1/4$, respectively. The dashed lines are polynomial fittings (see the main text for details) to the QMC data from $L = 6$ to $L = 12$. The interaction parameters are the same as in Fig. 2.

![Fig. 4](image-url)  
**Fig. 4.** (a) The extrapolation of $F/L^2 = \langle O^\dagger O \rangle$ in the limit of $L \to \infty$ versus $x$, where $O$ represents operators for the AF\textsubscript{z} and SC order parameters. The AF\textsubscript{z} ordering is suppressed beyond a critical doping $x_c \approx 0.11$, and the SC order coexists with the AF\textsubscript{z} one at small dopings $0 < x < x_c$. The interaction parameters are the same as in Fig. 2. (b) The single particle gap $\Delta_{1p}$ at all doping levels and the spin gap $\Delta_{AFz}$ at $x > x_c$. We next study the excitation gaps by calculating the imaginary-time-displaced correlation functions

$$\chi(\tau) = \langle T_\tau O(\tau)O^\dagger(0) \rangle,$$

where $T_\tau$ means time ordering. The long-time behavior of $\chi(\tau)$ is related to the excitation gap $\Delta_O$. As explained in S. M. V, we measure the mean gap defined as $\Delta_O = (E_O + E_{O\uparrow} - 2E_0)/2$ where $E_0$ is the ground state energy and $E_0$ (2$E_0$) gives the lowest energy excited by $O$ ($O^\dagger$). This gap can be extracted from $\chi(\tau)\chi(-\tau) \sim e^{-2\Delta_O \tau}$ for $\tau \to \infty$. For the single-particle gap, $O$ is chosen as $\psi_\alpha$ with $\alpha = 1 \sim 4$, which yields the diagonal terms of the single-particle Green’s function $G_{\alpha\alpha}(\tau)$. We use the averaged results of $G_{\alpha\alpha}(\tau)$ to yield the single-particle gap $\Delta_{1p}$ as plotted in Fig. 4 (a). In the whole phase diagram, the single-particle excitations are all gapped, and $\Delta_{1p}$ reaches the order of the band width in the antiferromagnetic order dominated region, indicating the existence of a Mott gap. We also calculate the spin gap $\Delta_{AFz}$ associated with $O = N_z$ in the spin disordered region, which is also plotted in Fig. 4 (b). It grows up at $x > x_c$ consistent with the vanishing of the AF\textsubscript{z} order.

**The SU(2) symmetric case** We briefly discuss the consequence if the SU(2) symmetry is preserved. The QMC simulations are performed by setting $g_{2,3,4} = \frac{16}{3}$ and also $g_c = g_{1,5} = 0$, which corresponds to the case of $U = 4, J_\perp = J_z = \frac{16}{3}, V = t_\perp = 0$. The finite-size
In summary, we have performed the projector QMC simulation based on the auxiliary field method on the bilayer SZH model, which is free of the sign problem. A quantum phase transition occurs from an Ising anisotropic AF insulating phase, or, an SU(2) invariant Mott insulating phase without the AF ordering, to a rung-singlet SC phase with an extended $s$-wave symmetry driven by doping. In the coexistence regime between the AF$_z$ and SC orders, their coupling leads to an enhanced tPDW correlation as a consequence of the symmetry principle. This work provides a reliable reference point for studying superconductivity and other competing orders by doping Mott insulators. Furthermore, the present study can be generalized to other bilayer geometries such as honeycomb or triangular lattices which may be relevant to certain materials and are left as future works.

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SUPPLEMENTAL MATERIALS

We present the detailed information about the model Hamiltonian and the quantum Monte Carlo (QMC) method, including the definition of \( \Gamma \)-matrices, the projector QMC algorithm, the scalings of \( \Delta r \) and \( \beta \), the calculation of excitation gaps, and the spatial correlations.

I. Definition of \( \Gamma \)-matrices

Following the convention in Ref. [38], we define the five \( \Gamma \)-matrices as follows:

\[
\Gamma^1 = \begin{pmatrix} 0 & -iI \\ iI & 0 \end{pmatrix}, \quad \Gamma^{2,3,4} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix}, \\
\Gamma^5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},
\]

where \( I \) and \( \vec{\sigma} \) are the \( 2 \times 2 \) unit and Pauli matrices. They satisfy the anti-commutation relation of

\[
\{\Gamma^a, \Gamma^b\} = 2\delta_{ab}.
\]

Their commutators give rise to the 10 generators of the Sp(4) group as

\[
\Gamma^{ab} = -\frac{i}{2} [\Gamma^a, \Gamma^b] \quad (1 \leq a, b \leq 5).
\]

The identity matrix, \( \Gamma^a \) \( (1 \leq a \leq 5) \) and \( \Gamma^{ab} \) \( (1 \leq a < b \leq 5) \) span the complete basis for the 16 bilinear operators in the particle-hole channel for 4-component fermions defined as

\[
n_i = \psi_{i,\alpha}^\dagger \psi_{i,\alpha},
\]

\[
n_i^a = \frac{1}{2} \psi_{i,\alpha}^\dagger \Gamma^a \psi_{i,\beta},
\]

\[
\Gamma_{i}^{ab} = -\frac{1}{2} \psi_{i,\alpha}^\dagger \Gamma^{ab} \psi_{i,\beta}.
\]

In the context of the bilayer model in the main text, we have

\[
n_i = c_{i,\sigma}^\dagger c_{i,\sigma} + d_{i,\sigma}^\dagger d_{i,\sigma},
\]

\[
n_i^1 = -\frac{i}{2} (d_{i,\sigma}^\dagger c_{i,\alpha} - h.c.),
\]

\[
n_i^3 = \frac{1}{2} (d_{i,\sigma}^\dagger c_{i,\alpha} + h.c.),
\]

\[
n_i^{2,3,4} = c_{i,\alpha}^\dagger \left( \frac{\vec{\sigma}}{2} \right)_{\alpha\beta} c_{i,\beta} - d_{i,\alpha}^\dagger \left( \frac{\vec{\sigma}}{2} \right)_{\alpha\beta} d_{i,\beta},
\]

where \( n_i \) is the total particle number on the rung, \( n_i^1 \) and \( n_i^3 \) are the bond current and bond strength along the rung, respectively, and \( n_i^{2,3,4} \) are the bond Neél order. We define the Kramers symmetry as

\[
\mathcal{T} = \Gamma^1 \Gamma^3 C,
\]
where \( C \) is the complex conjugate. Physically, \( T \) is the combination of the usual time-reversal transformation and the flipping of the upper and lower layers. It is easy to check that the above 6 bilinear operators are even under this Kramers operations.

The other 10 bilinear operators are odd under \( T \), which can be organized as

\[
\begin{align*}
\text{Re} \vec{\pi}_i &= e_{\alpha\beta}^i \left( \frac{\sigma}{2} \right)_{\alpha\beta} d_{i\beta} + \text{h.c.}, \\
\text{Im} \vec{\pi}_i &= -i e_{\alpha\beta}^i \left( \frac{\sigma}{2} \right)_{\alpha\beta} d_{i\beta} - \text{h.c.}, \\
\vec{S}_i &= c_{i\alpha}^\dagger \left( \frac{\sigma}{2} \right)_{\alpha\beta} c_{i\beta} + d_{i\alpha}^\dagger \left( \frac{\sigma}{2} \right)_{\alpha\beta} d_{i\beta}, \\
Q_i &= \frac{1}{2} (e_{\alpha\beta}^i c_{i\sigma} - d_{i\sigma}^\dagger d_{i\sigma}),
\end{align*}
\]

where \( \text{Re} \vec{\pi}_i \) is the spin-channel bonding strength, \( \text{Im} \vec{\pi}_i \) is the spin current along the rung, \( \vec{S}_i \) is the total spin of the rung, and \( Q_i \) is the charge-density order of the rung.

II. The projector QMC algorithm

We adopt the projector determinant QMC method [42] to study the model Hamiltonian shown in Eq. 1 in the main text. The basic idea is to apply the projection operator \( e^{-\beta H/2} \) on a trial wave function \( |\Psi_T\rangle \). If \( \langle\Psi_G|\Psi_T\rangle \neq 0 \) and there exists a nonzero gap between \( |\Psi_G\rangle \) and the first excited state, \( |\Psi_G\rangle \) is arrived as the projection time \( \beta \to \infty \),

\[
|\Psi_G\rangle = \lim_{\beta \to \infty} e^{-\beta H/2} |\Psi_T\rangle,
\]

where the projection time \( \beta \) can be divided into \( M \) slices with \( \beta = M \Delta \tau \), and the trial wave function can be written by filling \( N_e \) electrons,

\[
|\Psi_T\rangle = \prod_{i} \prod_{j=1}^{N_e} c_{i\sigma}^j |0\rangle.
\]

Here \( i, j \) contains both site and flavor indices and \( |0\rangle \) labels the fermion vacuum. In practice, \( |\Psi_T\rangle \) can be chosen as the ground state of a free fermion Hamiltonian. The scattering matrix \( \langle\Psi_T|e^{-\beta H}|\Psi_T\rangle \) is obtained by integrating out the fermionic degrees of freedom,

\[
\langle\Psi_T|e^{-\beta H}|\Psi_T\rangle = \sum_{\{\sigma\}} \prod_{i} \gamma_i(\sigma_i)|\det(P^\dagger B_L B_{L-1}...B_1 P)|,
\]

where \( \sigma_i \) labels the auxiliary discrete boson field (see below). The scattering matrix Eq. S10, which plays the role of the partition function, serves as the basis of the projector determinant QMC algorithm. The \( \{\sigma_i\} \) fields are then sampled by using the standard Monte Carlo technique.

In order to obtain Eq. S11, two preliminary steps are needed. The second order Suzuki-Trotter decomposition

\[
e^{-\Delta \tau (K+V)} = e^{-\Delta \tau K/2} e^{-\Delta \tau V} e^{-\Delta \tau K/2} + o(\Delta \tau)^2
\]

is first used to separate the kinetic \( (K) \) and interaction \( (V) \) terms in each time slice, and then the \( e^{-\Delta \tau V} \) term is decoupled by using the discrete Hubbard-Stratonovich transformation,

\[
eg^{gX^2} = \sum_{\sigma=\pm1,...,\pm I_{max}} \gamma(\sigma) e^{\lambda(\sigma)X},
\]

where \( \sigma \) is the discrete Hubbard-Stratonovich field. If eigenvalues \( \text{eig}(X) = \{0, \pm 1\} \), the maximal value of \( \sigma \), \( I_{max} \) can be set as 1 [23] along with the choices of \( \gamma(\sigma) \) and \( \lambda(\sigma) \) as

\[
\gamma(\pm 1) = \frac{1}{2}, \quad \lambda(\pm 1) = \pm \cosh^{-1}(e^g).
\]

If \( \text{eig}(X) = \{0, \pm 1, \pm 2, \pm 3\} \), we need set \( I_{max} = 2 \) and choose

\[
\begin{align*}
\gamma(\pm 1) &= \frac{-a(3 + a^2) + d}{4d}, \\
\gamma(\pm 2) &= \frac{a(3 + a^2) + d}{4d}, \\
\eta(\pm 1) &= \pm \cosh^{-1}\left\{ \frac{a + 2a^3 + a^5 + (a^2 - 1)d}{4} \right\}, \\
\eta(\pm 2) &= \pm \cosh^{-1}\left\{ \frac{a + 2a^3 + a^5 - (a^2 - 1)d}{4} \right\},
\end{align*}
\]

where \( a = e^g, \quad d = \sqrt{8 + a^2 (3 + a^2)^2} \) [54]. In our case, \( X = \psi^\dagger T^2, 3, 4 \psi \), whose eigenvalues are among \( 0, \pm 1, \pm 2 \), hence, the latter Hubbard-Stratonovich transformation is applied.

III. The \( \Delta \tau \) and \( \beta \)-scalings

In the projector QMC algorithm, the systematic error mainly comes from two origins: the finite time step \( \Delta \tau \) and the finite projection time \( \beta \). In the following, we perform the error analysis on both \( \Delta \tau \) and \( \beta \). In this section, we employ the parameter values for \( U = 2.5, J_{\perp} = 1, J_z = 8, V = t_{\perp} = 0 \) for simulations below.

For the Suzuki-Trotter decomposition defined in Eq. S11, detailed calculation shows that its error is at the order of max\{\text{tr}\{g_i^2, P^2 g_i\}(\Delta \tau)^3\}. In Fig. S1, scalings of the antiferromagnetic structure factors along the \( z, x(y) \) directions, and the superconductivity structure factor \( \nu s. \Delta \tau \) are plotted for \( x = 0 \) in (a) and \( x = \frac{1}{4} \) in (b). The slopes of these scaling lines are nearly independent on the lattice size \( L \) for all three orders. Therefore, we only need to check the small lattice size. Due to the
FIG. S1. (Color online) The $\Delta \tau$-dependence of the structure factors for various order parameters for $x = 0$ (a) and $x = \frac{1}{4}$ (b) with $L = 4$ (solid lines) and $L = 6$ (dashed lines). AFz, and AFx(y) represent the antiferromagnetic order along the $z$-direction, and that along the $x$ or $y$-direction, respectively, and SC represents the superconducting order. The interacting parameter values are $U = 2.5, V = t_\perp = 0, J_\perp = 1$, and $J_z = 8$.

FIG. S2. (Color online) The $\beta$-dependence of structure factors of various order parameters for $x = 0$ (a) and $x = \frac{1}{4}$ (b) with $L = 4$ (solid lines) and $L = 6$ (dashed lines). The symbols and the interacting parameter values are the same as those presented in Fig. S1.

convergence of the finite $\Delta \tau$ scaling, we use the value of $\Delta \tau = 0.1$ in all the simulations.

We further check the effect of the finite projection time $\beta$. In Fig. S2, the scalings of the antiferromagnetic structure factors along the $z$ and $x(y)$ directions, and the superconducting structure factor $v.s. \beta$ are presented. For each curve, $\beta_c$ is defined as the convergence projection time after which the structural factors converge. It is shown that the antiferromagnetic order parameter along the $x(y)$ direction and the superconducting order parameter converge very quickly for both $x = 0$ and $x = 1/4$. The corresponding $\beta_c$ is found to be around 8. For the antiferromagnetic order along the $z$-direction, we set $\beta_c = 16$ should be enough for $L = 4$, and $\beta_c = 24$ for $L = 6$ as well. This indicates that $\beta_c L = 4L$ is safe for convergence, which is taken for all the simulations presented in the main text for accurate numeric results.

IV. Spatial correlations

FIG. S3. The spatial correlation functions at different doping levels with system size $L = 4, 6$ and 8. The correlation functions for the AFz and SC orders at $x = 0$ are plotted in (a) and (b), respectively; those at $x = 1/16$ are plotted in (c) and (d) ($x = 1/18$ for the case of $L = 6$), respectively; those at $x = 1/4$ are plotted in (e) and (f), respectively. The squares of the order parameters obtained by the finite size scaling on the structure factors in the main text are plotted with dashed lines for comparison.

To demonstrate the SC long-range order after doping and its coexistence with the AFz order, we examine their spatial correlations $\langle O(0,0)O(r,r) \rangle$ [55]. The results are presented in Fig. 4 at three typical doping levels, i.e., $x = 0, 1/16, 1/4$, which correspond to the cases with only the AFz order, the coexistence of the AFz and SC orders, and only the SC order, respectively. For the system size with $L = 6$, $x = 1/18$ is used instead due to its commensurability with the system.

For all of these doping levels, the spatial correlations saturate at large distances. As $L$ increases, the farthest correlation functions approach the values obtained via the finite-size scalings on the corresponding structure factors in the main text. The consistency between two approaches demonstrates that the long-range orderings of the AFz and SC are reliable.

V. Calculation of excitation gaps

As explained in the main text, we calculate the spectra gap functions through the imaginary-time displaced correlation functions $\chi(\tau) = T_\tau \langle O(\tau)O^\dagger(0) \rangle$. Since our
FIG. S4. The imaginary time Green’s functions. $G(\tau)$ is plotted at different dopings. Due to the particle-hole symmetry at half-filling, the relation of $G(\tau) = -G(-\tau)$ is satisfied, while this symmetry is not held away from half-filling. We employ $[-G(\tau)G(-\tau)]$ to extract the mean single particle gap, plotted in (b), which shows very weak size dependence.

QMC works in the canonical ensemble, we can only obtain the energy difference directly through $\chi(\tau) \sim e^{-(E_{O^1}-E_0)\tau}$ for $\tau \to \infty$ and $\chi(\tau) \sim e^{E_O-E_0}\tau$ for $\tau \to -\infty$, where $E_0$ is the ground state energy and $E_O(E_{O^1})$ gives the lowest energy excited by $O(O^1)$. On the other hand, the physical gap should take the chemical potential into account, i.e. $\Delta_O = E_O - E_0 - \mu N_O$ where $N_O$ is the particle number of the excited states. Nevertheless, the relation between particle number $N$ and $\mu$ is generally complicated especially for an interacting model. We use the average of $\Delta_O$ and $\Delta_{O^1}$ as the excitation gap, in which $\mu$ does not appear explicitly.

In Fig. S4 (a), we plot the single-particle Green’s function $G(\tau)$ as an example to clarify our points. Only at half-filling, $G(\tau)$ shows the particle-hole symmetry, i.e., $G(\tau) = -G(-\tau)$. Away from the half-filling, the particle-hole symmetry is broken. If we directly take the slope of log$[G(\tau)]$ versus $\tau$ as the excitation gap, we even obtain a negative value, for example, at $x = 1/4$. According to the above discussions, we extract the mean gaps from log$[-G(\tau)G(-\tau)]$, as shown in Fig. S4(b), which show very small size-dependences.