Rigorous demonstration of pair-density-wave superconductivity in the σ_z-Hubbard model

Xingchuan Zhu [1,*] Junsong Sun,[2,*] Shou-Shu Gong [3,4] Wen Huang [5] Shiping Feng [6]
Richard T. Scalettar [7] and Huaiming Guo[2,†]
[1]School of Intelligent Manufacturing, Nanjing University of Science and Technology, Nanjing 210094, China
[2]School of Physics, Beihang University, Beijing 100191, China
[3]School of Physical Sciences, Great Bay University, Dongguan 523000, China
[4]Great Bay Institute for Advanced Study, Dongguan 523000, China
[5]Shenzhen Institute for Quantum Science and Engineering, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China
[6]Department of Physics, Beijing Normal University, Beijing 100875, China
[7]Department of Physics and Astronomy, University of California, Davis, California 95616, USA

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Describing and achieving "unconventional" superconductivity remains a forefront challenge in quantum many-body physics. Here, we use a unitary mapping, combined with the well-established properties of the attractive Hubbard model, to demonstrate rigorously a Hamiltonian with a low-temperature pair-density-wave (PDW) phase. We also show that the same mapping, when applied to the widely accepted properties of the repulsive Hubbard model, leads to a Hamiltonian exhibiting triplet d-wave PDW superconductivity and an unusual combination of ferro- and antiferromagnetic spin correlations. We then demonstrate the persistence of the d-wave PDW in a Hamiltonian derived from the mapping of the extended t-J model in the large-U limit. Furthermore, through strategic manipulation of the nearest-neighbor hopping signs of spin-down electrons, we illustrate the attainability of PDW superconductivity at other momenta. The intertwining of different magnetic and exotic pairing correlations noted here may have connections to experimental observations in spin-triplet candidates such as UTe_2.

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I. INTRODUCTION

Conventional BCS superconductivity describes the pairing of a singlet (s-wave) pair of fermions with zero momentum, that is, a nonzero expectation value of the off-diagonal order parameter $\Delta_s(k) = c_{-k\downarrow} c_{k\uparrow}$. This low-temperature phase is typically achieved through an effective retarded attractive interaction mediated by electron-phonon coupling. Shortly after BCS theory, the possibility of nonzero momentum pairs was noted by Fulde and Ferrell [1], and by Larkin and Ovchinnikov [2] (FFLO). Achieving such "FFLO" pairing proved very challenging but has been reported in heavy fermion systems such as $CeCoIn_5$ [3,4], and in ultracold atoms [5–7].

Other "unconventional" superconductors include those in which the Cooper wave function exhibits more complex patterns in real space, such as the nodes in the d-wave symmetry pairs of the cuprate materials [8–10], triplet superconductors which have nonzero total spin [11], pair density waves [12] in which the order parameter varies spatially with vanishing spatial average, and η pairs which are exact (high-energy) eigenstates of the Hubbard Hamiltonian exhibiting off-diagonal long-range order [13–15], etc.

Some of the unconventional superconductors noted above are (easily) achieved experimentally; others are less so. A key question for theory is what Hamiltonians give rise to the different types of "exotic" pairing. For example, in the case of the cuprates, the sufficiency of the repulsive Hubbard model continues to be debated [16,17]. As for a pair-density-wave (PDW) phase, obtaining a stable one in two dimensions is an even greater challenge [18–39]. In this paper, we present a pathway towards realizing PDW superconductivity in the σ_z-Hubbard model. Our key observation is that a unitary transformation, combined with known results of the conventional Hubbard model, allows us to identify Hamiltonians which rigorously must exhibit low-temperature unconventional PDW superconductivity.

II. THE HUBBARD MODEL

We begin with the celebrated Hubbard model

$$\mathcal{H} = -t \sum_{\langle ij\rangle\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) - \mu \sum_i (n_{i\uparrow} + n_{i\downarrow}) + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right), \quad (1)$$

which describes spin $\sigma = \uparrow, \downarrow$ fermions hopping on a lattice and interacting with an on-site interaction U. When the interaction is attractive ($U < 0$) the phase diagram on a

*These authors contributed equally to this work.
†Contact author: hmguo@buaa.edu.cn

square lattice is well understood qualitatively and quantitatively [40–42]: At half filling ($\mu = 0$) the ground state exhibits simultaneous long-range charge-density-wave (CDW) and s-wave superconducting (SC) orders. When doped ($\mu \neq 0$) the SC-CDW degeneracy is broken, and there is a finite-temperature (Kosterlitz-Thouless) transition to a SC phase. This description has been confirmed by quantum Monte Carlo (QMC) calculations which, owing to the absence of a sign problem, can be carried out to arbitrarily low temperatures.

A full understanding of the repulsive model with a large $U > 0$ is more elusive. At half filling there is long-range antiferromagnetic (AFM) order which occurs only at $T = 0$ on a square lattice owing to the continuous Heisenberg spin symmetry and the Mermin-Wagner theorem [43]. However, when doped, QMC fails to reach low T because of the sign problem. A d-wave SC phase, with intricate "striped" charge and spin patterns, is suggested by many calculations [sometimes with the addition of further next-nearest-neighbor (NNN) hopping], but the final determination of the various orders remains under discussion [44–53].

Before introducing the main results of this work, it is useful to review the well-known (partial) particle-hole transformation $c_{i\downarrow} \to (-1)^{i_x+i_y} c_{i\downarrow}^\dagger$ which links the descriptions of the properties of the attractive and repulsive cases. Here, $(-1)^{i_x+i_y}$ indicates opposite phases on the two sublattices of the (bipartite) square lattice. Under this transformation, the kinetic energy remains unchanged. The down-spin density $n_{i\downarrow} \leftrightarrow 1 - n_{i\downarrow}$ and, as a consequence the sign of U is reversed, mapping attraction to repulsion and vice versa. The roles of charge and spin operators are interchanged $n_{i\uparrow} + n_{i\downarrow} \leftrightarrow n_{i\uparrow} - n_{i\downarrow}$, so that the chemical potential μ and Zeeman B_z terms map into one another (to within an irrelevant energy shift) and correlations of the Z component of the spin map onto density correlations. Finally, the XY spin operators map onto s-wave pairing $c_{i\uparrow}^\dagger c_{i\downarrow} \leftrightarrow c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$.

With those mappings in place, the connections between the attractive and repulsive Hubbard models become clear. The fact that the square lattice repulsive Hubbard model has degenerate Z and XY spin order in its ground state and half filling immediately implies the degenerate CDW and SC patterns in the attractive case. Likewise, the fact that a Zeeman field B_z causes AFM Heisenberg spins to "lie down" and order in the XY plane perpendicular to the field is then connected to the preference for SC correlations over CDW ones in the attractive Hubbard model for μ nonzero. We will now show how an alternate canonical transformation lends similar insight into exotic superconductivity.

III. ATTRACTIVE σ_z-HUBBARD MODEL

We then apply the unitary transformation, $c_{i\downarrow} \to \text{sgn}(i) c_{i\downarrow}$, to the attractive Hubbard model, resulting in the σ_z-Hubbard model defined by the Hamiltonian [54–56],

$$\mathcal{H}_{\sigma_z} = -t \sum_{\langle ij \rangle} \sum_{\alpha\beta} c_{i\alpha}^\dagger \sigma_z^{\alpha\beta} c_{j\beta} - \mu \sum_{i,\alpha} n_{i\alpha} + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right), \quad (2)$$

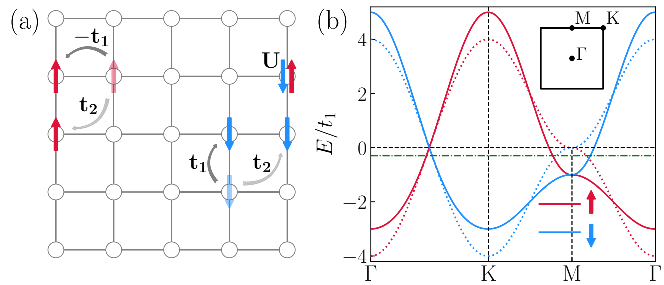

FIG. 1. (a) A schematic view of the extended σ_z-Hubbard model on a square lattice, where t_1 ($-t_1$) is the NN hopping parameter of the spin-up (spin-down) fermion, t_2 represents the NNN hopping amplitude, and U is the on-site Hubbard interaction. Up and down arrows correspond to spin-up and spin-down electrons, respectively. (b) Band structures of the noninteracting terms in Eq. (1) with $t_2 = 0$ (dotted line) and $t_2 = 0.25$ (solid line). The inset displays the first Brillouin zone, on which the high-symmetry points are marked.

where σ_z represents the Z component of the Pauli matrix, resulting in opposite signs in the hopping amplitudes for the spin-up and spin-down subsystems [see Fig. 1(a)]. In the following, we begin with the σ_z-Hubbard model and investigate its physical properties. It is clear that the Hamiltonian in Eq. (2) is invariant under the usual translation transformation.

The phase diagram of the attractive Hubbard model can be transformed back to derive that of the attractive σ_z-Hubbard model. It is observed that while the CDW remains unaffected, the s-wave SC phase is altered. Specifically, the on-site pairing transforms back as $\Delta_j = c_{j\downarrow} c_{j\uparrow} \to \Delta_j = \text{sgn}(j) c_{j\downarrow} c_{j\uparrow}$. Therefore, the pairing remains on site but with an alternating sign, indicating that the system displays s-wave PDW superconductivity. The pairing function can be written as $\Delta^\dagger = \frac{1}{\sqrt{N}} \sum_j (-1)^{j_x+j_y} c_j^\dagger c_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{-\mathbf{k}+\mathbf{K}_0}^\dagger$ with $\mathbf{K}_0 = (\pm\pi, \pm\pi)$. Therefore a PDW state, in which an electron at momentum $\mathbf{k}$ pairs up with another at momentum $-\mathbf{k} + \mathbf{K}_0$, resulting in a Cooper pair carrying net momentum $\mathbf{K}_0$, must rigorously be the low-temperature phase of the attractive σ_z-Hubbard model.

It has been well established that the Fermi-surface topology plays a crucial role in Cooper pair formation. To investigate the origin of PDW in the σ_z-Hubbard model, we plot the noninteracting Fermi surface in Fig. 2(a). In contrast to the normal spin-independent hopping scenario where the Fermi surface is spin degenerate, the σ_z hopping term generates a spin-dependent Fermi surface. Since the dispersion of the two spin species satisfies the condition $\xi_{\uparrow,\mathbf{k}} = \xi_{\downarrow,-\mathbf{k}+\mathbf{K_0}}$, the spin-up and spin-down Fermi surfaces are of identical shape and are centered around the Γ and K points, respectively. The above relation also indicates perfect nesting in the particle-particle channel with the center-of-mass momentum $\mathbf{K}_0$. Hence, in the presence of an on-site attractive interaction, a PDW order with modulation wave vector $\mathbf{K}_0$ will develop.

IV. REPULSIVE σ_z-HUBBARD MODEL

We next consider the repulsive case, $U > 0$. Introducing a NNN hopping term t_2 into the Hamiltonian in Eq. (2), the total

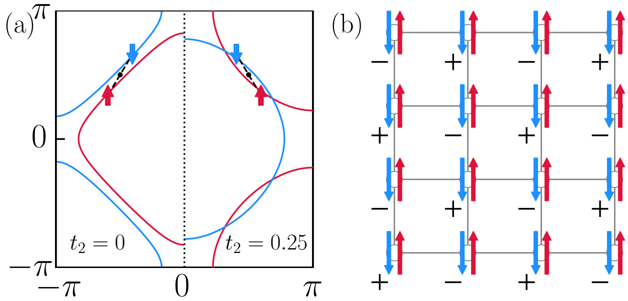

FIG. 2. (a) Fermi surfaces of the spin-up and spin-down electrons at $\mu = -0.3$, in which a pair of electrons with different spins on the nested Fermi surface is demonstrated. The Fermi surfaces are C_4 symmetric, therefore only the left (right) half of them are shown for $t_2 = 0$ ($t_2 = 0.25$). (b) A schematic view of the s-wave PDW with center-of-mass momentum (π, π) in the attractive σ_z-Hubbard model on a square lattice.

Hamiltonian becomes

$$\mathcal{H} = -t_1 \sum_{\langle ij\rangle} \sum_{\alpha\beta} c_{i\alpha}^{\dagger} \sigma_z^{\alpha\beta} c_{j\beta} + t_2 \sum_{\langle\langle ij\rangle\rangle\alpha} \hat{c}_{i\alpha}^{+} \hat{c}_{j\alpha} + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) - \mu \sum_{i,\alpha} n_{i\alpha}, \quad (3)$$

where $\langle\langle ij\rangle\rangle$ denotes next-nearest neighbors, and t_2 is the NNN hopping amplitude. Under the same unitary transformation in the previous section, the above extended σ_z-Hubbard model transforms into a normal extended one. The inclusion of the NNN hopping term is essential at large U as it may play a key role in generating long-range SC correlation and establishing a delicate balance between CDW, spin density wave, and superconductivity [48,53,57,58]. Recent comprehensive density matrix renormalization group (DMRG) studies have revealed the intertwined CDW and SC correlations on four-leg systems [47–49], as well as an emergent d-wave SC phase on wider systems with a moderate $t_2 > 0$ [53].

The magnetic order can be characterized by the spin correlation functions defined as $C^z(ij) = \langle S_i^z S_j^z\rangle = \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow})\rangle$ and $C^{xy}(ij) = \langle S_i^+ S_j^-\rangle = \langle c_{i\uparrow}^+ c_{i\downarrow} c_{j\downarrow}^+ c_{j\uparrow}\rangle$. Under the transformation, $C^{xy}(ij)$ will change its sign when i and j belong to different sublattices, whereas $C^z(ij)$ will remain unchanged. The magnetic properties of the normal extended Hubbard model [connected to Eq. (3) through the unitary transformation] have been well established at half filling, exhibiting an AFM ground state [16,17,46,59]. Consequently, the Hamiltonian in Eq. (3) will exhibit unconventional long-range magnetic order, which is ferromagnetic (antiferromagnetic) in the XY plane (Z direction).

Similarly, in diagnosing the SC order, if the pair correlation function involves the spin-singlet pair annihilation operator $\Delta(ij) = \frac{1}{\sqrt{2}}(c_{i\uparrow} c_{j\downarrow} - c_{i\downarrow} c_{j\uparrow})$, it is straightforward to infer that the transformation will convert the spin-singlet pair operator to $\Delta(ij) = \pm\frac{1}{\sqrt{2}}(c_{i\uparrow} c_{j\downarrow} + c_{i\downarrow} c_{j\uparrow})$ for the nearest-neighbor (NN) pairing (as is the case for the most-studied d-wave in the normal repulsive Hubbard model), where $+$ $(-)$ corresponds to the negative sign of the transformation situated on site i (j). Then, the NN pairings $c_{i\uparrow} c_{j\downarrow}$ and $c_{j\uparrow} c_{i\downarrow}$, which are equivalent in the spin-singlet scenario, will exhibit a sign difference under the unitary transformation, giving rise to a spin-triplet state. Therefore, the additional symbol $\pm$ will not only produce a net momentum $\mathbf{K}_0$ for the d-wave pairs but also alter the nature of the pairing, leading to the emergence of a d-wave PDW triplet superconductor with a center of mass momentum $\mathbf{K}_0$ [60].

The various types of correlations mentioned above can be transformed back by the gauge transformation and are used to characterize the ground-state properties of the extended σ_z-Hubbard model. While the charge density correlations and spin-z correlations remain unchanged, the SC correlations transform into those of spin-triplet d-wave pairings at momentum $\mathbf{K}_0$, and the transverse spin correlation transitions to be ferromagnetic (FM). Therefore, considering that spin-singlet d-wave superconductivity dominates in the doped normal extended Hubbard model [48,49,52,53], it is reasonable to suggest that the extended σ_z-Hubbard model may support a spin-triplet d-wave PDW SC ground state with the center-of-mass momentum $\mathbf{K}_0$. It is noted that the conversion of the pairing symmetry is accompanied by changes in the transverse magnetic property, i.e., from AFM to FM corresponding to the shift from singlet to triplet pairings. This may imply the significant role of FM spin fluctuations in mediating the formation of spin-triplet pairs of electrons.

To confirm the existence of the d-wave triplet SC at momentum $\mathbf{K}_0$ in the extended σ_z-Hubbard model given by Eq. (3), we conduct determinantal quantum Monte Carlo (DQMC) calculations of the d-wave pairing susceptibility at momentum $\mathbf{K}_0$, defined as follows [61],

$$P_d = \frac{1}{N} \int_0^\beta d\tau \sum_{ij} \left\langle \Delta_i^d(\tau) \Delta_j^{d\dagger}(0) \right\rangle e^{i\mathbf{K}_0 \cdot (\mathbf{r}_j - \mathbf{r}_i)},$$

where $\Delta_i^d(\tau) = \sum_j f_{ij}^d e^{\tau H} c_{i\uparrow} c_{j\downarrow} e^{-\tau H}$ represents the time-dependent pairing operator with a form factor $f_{ij}^d = 1$ (-1) for the bond in the X (Y) direction between sites i and j. The interaction vertex Γ_d can be extracted from P_d and the uncorrelated susceptibility $\bar{P}_d$ as follows: $\Gamma_d = \frac{1}{P_d} - \frac{1}{\bar{P}_d}$ [62,63].

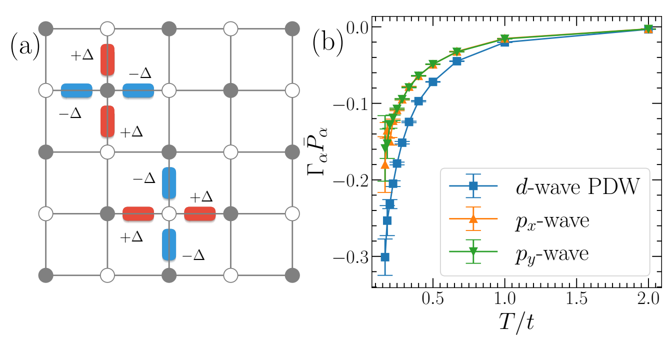

FIG. 3. (a) A schematic demonstration of the d-wave PDW with center-of-mass momentum (π, π) in the extended repulsive σ_z-Hubbard model on a square lattice. (b) The measured $\Gamma_\alpha \bar{P}_\alpha$ of the pairing instability as a function of temperature for various paring symmetries at a filling of $\rho = 0.95$. The parameters used are $t'/t = 0.25$ and $U/t = 4$, with a lattice size of $L = 8$.

When $\Gamma_d \bar{P}_d < 0$, the corresponding pairing interaction is attractive. As $\Gamma_d \bar{P}_d \to -1$, P_d tends to diverge, indicating a SC instability. Figure 3(b) illustrates the product $\Gamma_d \bar{P}_d$ for the d-wave pairing susceptibility at momentum $\mathbf{K}_0$. As the temperature decreases, we find $\Gamma_d \bar{P}_d$ is the most negative, suggesting this pairing will dominate the SC instability. For comparison, we also calculate $\Gamma_\alpha \bar{P}_\alpha$ for the p-wave triplet at zero momentum, which is less dominant.

V. THE LARGE-U LIMIT

In the large-U limit, the double occupancy on a lattice site is excluded, and the extended σ_z-Hubbard model is reduced to an extended σ_z-t-J-like Hamiltonian [64],

$$\begin{aligned}\mathcal{H} = &-t_1 \sum_{\langle ij\rangle}\sum_{\alpha\beta} c^\dagger_{i\alpha}\sigma_z^{\alpha\beta} c_{j\beta} + t_2 \sum_{\langle\langle ij\rangle\rangle\alpha} \hat{c}^+_{i\alpha}\hat{c}_{j\alpha}\\ &- \sum_{\langle ij\rangle}\left[J_1\left(S_i^x S_j^x + S_i^y S_j^y\right) - J_1 S_i^z S_j^z + J_1 \frac{1}{4}\hat{n}_i\hat{n}_j\right]\\ &+ \sum_{\langle\langle ij\rangle\rangle} J_2\left(\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j - \frac{1}{4}\hat{n}_i\hat{n}_j\right),\end{aligned} \tag{4}$$

where the exchange coupling is $J_{1(2)} = \frac{4t_{1(2)}^2}{U}$ with the ratio $J_2/J_1 = t_2^2/t_1^2$. Here, the FM nature of the XY component of the NN Heisenberg term J_1 aligns with the magnetic properties observed in Eq. (3). Under the transformation, the above Hamiltonian becomes the normal extended t-J model, on which recent DMRG calculations have been conducted for six- and eight-leg cylinders, uncovering a robust d-wave SC phase in the case of electron doping ($t_2 > 0$) [65–70]. It has been demonstrated that the SC phase exhibits a power-law pairing correlation that decays much slower than the charge density and spin correlations. Furthermore, it is found that spin-singlet d-wave superconductivity can also emerge at the hole-doped side ($t_2 < 0$) near the optimal 1/8 doping level on the wider eight-leg system [69,70]. Correspondingly, it is reasonable to propose that the σ_z-t-J-like model in Eq. (4) could potentially give rise to a d-wave PDW triplet superconductor with a center-of-mass momentum $\mathbf{K}_0$ within the proper parameter region of the normal extended t-J model, where the SC phase is observed [65–73].

VI. THE $(\pi, 0)$ PDW SUPERCONDUCTIVITY

The PDW SC ground state with a different center-of-mass momentum can be achieved by appropriately manipulating the NN hopping signs of the spin-down electrons. In the case of $(\pi, 0)$, we can select the NN hoppings as follows,

$$\mathcal{H}_{(\pi,0)} = -t\sum_{i,\alpha\beta} c^\dagger_{i\alpha}\sigma_z^{\alpha\beta} c_{i\pm\hat{x}\beta} - t\sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\pm\hat{y}\sigma}, \tag{5}$$

where an additional sign is present when the spin-down electrons hop in the x direction. This additional sign can be eliminated by the following unitary transformation:

$$c_{i\downarrow} \to (-1)^{i_x} c_{i\downarrow}. \tag{6}$$

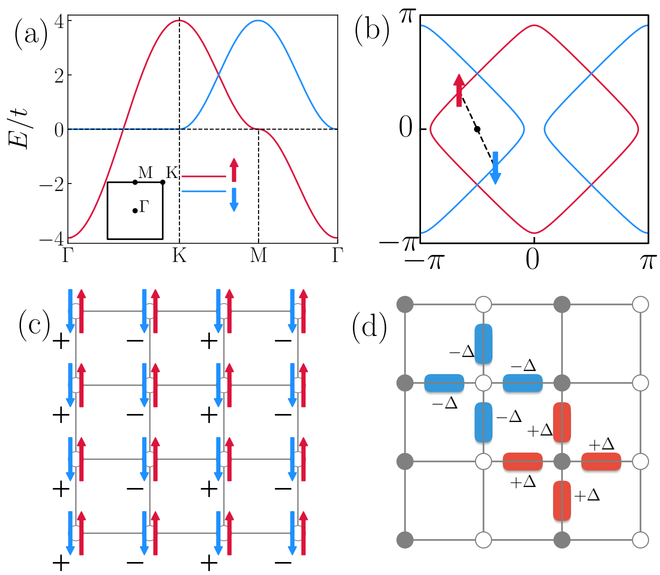

FIG. 4. (a) Band structures of the noninteracting Hamiltonian in Eq. (5). (b) Fermi surfaces of the spin-up and spin-down electrons at filling $\rho = 0.95$, in which the nesting of the Fermi surface is illustrated. Schematic views of the s-wave (c) and extended s-wave (d) PDWs with center-of-mass momentum $(\pi, 0)$ in the modified σ_z-Hubbard model on a square lattice.

Through a similar analysis, the corresponding attractive Hubbard model supports a s-wave PDW state with a center-of-mass momentum of $(\pi, 0)$. Similarly, the dispersion of the two spins has the relation $\xi_{\uparrow,\mathbf{k}} = \xi_{\downarrow,-\mathbf{k}+\mathbf{K_0}}$ with $\mathbf{K_0} = (\pi, \mathbf{0})$ and their Fermi surfaces are again nested in the particle-particle channel with center-of-mass momentum $\mathbf{K_0}$ [see Fig. 4(b)]. By substituting the NN hopping term with the one in Eq. (5) in the Hamiltonian Eq. (3), the modified repulsive Hubbard model exhibits an extended s-wave PDW state with a center-of-mass momentum of $(\pi, 0)$. The pairings in the X direction transition to triplet, accompanied by FM spin correlations in the X component along this direction. These results extend to the corresponding model in the large-U limit, which deviates from Eq. (4) in the NN hoppings [replaced by Eq. (5)] and NN exchange couplings (FM for the X component along the X direction). Finally, by rotating the Hamiltonian by 90°, PDW superconductivity with a center-of-mass momentum $(0, \pi)$ can also be realized.

VII. CONCLUSIONS

We explicitly demonstrate the presence of PDW superconductivity in the σ_z-Hubbard model and its related extensions, such as incorporating long-range hoppings and the large-U limit. These modified Hubbard or t-J models can be transformed into normal ones through unitary transformations, where their physical properties have been thoroughly established. The attractive σ_z-Hubbard model supports an s-wave PDW phase, whereas the repulsive extended σ_z-Hubbard model features a d-wave PDW state. Both PDW phases possess a center-of-mass momentum at (π, π). Specifically, the

d-wave PDW at momentum (π, π) is a triplet, corresponding to which the spin correlations in the XY component are ferromagnetic. The d-wave PDW persists in the extended σ_z-t-J-like model derived from the extended σ_z-Hubbard model in the large-U limit. Finally, we discover that a PDW superconductivity at momentum $(\pi, 0)$ can also be achieved by appropriately manipulating the NN hopping signs of the spin-down electrons. Our study provides a microscopic mechanism for the PDW superconductivity, and will deepen the understanding of this exotic SC state [74–79]. Specifically, while recent experiments have identified UTe_2 as a candidate for a spin-triplet PDW state near an FM instability [78], the AFM fluctuations detected by inelastic neutron scattering seem highly unusual [79]. Nonetheless, the d-wave PDW at momentum (π, π) mentioned here inherently exhibits a coexistence of these intertwined orders. Therefore, the σ_z-Hubbard model proposed here may have a connection to such quantum materials, a topic we leave for further study.

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