

Spin texture and spin current in excitonic phases of the two-band Hubbard modelHisao Nishida,¹ Shohei Miyakoshi,² Tatsuya Kaneko,³ Koudai Sugimoto,⁴ and Yukinori Ohta¹¹*Department of Physics, Chiba University, Chiba 263-8522, Japan*²*Computational Quantum Matter Research Team, RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan*³*Computational Condensed Matter Physics Laboratory, RIKEN Cluster for Pioneering Research (CPR), Wako, Saitama 351-0198, Japan*⁴*Center for Frontier Science, Chiba University, Chiba 263-8522, Japan*

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Using the mean-field approximation, we study the k -space spin textures and local spin currents emerged in the spin-triplet excitonic insulator states of the two-band Hubbard model defined on the square and triangular lattices. We assume a noninteracting band structure with a direct band gap and introduce s -, p -, d -, and f -type cross-hopping integrals, i.e., the hopping of electrons between different orbitals on adjacent sites with four different symmetries. First, we calculate the ground-state phase diagrams in the parameter space of the band filling and interaction strengths, whereby we present the filling dependence of the amplitude and phase of the excitonic order parameters. Then, we demonstrate that the spin textures (or asymmetric band structures) are emerged in the Fermi surfaces by the excitonic symmetry breaking when particular phases of the order parameter are stabilized. Moreover, in the case of the p -type cross-hopping integrals, we find that the local spin current can be induced spontaneously in the system, which does not contradict the Bloch theorem for the absence of the global spin current. The proofs of the absence of the global spin current and the possible presence of the local spin currents are given on the basis of the Bloch theorem and symmetry arguments.

DOI: [10.1103/PhysRevB.99.035119](https://doi.org/10.1103/PhysRevB.99.035119)**I. INTRODUCTION**

The excitonic phase, which is sometimes referred to as the excitonic insulator phase, is the state where valence-band holes and conduction-band electrons in small band-gap semiconductors or small band-overlap semimetals form pairs (or excitons) due to weakly screened Coulomb interactions, and a macroscopic number of the pairs condense into a quantum state acquiring the phase coherence. Although the excitonic phase was predicted to occur more than half a century ago as a spontaneous hybridization between the valence and conduction bands and has attracted much attention because a theoretical framework similar to that of BCS superconductors can be applied [1–7], the lack of candidate materials delayed our understandings of this phase until recently. However, the progress in this research field has been made rapidly in recent years owing to the discovery of some candidate materials. The spin-singlet excitonic phase has been suggested to emerge in some transition-metal chalcogenides such as $1T$ -TiSe₂ [8–13] and Ta₂NiSe₅ [14–21], and the spin-triplet excitonic phase has also been suggested to emerge in some cobalt oxide materials located in the crossover regime between the high-spin and low-spin states [22–31]. Since these materials are transition-metal compounds, the relevant properties should be considered within the framework of the physics of strong electron correlations using the Hubbard-like lattice models [32–42].

In a series of such studies, Kuneš and Geffroy [43] discussed the effects of cross-hopping integrals on the excitonic states in the two-band Hubbard model, where the cross hopping is defined as the hopping of electrons between different orbitals on the adjacent sites. The hopping integral between

different orbitals on the same site vanishes exactly because of the orthogonality of the orbitals, but the cross-hopping integrals between the adjacent sites can have a finite value [44]. Since the hybridization between the orthogonal orbitals occurs spontaneously due to interorbital Coulomb interactions in the excitonic phase, one may naturally expect that the hybridization caused by the cross-hopping integrals should affect the excitonic phase significantly. Kuneš and Geffroy, in particular, showed that the k -space spin texture, similar to the one derived from the Rashba-Dresselhaus spin-orbit coupling, can appear in the spin-triplet excitonic phases even in centrosymmetric lattices without any intrinsic spin-orbit coupling.

Kuneš and Geffroy [43] also argued that the spontaneous spin currents can appear if the order parameters of the spin-triplet excitonic phase are imaginary. Using different models with certain cross-hopping integrals, Volkov *et al.* [45,46] discussed the relationship between the excitonic phase and imaginary order parameters and showed that the spin current of the orbital off-diagonal components can remain finite, but the total spin current including both the orbital diagonal and off-diagonal components vanishes exactly. Thus, they concluded that the global spin currents can never appear spontaneously in the equilibrium excitonic phase. Geffroy *et al.* [47] also pointed out the absence of the global spin current. This result is consistent with the Bloch theorem [48,49] that claims that the global spin current does not appear spontaneously in the ground state. The existence of the spontaneous global spin current is thus unlikely to occur in the excitonic phases of strongly correlated electron systems.

In this paper, motivated by the above developments in the field, we study the excitonic phases of the two-band Hubbard

models with cross-hopping integrals within the mean-field approximation. We assume the square and triangular lattices in two dimensions and examine the cross-hopping integrals of four types, i.e., s , p , d , and f types. We thus calculate the ground-state phase diagram of the models and clarify the behaviors of the excitonic order parameters, Fermi surfaces, band dispersions, and spin currents. In particular, we discuss the relationship between the global spin currents and excitonic phase with imaginary order parameters. We thereby find that the spin textures are emerged in the Fermi surfaces by the excitonic symmetry breaking when particular phases of the order parameter are stabilized and that the local spin current can be induced in the system with the p -type cross-hopping integral. The proofs of the absence of the global spin current and the possible presence of the local spin currents are also given on the basis of the Bloch theorem and symmetry arguments. We thus present a comprehensive understanding of the spin textures and spin currents in the spin-triplet excitonic phases of the two-band Hubbard model.

The rest of this paper is organized as follows. In Sec. II, we introduce the two-band Hubbard model with the cross hopping integrals and derive the self-consistent equations for obtaining the ground state of the model in the mean-field approximation. In Sec. III, we present the calculated results for the phase diagram of the system, k -space spin texture, features of the order parameters, and the local and global spin currents of the system. We summarize our results in Sec. IV. Appendices are provided to show the proofs of the absence of the global spin currents and the possible presence of the local spin currents in the excitonic phases of the model.

II. MODEL AND METHOD

A. Model

We consider the two-band Hubbard model defined on the two-dimensional lattices. The Hamiltonian is written as

$$\hat{H} = \hat{H}_t + \hat{H}_{\text{int}}, \quad (1)$$

$$\begin{aligned} \hat{H}_t = & \sum_{j,\tau,\sigma} (t_c \hat{c}_{j+\tau,\sigma}^\dagger \hat{c}_{j,\sigma} + t_f \hat{f}_{j+\tau,\sigma}^\dagger \hat{f}_{j,\sigma} + \text{H.c.}) \\ & + \sum_{j,\tau,\sigma} (V_{1,\tau} \hat{c}_{j+\tau,\sigma}^\dagger \hat{f}_{j,\sigma} + V_{2,\tau} \hat{f}_{j+\tau,\sigma}^\dagger \hat{c}_{j,\sigma} + \text{H.c.}) \\ & + \frac{D}{2} \sum_{j,\sigma} (\hat{n}_{j,\sigma}^c - \hat{n}_{j,\sigma}^f) - \mu \sum_{j,\sigma} (\hat{n}_{j,\sigma}^c + \hat{n}_{j,\sigma}^f), \quad (2) \end{aligned}$$

$$\hat{H}_{\text{int}} = \sum_j (U_c \hat{n}_{j,\uparrow}^c \hat{n}_{j,\downarrow}^c + U_f \hat{n}_{j,\uparrow}^f \hat{n}_{j,\downarrow}^f) + U' \sum_{j,\sigma,\sigma'} \hat{n}_{j,\sigma}^c \hat{n}_{j,\sigma'}^f, \quad (3)$$

where $\hat{c}_{j,\sigma}^\dagger$ ($\hat{f}_{j,\sigma}^\dagger$) and $\hat{c}_{j,\sigma}$ ($\hat{f}_{j,\sigma}$) are the creation and annihilation operators of an electron on the conduction (c) orbital [valence (f) orbital] at site j with spin σ . We define the number operators $\hat{n}_{j,\sigma}^c = \hat{c}_{j,\sigma}^\dagger \hat{c}_{j,\sigma}$ and $\hat{n}_{j,\sigma}^f = \hat{f}_{j,\sigma}^\dagger \hat{f}_{j,\sigma}$. In \hat{H}_t , D is the on-site energy splitting, μ is the chemical potential, t_c and t_f are the hopping integrals between the same orbitals on the nearest-neighbor sites, and $V_{1,\tau}$ and $V_{2,\tau}$ are the hopping integrals between the different orbitals on

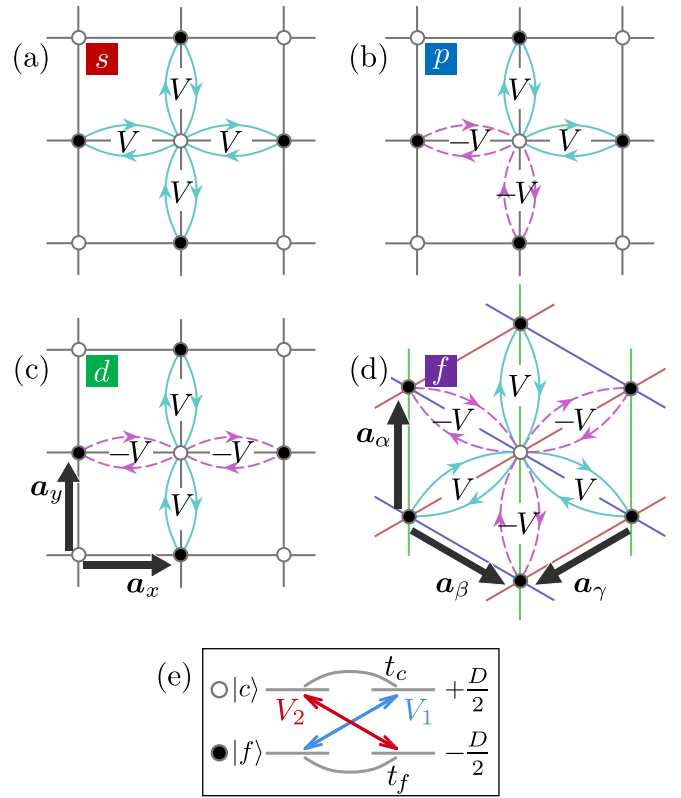


FIG. 1. Schematic representations of (a) the s -, (b) p -, (c) d -, and (d) f -type cross-hopping integrals defined on either the square or triangular lattice. The blue bonds indicate $V_{1,\tau} = V_{2,\tau} = V$ and the purple bonds indicate $V_{1,\tau} = -V_{2,\tau} = V$. In (e), the direct hoppings (t_c and t_f) and cross hoppings (V_1 and V_2) are illustrated. The primitive translation vectors are $\mathbf{a}_x = (1, 0)$ and $\mathbf{a}_y = (0, 1)$ in (c), and $\mathbf{a}_\alpha = (0, 1)$, $\mathbf{a}_\beta = (\sqrt{3}/2, -1/2)$, and $\mathbf{a}_\gamma = (-\sqrt{3}/2, -1/2)$ in (d).

the nearest-neighbor sites. $V_{1,\tau}$ and $V_{2,\tau}$ are referred to as the cross-hopping integrals. Note that $j + \tau$ indicates the nearest-neighbor site of j , where j runs over all sites in the system and τ denotes the primitive translation vector \mathbf{a}_τ illustrated in Fig. 1(c) for the square lattice and Fig. 1(d) for the triangular lattice. In \hat{H}_{int} , U_c and U_f are the intraorbital Coulombic repulsive interactions, and U' is the interorbital Coulombic repulsive interaction. This model is illustrated in Fig. 1, where \mathbf{a}_τ is the vector from site j to site $j + \tau$ (or the primitive translation vector). The Fourier transformation of Eq. (2) reads

$$\hat{H}_t = \sum_{k,\sigma} (\hat{c}_{k,\sigma}^\dagger \hat{f}_{k,\sigma}^\dagger) \begin{pmatrix} \varepsilon_c(\mathbf{k}) & \gamma(\mathbf{k}) \\ \gamma^*(\mathbf{k}) & \varepsilon_f(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \hat{c}_{k,\sigma} \\ \hat{f}_{k,\sigma} \end{pmatrix}, \quad (4)$$

where the matrix elements are

$$\varepsilon_c(\mathbf{k}) = 2t_c \sum_{\tau} \cos k_{\tau} + \frac{D}{2} - \mu, \quad (5)$$

$$\varepsilon_f(\mathbf{k}) = 2t_f \sum_{\tau} \cos k_{\tau} - \frac{D}{2} - \mu, \quad (6)$$

$$\gamma(\mathbf{k}) = 2 \sum_{\tau} (V_{\tau} \cos k_{\tau} + i V'_{\tau} \sin k_{\tau}), \quad (7)$$

with $V_\tau = (V_{1,\tau} + V_{2,\tau})/2$, $V'_\tau = (V_{1,\tau} - V_{2,\tau})/2$, and $k_\tau = \mathbf{k} \cdot \mathbf{a}_\tau$. We assume the hopping integrals as $-t_c = t_f = t = 1$ (direct gap) and set $D = 6$ and $U_c = U_f = U$ throughout the paper.

We consider four types of the cross-hopping integrals, i.e., s , p , d , and f types, where s , p , and d types are for the square lattice and f type is for the triangular lattice. The signs of $V_{1,\tau}$ and $V_{2,\tau}$ for each type are shown in Fig. 1. We set $V_{1,\tau} = V_{2,\tau} = V_{1,-\tau} = V_{2,-\tau}$ for the s and d types and $V_{1,\tau} = -V_{2,\tau} = -V_{1,-\tau} = V_{2,-\tau}$ for the p and f types, where $-\tau$ denotes the primitive translation vector in the opposite direction, $-\mathbf{a}_\tau$. Thus, we rewrite Eq. (7) as

$$\gamma(\mathbf{k}) = 2(V_x \cos k_x + V_y \cos k_y) \quad (8)$$

for s type,

$$\gamma(\mathbf{k}) = 2i(V'_x \sin k_x + V'_y \sin k_y) \quad (9)$$

for p type,

$$\gamma(\mathbf{k}) = 2(V_x \cos k_x - V_y \cos k_y) \quad (10)$$

for d type, and

$$\gamma(\mathbf{k}) = 2i \sum_{\tau=\alpha,\beta,\gamma} V'_\tau \sin k_\tau \quad (11)$$

with $k_\gamma = -k_\alpha - k_\beta$ for f type. Hereafter, we assume $V_\tau = V'_\tau = V = 0.1t$. Note that the space inversion of the s - and d -type cross-hopping integrals has even parity, while that of the p - and f -type ones has odd parity. Also, when there are no cross-hopping integrals, the ground state of our two-band model at half filling is a band insulator for $U', D \gg U$, while it is a Mott insulator for $U', D \ll U$, and the excitonic insulator state appears in the intermediate region [44,50,51].

B. Mean-field theory

We use the mean-field theory to obtain the ground state of the model. The excitonic order parameter is given by

$$\begin{aligned} \Phi_q &= \frac{1}{L^2} \sum_{j,\sigma,\sigma'} e^{-iq \cdot \mathbf{r}_j} \langle \hat{c}_{j,\sigma}^\dagger T_{\sigma,\sigma'}(l) \hat{f}_{j,\sigma'} \rangle \\ &= \frac{1}{L^2} \sum_{\mathbf{k},\sigma,\sigma'} \langle \hat{c}_{\mathbf{k}+\mathbf{q},\sigma}^\dagger T_{\sigma,\sigma'}(l) \hat{f}_{\mathbf{k},\sigma'} \rangle, \end{aligned} \quad (12)$$

where $T(l) = l_0 I + \mathbf{l} \cdot \boldsymbol{\sigma}$ with $l = (l_0, \mathbf{l})$ and $\mathbf{l} = (l_1, l_2, l_3)$, satisfying $l_0^2 + \mathbf{l} \cdot \mathbf{l} = 1$ for real numbers l_r ($r = 0, 1, 2, 3$). L^2 is the number of lattice sites in the system. In this paper, we assume the spin-triplet excitonic order of the spin direction along the z axis: i.e., $T(l) = \sigma_z$. Note that the energy of the spin-singlet excitonic order ($l_0 \neq 0$ and $\mathbf{l} = 0$) and that of the spin-triplet excitonic order ($l_0 = 0$ and $\mathbf{l} \neq 0$) are the same in the present model. However, we implicitly assume the presence of the exchange interactions like Hund's rule coupling, which stabilizes the spin-triplet excitonic order [38]. We do not consider the spin-singlet excitonic order, which may be stabilized in the presence of strong electron-phonon couplings [39].

If we restrict ourselves to the case $\mathbf{q} = 0$ (direct gap), the excitonic ordering changes the matrix $\gamma(\mathbf{k})$ as

$$\gamma(\mathbf{k}) \rightarrow \gamma'_\sigma(\mathbf{k}) = \gamma(\mathbf{k}) - \frac{U'}{2} \sigma \Phi_0^*. \quad (13)$$

The symmetry of the excitonic order depends on the phases of the hybridization term $\gamma(\mathbf{k})$ and order parameter Φ_0 . The mean-field Hamiltonian of the two-band Hubbard model may then read

$$\hat{\mathcal{H}}_{\text{MF}} = \sum_{\mathbf{k},\sigma} (\hat{c}_{\mathbf{k},\sigma}^\dagger \hat{f}_{\mathbf{k},\sigma}^\dagger) \begin{pmatrix} \varepsilon'_c(\mathbf{k}) & \gamma'_\sigma(\mathbf{k}) \\ \gamma'^*_\sigma(\mathbf{k}) & \varepsilon'_f(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k},\sigma} \\ \hat{f}_{\mathbf{k},\sigma} \end{pmatrix} + 2L^2 \varepsilon_0, \quad (14)$$

with

$$\varepsilon'_c(\mathbf{k}) = 2g_c(\mathbf{k}) + \frac{D}{2} - \frac{n}{4}(U - 2U') - \mu_0, \quad (15)$$

$$\varepsilon'_f(\mathbf{k}) = 2g_f(\mathbf{k}) - \frac{D}{2} + \frac{n}{4}(U - 2U') - \mu_0, \quad (16)$$

$$\gamma'_\sigma(\mathbf{k}) = 2h(\mathbf{k}) - \frac{U'}{2} \sigma |\Phi_0^\dagger| e^{-i\phi}, \quad (17)$$

$$\varepsilon_0 = -\left(\frac{N}{4}\right)^2 (U + 2U') - \left(\frac{n}{4}\right)^2 (U - 2U') + \frac{U'}{4} |\Phi_0^\dagger|^2, \quad (18)$$

where we define $g_{c(f)}(\mathbf{k}) = t_{c(f)} \sum_\tau \cos k_\tau$, $h(\mathbf{k}) = \sum_\tau (V_\tau \cos k_\tau + i V'_\tau \sin k_\tau)$, and $\mu_0 = \mu - \frac{N}{4}(U + 2U')$. The number of electrons per unit cell is given by $N = \frac{1}{L^2} \sum_{\mathbf{k},\sigma} (\langle \hat{n}_{\mathbf{k},\sigma}^f \rangle + \langle \hat{n}_{\mathbf{k},\sigma}^c \rangle)$, where $N = 2$ is for the half-filled band, and the difference between the numbers of c and f electrons is given by $n = \frac{1}{L^2} \sum_{\mathbf{k},\sigma} (\langle \hat{n}_{\mathbf{k},\sigma}^f \rangle - \langle \hat{n}_{\mathbf{k},\sigma}^c \rangle)$.

We define the $\mathbf{q} = 0$ spin-triplet excitonic order parameter as

$$\Phi_0^\dagger = |\Phi_0^\dagger| e^{i\phi} = \frac{1}{L^2} \sum_{\mathbf{k},\sigma} \sigma \langle \hat{c}_{\mathbf{k},\sigma}^\dagger \hat{f}_{\mathbf{k},\sigma} \rangle, \quad (19)$$

where ϕ is the phase of the complex order parameter and $\sigma = \pm 1$. The mean-field Hamiltonian can be diagonalized by the Bogoliubov transformation

$$\begin{pmatrix} \hat{\alpha}_{\mathbf{k},\sigma,+} \\ \hat{\alpha}_{\mathbf{k},\sigma,-} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k},\sigma} & e^{i\theta_{\mathbf{k},\sigma}} v_{\mathbf{k},\sigma} \\ e^{-i\theta_{\mathbf{k},\sigma}} v_{\mathbf{k},\sigma} & -u_{\mathbf{k},\sigma} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k},\sigma} \\ \hat{f}_{\mathbf{k},\sigma} \end{pmatrix}, \quad (20)$$

where we take $u_{\mathbf{k},\sigma}$ and $v_{\mathbf{k},\sigma}$ to be real, and $v_{\mathbf{k},\sigma}$ is multiplied by the phase factor $e^{i\theta_{\mathbf{k},\sigma}}$. This assumption does not lose generality because the relative phase of $u_{\mathbf{k},\sigma}$ and $v_{\mathbf{k},\sigma}$ is fixed in the Bogoliubov transformation. Since the Bogoliubov transformation is unitary, the identity $|u_{\mathbf{k},\sigma}|^2 + |v_{\mathbf{k},\sigma}|^2 = 1$ is satisfied. Thus, we obtain the diagonalized mean-field Hamiltonian as

$$\hat{\mathcal{H}}_{\text{MF}} = \sum_{\mathbf{k},\sigma} (E_{\mathbf{k},\sigma}^+ \hat{\alpha}_{\mathbf{k},\sigma,+}^\dagger \hat{\alpha}_{\mathbf{k},\sigma,+} + E_{\mathbf{k},\sigma}^- \hat{\alpha}_{\mathbf{k},\sigma,-}^\dagger \hat{\alpha}_{\mathbf{k},\sigma,-}) + 2L^2 \varepsilon_0, \quad (21)$$

with the quasiparticle band dispersions

$$E_{k,\sigma}^{\pm} = \eta_k \pm \sqrt{\xi_k^2 + |\gamma'_\sigma(\mathbf{k})|^2}, \quad (22)$$

$$\eta_k = \frac{1}{2}(\varepsilon'_c(\mathbf{k}) + \varepsilon'_f(\mathbf{k})), \quad (23)$$

$$\xi_k = \frac{1}{2}(\varepsilon'_c(\mathbf{k}) - \varepsilon'_f(\mathbf{k})). \quad (24)$$

The transformation coefficients and complex phase factor are given by

$$u_{k,\sigma}^2 = \frac{1}{2} \left(1 + \frac{\xi_k}{\sqrt{\xi_k^2 + |\gamma'_\sigma(\mathbf{k})|^2}} \right), \quad (25)$$

$$v_{k,\sigma}^2 = \frac{1}{2} \left(1 - \frac{\xi_k}{\sqrt{\xi_k^2 + |\gamma'_\sigma(\mathbf{k})|^2}} \right), \quad (26)$$

$$e^{i\theta_{k,\sigma}} = \frac{\gamma'_\sigma(\mathbf{k})}{|\gamma'_\sigma(\mathbf{k})|}. \quad (27)$$

Thus, the self-consistent equations are given by

$$N = \frac{1}{L^2} \sum_{k,\sigma} [f(E_{k,\sigma}^+) + f(E_{k,\sigma}^-)], \quad (28)$$

$$n = \frac{1}{L^2} \sum_{k,\sigma} (u_{k,\sigma}^2 - v_{k,\sigma}^2) [f(E_{k,\sigma}^+) - f(E_{k,\sigma}^-)], \quad (29)$$

$$\Phi_0^l = \frac{1}{L^2} \sum_{k,\sigma} \sigma u_{k,\sigma} v_{k,\sigma} e^{-i\theta_{k,\sigma}} [f(E_{k,\sigma}^+) - f(E_{k,\sigma}^-)], \quad (30)$$

where we define the Fermi distribution function $f(E_{k,\sigma}^{\pm}) = \langle \hat{\alpha}_{k,\sigma,\pm}^\dagger \hat{\alpha}_{k,\sigma,\pm} \rangle = 1/(1 + e^{\beta E_{k,\sigma}^{\pm}})$ using the reciprocal temperature β . We carry out the following calculations at zero temperature.

III. RESULTS AND DISCUSSION

A. Order parameter and k -space spin textures

Let us first discuss the excitonic order parameter focusing on its phase, which can cause the k -space spin textures. When the cross hopping is introduced, the phase of the excitonic order parameter is fixed to a certain value that depends on both types of the cross hopping and electron filling N [43]. The calculated results for the phase diagram are summarized in Fig. 2; the results in the parameter space of (N, U') at $U = 9$ are shown in Figs. 2(a)–2(d) and the results in the parameter space of (N, U) at $U' = 5$ are shown in Figs. 2(e)–2(h). The calculated results for the amplitude $|\Phi_0^l|$ and phase ϕ of the order parameter are also shown in Figs. 2(i)–2(l) at $U = 9.5$ and $U' = 5$ as a function of N . In the normal phase where the order parameter is zero, the system is a band insulator at half filling ($N = 2$) and a metal at $N < 2$. As the number of electrons decreases from $N = 2$, the required U for the excitonic phase transition increases. In the excitonic phase, the phase of the order parameter strongly depends on the types of the cross hopping and N . When the cross hopping is present, the k -space spin texture can emerge, where the splitting of the up-spin and down-spin bands occurs in the excitonic phase as is illustrated in Fig. 3 and Fig. 4. In the following, we discuss

the k -space spin texture in the even-parity (s - and d -type) and odd-parity (p - and f -type) cross-hopping cases separately.

For the s - and d -type cross-hopping integrals (even-parity case), we find that the phase is fixed to $\phi = \pi/2$ at $N = 2$, which decreases with decreasing N monotonically to zero. A finite value of the magnetization emerges, whose sign is opposite to the direction of the excitonic order parameter, in agreement with the preceding study [43]. We define the magnetization of each orbital ($\ell = c, f$) as $m_0^\ell = \frac{1}{2L^2} \sum_{k,\sigma} \sigma \langle \hat{n}_{k,\sigma}^\ell \rangle$, which is calculated in the mean-field approximation $\varepsilon'_\ell(\mathbf{k}) \rightarrow \varepsilon'_\ell(\mathbf{k}) - U\sigma m_0^\ell$ and $\varepsilon_0 \rightarrow \varepsilon_0 + U/2[(m_0^c)^2 + (m_0^f)^2]$. In the case of s -type cross hopping, there occurs the mixing between the orbital diagonal component of the order parameters (or magnetization) and the orbital off-diagonal component of the order parameter (or excitonic order), so that the excitonic order is accompanied necessarily by the magnetization. From Eqs. (17) and (22), we find that the quasiparticle band splits at $\phi \neq \pi/2$ since $h(\mathbf{k})$ is real.

The calculated k -space spin textures (or spin-dependent Fermi surfaces) are shown in Figs. 3(a) and 3(c) for the s - and d -type even-parity cross-hopping integrals, respectively, and the corresponding quasiparticle band dispersions are shown in Figs. 4(a), 4(b), and 4(e). The time-reversal symmetry breaking by the excitonic ordering leads to $E_{k,\sigma}^{\pm} = E_{k,\sigma}^{\pm}$ and $E_{k,\sigma}^{\pm} \neq E_{-k,-\sigma}^{\pm}$, whereby the degeneracy of the up-spin and down-spin bands is lifted along the ω direction. In the case of the s -type cross-hopping integral, the excitonic order splits the up-spin and down-spin bands along the ω direction in the entire k space, resulting in the net spin polarization. In the d -type cross-hopping integral, the excitonic order splits the spin bands as well, but due to the k -dependent spin occupation of the bands (or spin texture), the net spin polarization vanishes. Such a difference caused by the cross-hopping integrals affects the self-consistent equations, thereby giving rise to a qualitative difference in the orders of the excitonic phase transitions [see Figs. 2(i) and 2(k)].

On the other hand, for the p - and f -type cross-hopping integrals (odd-parity case), we find that the phase is fixed to $\phi = 0$ at $N = 2$, increases continuously with decreasing N , and reaches a constant value $\pi/2$ at $N < 1.96$ for the p type and at $N < 1.98$ for the f type. We also find that the excitonic order parameter continuously decreases with decreasing N . Since $h(\mathbf{k})$ is pure imaginary, the degeneracy of the up-spin and down-spin bands is lifted along the k direction (rather than the ω direction) when $\phi \neq 0$. The k -space spin textures are shown in Figs. 3(b) and 3(d) for the p - and f -type cross-hopping integrals, respectively, and the corresponding quasiparticle band dispersions are shown in Figs. 4(c), 4(d), and 4(f). The inversion symmetry breaking by the excitonic ordering leads to $E_{k,\sigma}^{\pm} \neq E_{-k,\sigma}^{\pm}$ and $E_{k,\sigma}^{\pm} = E_{-k,-\sigma}^{\pm}$, whereby the splitting of the up-spin and down-spin bands emerges. The splitting characteristic of the inversion symmetry breaking is clearly visible in the $X'-\Gamma-X$ line of the Brillouin zone [see Figs. 4(c) and 4(d)] as well as in the $K-\Gamma-K'$ line of the Brillouin zone [see Fig. 4(f)].

B. Spin currents

Next, let us discuss the local and global spin currents in the excitonic phases of our model. The global spin current may be

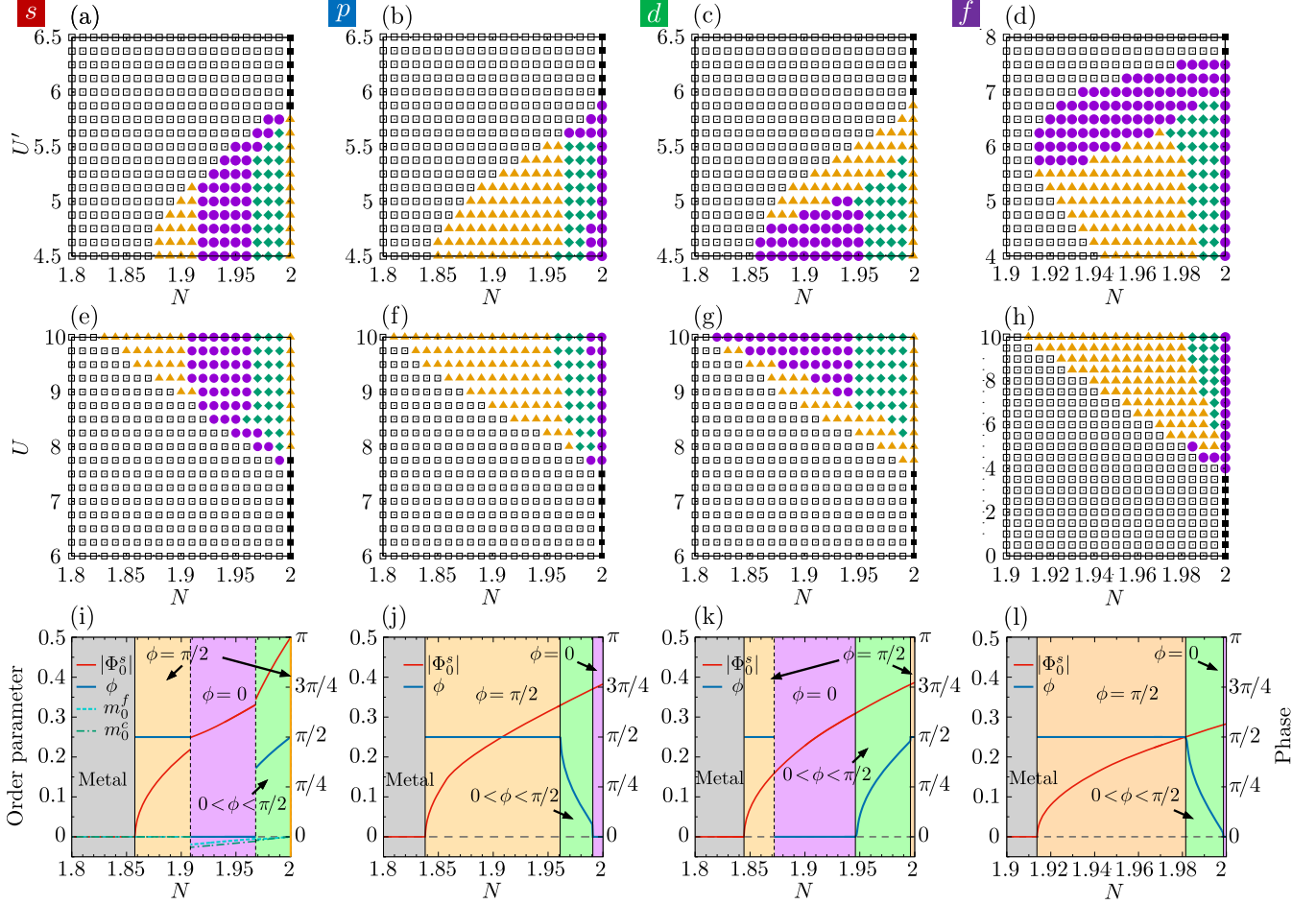


FIG. 2. Calculated phase diagrams of our model in the parameter space of (N, U') at $U = 9$ (upper panels) and (N, U) at $U' = 5$ (middle panels), where N is the number of electrons per site. The cross-hopping integrals of (a),(e) s , (b),(f) p , (c),(g) d , and (d),(h) f type are assumed. Circles, diamonds, and triangles in the phase diagrams represent the excitonic phases with the phase $\phi = 0$, $0 < \phi < \pi/2$, and $\phi = \pi/2$, respectively, and squares represent the normal phase. In the lower panels (i)–(l), we show the calculated amplitude $|\Phi_0^s|$ (red) and phase ϕ (blue) of the excitonic order parameter at $U = 9.5$ and $U' = 5$ as a function of N , where we assume the cross-hopping parameters of (i) s , (j) p , (k) d , and (l) f type. The solid and dotted lines at the phase boundaries represent the second- and first-order phase transitions, respectively.

defined as

$$\hat{\mathbf{J}}_{\text{tot}}^s = \frac{1}{L^2} \sum_{\mathbf{k}, \sigma} \frac{\sigma}{2} (\hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{f}_{\mathbf{k}, \sigma}^\dagger) \nabla_{\mathbf{k}} \begin{pmatrix} \varepsilon'_c(\mathbf{k}) & \gamma'_\sigma(\mathbf{k}) \\ \gamma'^*_{\sigma'}(\mathbf{k}) & \varepsilon'_f(\mathbf{k}) \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}, \sigma} \\ \hat{f}_{\mathbf{k}, \sigma} \end{pmatrix} \quad (31)$$

with $\nabla_{\mathbf{k}} = \sum_{\tau} \mathbf{a}_{\tau} \frac{\partial}{\partial k_{\tau}}$, which may be separated into the orbital diagonal component

$$\hat{\mathbf{J}}_{cc}^s + \hat{\mathbf{J}}_{ff}^s = -\frac{1}{L^2} \sum_{\tau, \mathbf{k}, \sigma} \sigma t_c \sin k_{\tau} \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} \mathbf{a}_{\tau} - \frac{1}{L^2} \sum_{\tau, \mathbf{k}, \sigma} \sigma t_f \sin k_{\tau} \hat{f}_{\mathbf{k}, \sigma}^\dagger \hat{f}_{\mathbf{k}, \sigma} \mathbf{a}_{\tau} \quad (32)$$

and orbital off-diagonal component

$$\hat{\mathbf{J}}_{cf}^s + \hat{\mathbf{J}}_{fc}^s = \frac{1}{L^2} \sum_{\tau, \mathbf{k}, \sigma} \sigma (-V_{\tau} \sin k_{\tau} + i V'_{\tau} \cos k_{\tau}) \hat{c}_{\mathbf{k}, \sigma}^\dagger \hat{f}_{\mathbf{k}, \sigma} \mathbf{a}_{\tau} + \frac{1}{L^2} \sum_{\tau, \mathbf{k}, \sigma} \sigma (-V_{\tau} \sin k_{\tau} - i V'_{\tau} \cos k_{\tau}) \hat{f}_{\mathbf{k}, \sigma}^\dagger \hat{c}_{\mathbf{k}, \sigma} \mathbf{a}_{\tau}. \quad (33)$$

Let us consider the diagonal component first. The expectation value of the diagonal component is given by

$$\langle \hat{\mathbf{J}}_{cc}^s \rangle + \langle \hat{\mathbf{J}}_{ff}^s \rangle = -\frac{t}{L^2} \sum_{\tau, \mathbf{k}, \sigma}^{\text{occ.}} \sigma \frac{\xi_{\mathbf{k}} \sin k_{\tau}}{\sqrt{\xi_{\mathbf{k}}^2 + |\gamma'_{\sigma}(\mathbf{k})|^2}} \mathbf{a}_{\tau}, \quad (34)$$

where occ. means the summation over the \mathbf{k} points at which the quasiparticle band $E_{\mathbf{k}, \sigma}^-$ is occupied. In the even-parity case, we have $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$ and $|\gamma'_{\sigma}(\mathbf{k})|^2 = |\gamma'_{\sigma}(-\mathbf{k})|^2$, which lead to $\langle \hat{\mathbf{J}}_{cc}^s \rangle + \langle \hat{\mathbf{J}}_{ff}^s \rangle = 0$ since the integrand of Eq. (34) becomes an odd function with respect to \mathbf{k} . Therefore, the diagonal

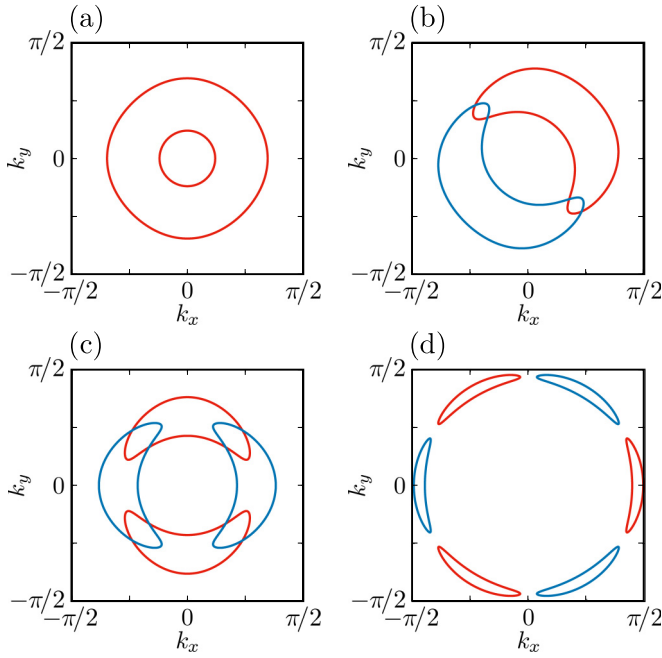


FIG. 3. Calculated k -space spin textures for the (a) s -, (b) p -, (c) d -, and (d) f -type cross-hopping integrals, where the up-spin (red) and down-spin (blue) Fermi surfaces are drawn. We assume $N = 1.94$ in (a), (b), and (c), and $N = 1.98$ in (d). We find $\phi = 0$ in (a) and (c) and $\phi = \pi/2$ in (b) and (d). We set $D = 6$, $U = 9.5$, and $U' = 5$. The areas enclosed by the dotted lines in Figs. 4(g) and 4(h) (see below) are shown.

component of the spin current never appears in the even-parity case. On the other hand, in the odd-parity case with $\phi \neq 0$ excitonic phases, we have $|\gamma'_\sigma(\mathbf{k})|^2 \neq |\gamma'_\sigma(-\mathbf{k})|^2$, which leads to $\langle \hat{\mathbf{J}}_{cc}^s \rangle + \langle \hat{\mathbf{J}}_{ff}^s \rangle \neq 0$. The diagonal component of the spin current calculated for the model with the p -type cross hopping is shown in Fig. 5, where the phase of the order parameter varies continuously from zero to $\pi/2$ with decreasing N [see Fig. 2(j)]. When $\phi = 0$, we have $|\gamma'_\sigma(\mathbf{k})|^2 = |\gamma'_\sigma(-\mathbf{k})|^2$, which leads to $\langle \hat{\mathbf{J}}_{cc}^s \rangle + \langle \hat{\mathbf{J}}_{ff}^s \rangle = 0$. However, when $\phi > 0$, the diagonal component acquires a finite value, which is caused by the spin-dependent band splitting as shown in Fig. 3(b). The value of the diagonal component increases until the phase reaches $\pi/2$, but it decreases by further decreasing N and vanishes when the excitonic order disappears.

Let us next consider the off-diagonal component of the spin current. V_τ and V'_τ in Eq. (33) depend on the types of the cross hopping: In the even-parity case, we have $V_\tau \neq 0$ and $V'_\tau = 0$, and in the odd-parity case, we have $V_\tau = 0$ and $V'_\tau \neq 0$. In the following, we consider the cases with the s - and p -type cross-hopping integrals.

For the s -type cross-hopping integral, we have the off-diagonal component of the spin current as

$$\langle \hat{\mathbf{J}}_{cf}^s \rangle + \langle \hat{\mathbf{J}}_{fc}^s \rangle = \frac{V}{L^2} \sum_{\tau, \mathbf{k}, \sigma}^{\text{occ.}} \sigma \frac{\text{Re}[\gamma'_\sigma(\mathbf{k}) \sin k_\tau]}{\sqrt{\xi_k^2 + |\gamma'_\sigma(\mathbf{k})|^2}} \mathbf{a}_\tau. \quad (35)$$

Since $\gamma'_\sigma(\mathbf{k}) = \gamma'_\sigma(-\mathbf{k})$ in any ϕ , the inversion symmetry remains in the excitonic phase. Therefore, the integrand of Eq. (35) is an odd function with respect to \mathbf{k} , so that $\langle \hat{\mathbf{J}}_{cf}^s \rangle +$

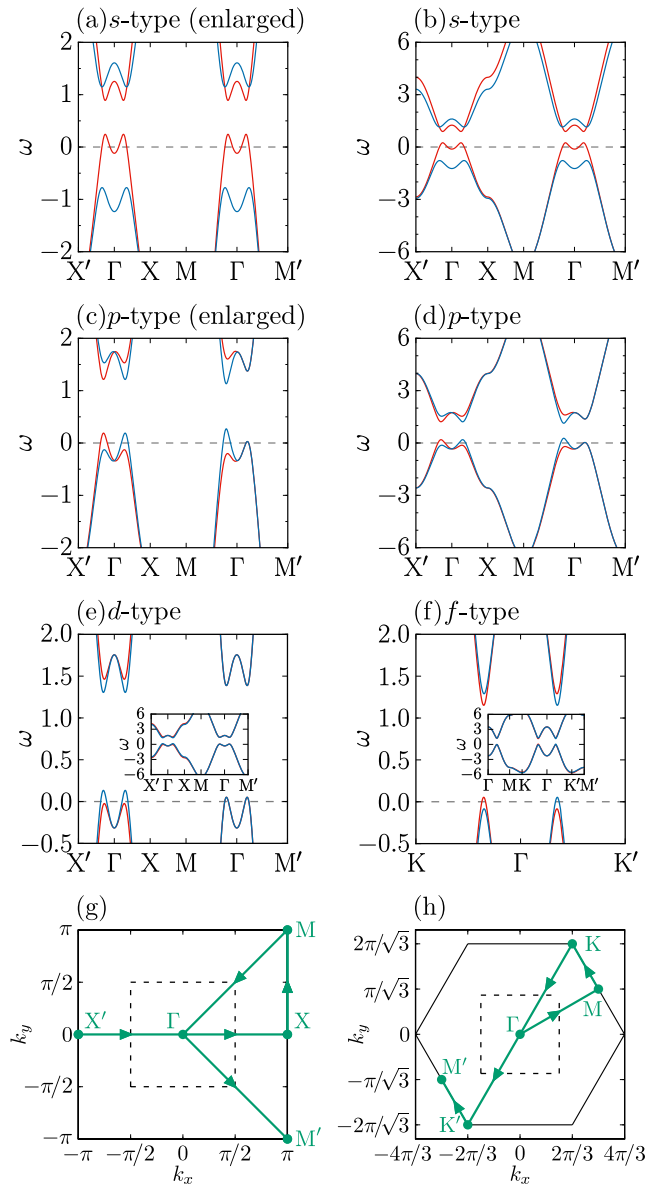


FIG. 4. Calculated quasiparticle band dispersions in the spin-triplet excitonic phases of our model. Their energies ω are plotted in the Brillouin zone. The up-spin (red) and down-spin (blue) bands are illustrated. We assume $N = 1.94$ for the s -, p -, and d -type cross-hopping integrals and $N = 1.98$ for the f -type cross-hopping integrals. We find $\phi = 0$ for the s and d type, and $\phi = \pi/2$ for the p and f type. We set $D = 6$, $U = 9.5$, and $U' = 5$. In (g) and (f), we show the Brillouin zones and the paths along which the band dispersions are drawn.

$\langle \hat{\mathbf{J}}_{fc}^s \rangle = 0$. The same discussion also applies to the case with the d -type cross-hopping integral.

For the p -type cross-hopping integral, we have the off-diagonal component as

$$\langle \hat{\mathbf{J}}_{cf}^s \rangle + \langle \hat{\mathbf{J}}_{fc}^s \rangle = -\frac{V}{L^2} \sum_{\tau, \mathbf{k}, \sigma}^{\text{occ.}} \sigma \frac{\text{Im}[\gamma'_\sigma(\mathbf{k}) \cos k_\tau]}{\sqrt{\xi_k^2 + |\gamma'_\sigma(\mathbf{k})|^2}} \mathbf{a}_\tau. \quad (36)$$

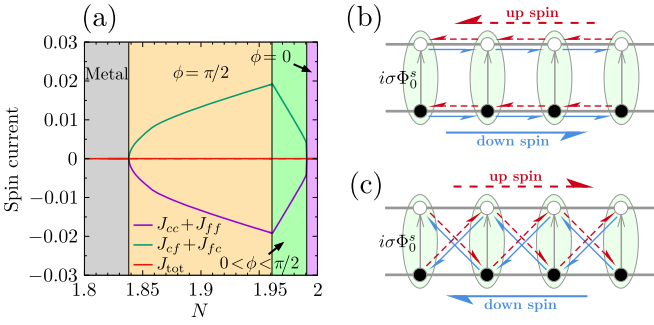


FIG. 5. (a) Calculated local and global spin currents as a function of the electron filling N , where we assume the p -type cross-hopping integral. We set $D = 6$, $U = 9.5$, and $U' = 5$. We also show schematic representations of the local spin currents in (b) and (c), where the diagonal and off-diagonal components are indicated, respectively.

Since $|\gamma'_\sigma(\mathbf{k})|^2 = |\gamma'_\sigma(-\mathbf{k})|^2$ and $\text{Im}[\gamma'_\sigma(\mathbf{k})] = 2V \sum_\tau \sin k_\tau$ at $\phi = 0$, the integrand of Eq. (36) becomes an odd function with respect to \mathbf{k} , which leads to $\langle \hat{\mathbf{J}}_{cf}^s \rangle + \langle \hat{\mathbf{J}}_{fc}^s \rangle = 0$. However, the inequality $\gamma'_\sigma(\mathbf{k}) \neq \gamma'_\sigma(-\mathbf{k})$ at $\phi = \pi/2$ breaks the inversion symmetry, which leads to $\langle \hat{\mathbf{J}}_{cf}^s \rangle + \langle \hat{\mathbf{J}}_{fc}^s \rangle \neq 0$. We obtain the same result whenever $\phi \neq 0$.

The calculated off-diagonal component of the spin current for the p -type cross-hopping integrals is shown in Fig. 5. One might think that this result contradicts the Bloch theorem that the current necessarily vanishes without external fields in the bulk systems. However, we find in Fig. 5 that the sum of the diagonal and off-diagonal components exactly vanishes as

$$\langle \hat{\mathbf{J}}_{\text{tot}}^s \rangle = \langle \hat{\mathbf{J}}_{cc}^s \rangle + \langle \hat{\mathbf{J}}_{ff}^s \rangle + \langle \hat{\mathbf{J}}_{cf}^s \rangle + \langle \hat{\mathbf{J}}_{fc}^s \rangle = 0, \quad (37)$$

which is consistent with the Bloch theorem. Thus, the global spin current always vanishes, in agreement with the identity at zero temperature [46,52]

$$\langle \hat{\mathbf{J}}_{\text{tot}}^s \rangle = \frac{1}{L^2} \sum_{\mathbf{k}, \sigma}^{\text{occ.}} \sigma \nabla_{\mathbf{k}} E_{\mathbf{k}, \sigma}^- = 0. \quad (38)$$

We should emphasize again that the global spin current never appears even if the cross-hopping integrals are added and the carriers are introduced. The same discussion can also be applied to the case of the f -type cross-hopping integrals. However, we note that the relation $\langle \hat{\mathbf{J}}_{\ell\ell'}^s \rangle = 0$ necessarily holds since we have $\sum_\tau \mathbf{a}_\tau = 0$ in the triangular lattice, which results in the vanishing local spin currents. As discussed in the study of superconductivity [48,49] and also in a recent paper by Geffroy *et al.* [47], the ground state containing a finite global current cannot be allowed in the equilibrium system. In our mean-field calculation, we actually find that there is no global spin current but there can be a finite local spin current. As shown here, the origin of the local spin current is the inversion-symmetry breaking in the excitonic phase. We again stress that the Bloch theorem does not prohibit the presence of the local spin currents. The detailed discussions on the absence of the global spin current and the presence of the local spin currents are found in Appendices A and B.

IV. SUMMARY

We studied the k -space spin textures and spin currents in the spin-triplet excitonic phase of the two-band Hubbard model defined on the square and triangular lattices by the mean-field approximation. We assumed the noninteracting band structure with a direct band gap and introduced the s -, p -, d -, and f -type cross-hopping integrals. We thus found that, depending on the types of the cross hopping, interaction strength, and electron filling, the phase of the excitonic order parameter is fixed to be imaginary, whereby the k -space spin texture and local spin current can emerge.

The even-parity cross-hopping integrals of the s and d type lift the spin degeneracy of the band dispersions by the breaking of the time-reversal symmetry, which leads to the k -space spin texture, whereas the local spin current exactly vanishes because the space-inversion symmetry remains in this system. On the other hand, the odd-parity cross-hopping integrals of the p and f type lift the spin degeneracy of the band structures by the breaking of the space-inversion symmetry, which leads to the k -space spin texture as well. Moreover, in the case of the p -type cross-hopping integral, the local spin currents of the diagonal and off-diagonal components remain finite when the excitonic order parameter has the imaginary value. The global spin current always vanishes, which is consistent with the Bloch theorem.

The experimental observation of the k -space spin textures and local spin currents may, therefore, be very useful for verification of the presence of the spin-triplet excitonic orders. We hope that our results will encourage experimental confirmations of the excitonic phases in real materials.

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APPENDIX A: ABSENCE OF THE GLOBAL SPIN CURRENT

Here, we discuss the absence of the global spin current in spin-triplet excitonic insulator states from the viewpoint of the Bloch theorem. First, we introduce the spin current from the continuity equation in the d -dimensional lattice containing L^d sites and define the global and local (or partial) spin currents. Next, we derive the Bloch theorem for the global spin current and examine its correspondence with the results of our mean-field calculations.

1. Global and local spin currents

The current operators may be derived from the continuity conditions of the Hamiltonian as [53]

$$\frac{\partial}{\partial t} \hat{S}_j^z = i[\hat{\mathcal{H}}, \hat{S}_j^z] = - \sum_{\tau} (\hat{J}_{(j,\tau)}^z - \hat{J}_{(j,-\tau)}^z), \quad (\text{A1})$$

where $\hat{J}_{(j,\tau)}^z$ denotes the operator of the spin current flowing out from site j to $j + \tau$ and $\hat{S}_j^z = 1/2 \sum_{\sigma} \sigma (\hat{n}_{j\sigma}^c + \hat{n}_{j\sigma}^f)$. We note that this argument is justified if and only if the system has the axial spin rotational symmetry about the z axis, R_z , and the expectation value of the z component of the total spin operator is conserved. Thus, we assume in the following discussions that the system has the symmetry R_z . The spin current operators $\hat{J}_{(j,\tau)}^z$ may then be divided into the orbital diagonal and orbital off-diagonal components as

$$\hat{J}_{(j,\tau),cc}^z = -it_c/2 \sum_{\sigma} \sigma (\hat{c}_{j+\tau,\sigma}^{\dagger} \hat{c}_{j,\sigma} - \text{H.c.}), \quad (\text{A2})$$

$$\hat{J}_{(j,\tau),ff}^z = -it_f/2 \sum_{\sigma} \sigma (\hat{f}_{j+\tau,\sigma}^{\dagger} \hat{f}_{j,\sigma} - \text{H.c.}), \quad (\text{A3})$$

$$\hat{J}_{(j,\tau),cf}^z = -iV_{1,\tau}/2 \sum_{\sigma} \sigma (\hat{c}_{j+\tau,\sigma}^{\dagger} \hat{f}_{j,\sigma} - \text{H.c.}), \quad (\text{A4})$$

$$\hat{J}_{(j,\tau),fc}^z = -iV_{2,\tau}/2 \sum_{\sigma} \sigma (\hat{f}_{j+\tau,\sigma}^{\dagger} \hat{c}_{j,\sigma} - \text{H.c.}). \quad (\text{A5})$$

Then, the global spin current flowing in the direction τ may be defined as

$$L^d \hat{J}_{\tau}^z = \sum_j \hat{J}_{(j,\tau)}^z = \frac{1}{2} \sum_{\mathbf{k}\sigma} \sigma (\hat{c}_{\mathbf{k},\sigma}^{\dagger} \hat{f}_{\mathbf{k},\sigma}^{\dagger}) \frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_{\tau}} \begin{pmatrix} \hat{c}_{\mathbf{k},\sigma} \\ \hat{f}_{\mathbf{k},\sigma} \end{pmatrix} \quad (\text{A6})$$

with

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \varepsilon_c(\mathbf{k}) & \gamma(\mathbf{k}) \\ \gamma^*(\mathbf{k}) & \varepsilon_f(\mathbf{k}) \end{pmatrix}, \quad (\text{A7})$$

where the τ denotes the vector from site j to site $j + \tau$. Note that the interaction terms of the Hamiltonian Eq. (3) do not contribute to the spin current operators.

Similarly, the partial spin current may be defined as

$$L^d \hat{J}_{\tau,ll'}^z = \sum_j \hat{J}_{(j,\tau),ll'}^z, \quad (\text{A8})$$

where l and l' ($= c, f$) denote the orbitals. We also define the difference between the orbital diagonal and orbital off-diagonal spin currents as

$$\begin{aligned} \hat{J}_{\tau}^{l'z} &= \hat{J}_{\tau,cc}^z + \hat{J}_{\tau,ff}^z - \hat{J}_{\tau,cf}^z - \hat{J}_{\tau,fc}^z \\ &= \frac{1}{2L^d} \sum_{\mathbf{k}\sigma} \sigma (\hat{c}_{\mathbf{k},\sigma}^{\dagger} \hat{f}_{\mathbf{k},\sigma}^{\dagger}) \tau_z \frac{\partial \mathcal{H}(\mathbf{k})}{\partial k_{\tau}} \tau_z \begin{pmatrix} \hat{c}_{\mathbf{k},\sigma} \\ \hat{f}_{\mathbf{k},\sigma} \end{pmatrix}, \quad (\text{A9}) \end{aligned}$$

where τ^z denotes the z component of the Pauli matrix. We may then obtain the orbital diagonal and orbital off-diagonal spin currents as $\hat{J}_{\tau}^{(+)} = \hat{J}_{\tau}^z + \hat{J}_{\tau}^{l'z}$ and $\hat{J}_{\tau}^{(-)} = \hat{J}_{\tau}^z - \hat{J}_{\tau}^{l'z}$, respectively.

Here, we note that the orbital-decomposed partial spin currents may be termed as the *local* spin currents if the orbitals are located in different spatial positions, as is assumed in the main text. The global (or total) spin current may then be defined as a sum of the local (or partial) spin currents. We also note that the global spin current if it exists may obviously be observed experimentally but the local spin currents should in principle be observed experimentally as well, which can lead to an experimental proof of the existence of the spin-triplet

excitonic insulator state. In the Appendices A and B, we use the term ‘‘partial’’ spin current rather than ‘‘local’’ spin current.

2. The Bloch theorem

Now, let us prove the Bloch theorem for our system, which states that the persistent spin current does not exist in thermal equilibrium without any external fields. The proof is carried out in the following two steps [49]. First, we introduce the excited state generated by an infinitesimal twisting of the spin-dependent Peierls phase in the hopping parameters. Secondly, using the inequality originated from the passivity (defined below) of thermal equilibrium states, we show on the basis of the dimensional analysis that a contradiction is lead if we assume the existence of the global spin current. In this proof, we assume that the system is under the periodic boundary condition in all the orthogonal directions.

First, we introduce the spin-dependent Peierls phase using the twist operator defined as

$$\hat{U}(\boldsymbol{\varphi}) = \exp \left(i \boldsymbol{\varphi} \cdot \sum_{l,j,\sigma} \sigma \hat{n}_{l,j,\sigma}^{\dagger} \mathbf{r}_j \right), \quad (\text{A10})$$

where $\boldsymbol{\varphi}$ denotes a vector in the reciprocal lattice space, which satisfies $L\boldsymbol{\varphi} \cdot \mathbf{a}_i = 0$ and its amplitude characterizes the intensity of the flux penetrating a one-dimensional ring. Thus, the vector $\boldsymbol{\varphi}$ can be written as

$$\boldsymbol{\varphi} = \frac{1}{L} \sum_j m_j \mathbf{b}_j = \mathcal{O}(L^{-1}), \quad m_j \in \mathbb{Z}, \quad (\text{A11})$$

where $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}$. Here, we assume the integers $m_j \in \mathbb{Z}$ are sufficiently smaller than L , so that the vector $\boldsymbol{\varphi}$ has the order of L^{-1} . Using this twist operator, the fermion creation and annihilation operators with momentum \mathbf{k} are transformed into the other fermion operators with momentum $\mathbf{k} - \sigma\boldsymbol{\varphi}$ as

$$\hat{U}^{\dagger}(\boldsymbol{\varphi}) \hat{c}_{\mathbf{k},\sigma} \hat{U}(\boldsymbol{\varphi}) = \hat{c}_{\mathbf{k}-\sigma\boldsymbol{\varphi},\sigma}, \quad (\text{A12})$$

$$\hat{U}^{\dagger}(\boldsymbol{\varphi}) \hat{c}_{\mathbf{k},\sigma}^{\dagger} \hat{U}(\boldsymbol{\varphi}) = \hat{c}_{\mathbf{k}-\sigma\boldsymbol{\varphi},\sigma}^{\dagger}, \quad (\text{A13})$$

$$\hat{U}^{\dagger}(\boldsymbol{\varphi}) \hat{f}_{\mathbf{k},\sigma} \hat{U}(\boldsymbol{\varphi}) = \hat{f}_{\mathbf{k}-\sigma\boldsymbol{\varphi},\sigma}, \quad (\text{A14})$$

$$\hat{U}^{\dagger}(\boldsymbol{\varphi}) \hat{f}_{\mathbf{k},\sigma}^{\dagger} \hat{U}(\boldsymbol{\varphi}) = \hat{f}_{\mathbf{k}-\sigma\boldsymbol{\varphi},\sigma}^{\dagger}, \quad (\text{A15})$$

where we note that the shifted momentum $\mathbf{k} - \sigma\boldsymbol{\varphi}$ is in the Brillouin zone. Because thermal equilibrium states are passive (or energetically stable) for any local unitary transformation [49,54], we can introduce the following inequality:

$$\omega_0(\hat{U}^{\dagger}(\boldsymbol{\varphi})[\hat{\mathcal{H}}, \hat{U}(\boldsymbol{\varphi})]) \geq 0, \quad (\text{A16})$$

where $\omega_0(\dots)$ is defined as the expectation value with respect to the infinite thermodynamical equilibrium state. In particular, if the N -fermion system has a unique ground state $|\Phi_0^{(N)}\rangle$ at zero temperature, $\omega_0(\dots)$ may be rewritten as

$$\omega_0(\dots) = \lim_{L \rightarrow \infty} \langle \Phi_0^{(N)} | \dots | \Phi_0^{(N)} \rangle, \quad (\text{A17})$$

where we take the infinite volume limit $L \rightarrow \infty$ so that the density $\rho = N/L^d$ converges to a finite positive constant.

Using the twist operator, we then obtain

$$\begin{aligned} \hat{U}^\dagger(\boldsymbol{\varphi})[\hat{\mathcal{H}}, \hat{U}(\boldsymbol{\varphi})] &= 2\boldsymbol{\varphi} \cdot \sum_{\mathbf{k}\sigma} \frac{\sigma}{2} (\hat{c}_{\mathbf{k},\sigma}^\dagger \hat{f}_{\mathbf{k},\sigma}^\dagger) \nabla_{\mathbf{k}} \mathcal{H}(\mathbf{k}) \begin{pmatrix} \hat{c}_{\mathbf{k},\sigma} \\ \hat{f}_{\mathbf{k},\sigma} \end{pmatrix} \\ &+ \mathcal{O}(L^{d-2}), \end{aligned} \quad (\text{A18})$$

where the first term of the right-hand side corresponds to the global spin current defined in Eq. (A6). If the system has a nonzero bulk spin current, this term is of the order of L^{d-1} . Thus, we find

$$\begin{aligned} \frac{1}{L^d} \omega_0(\hat{U}^\dagger(\boldsymbol{\varphi})[\hat{\mathcal{H}}, \hat{U}(\boldsymbol{\varphi})]) \\ = \frac{4\pi}{L} \sum_{\tau} m_{\tau} \omega_0(\hat{J}_{\tau}^z) + \mathcal{O}(L^{-2}) \geq 0, \end{aligned} \quad (\text{A19})$$

where we note that the vector $\boldsymbol{\varphi}$ is arbitrary, so that we can take any values of m_{τ} . Now, if we assume the presence of the positive global spin current, i.e., $\omega(\hat{J}_{\tau}^z) > 0$, then choosing all m_{τ} to be negative, we obtain $\sum_{\tau} m_{\tau} \omega_0(\hat{J}_{\tau}^z) < 0$, which contradicts the passivity condition Eq. (A16). Therefore, we find that the global spin current does not exist. In other words, the axial spin rotational symmetry about the z axis is not broken in the ground state of the system. We also note that the above argument cannot be applied to the case of the surface currents. If the system has only the surface currents, the leading order of Eq. (A19) becomes L^{-2} . Therefore, the Bloch theorem does not prohibit the existence of the surface currents. Similarly, the bulk spin current is robust against surface defects because of the same reasons. As discussed in Appendix B, such a dimensional analysis can also be applied to the proof of the existence of the partial spin currents, which are not prohibited by the Bloch-like theorem in general.

3. Absence of the global spin current in the mean-field approximation

Here, we discuss the validity of the Bloch theorem in the straightforward mean-field calculation. In general, the Bloch theorem is applicable to any interacting electron systems with the axial spin rotational symmetry and therefore should be valid in the mean-field approximation as well. Using the Hellmann-Feynman theorem [55], we obtain

$$\begin{aligned} \langle \hat{\mathbf{J}}_{\text{tot}}^s \rangle &= \frac{1}{L^d} \sum_{\tau, \mathbf{k}, \sigma} \sigma \left(\frac{\partial E_{\mathbf{k},\sigma}^+}{\partial \mathbf{k}_{\tau}} f(E_{\mathbf{k},\sigma}^+) + \frac{\partial E_{\mathbf{k},\sigma}^-}{\partial \mathbf{k}_{\tau}} f(E_{\mathbf{k},\sigma}^-) \right) \mathbf{a}_{\tau} \\ &= \frac{1}{L^d} \sum_{\mathbf{k}, \sigma, \nu=\pm} \sigma (\nabla_{\mathbf{k}} E_{\mathbf{k},\sigma}^{\nu}) f(E_{\mathbf{k},\sigma}^{\nu}), \end{aligned} \quad (\text{A20})$$

where ν denotes the band index. Using the density of states defined as

$$D_{\nu,\sigma}(E) dE = \frac{L^d}{(2\pi)^d} \left[\int_{E_{\mathbf{k},\sigma}^{\nu}=E} \frac{dl}{|\nabla_{\mathbf{k}} E_{\mathbf{k},\sigma}^{\nu}|} \right] dE, \quad (\text{A21})$$

where dl is the surface element in \mathbf{k} space satisfying $E_{\mathbf{k},\sigma}^{\nu} = E$, we can rewrite Eq. (A20) as

$$\begin{aligned} \langle \hat{\mathbf{J}}_{\text{tot}}^s \rangle &= \frac{1}{L^d} \sum_{\sigma, \nu} \sigma \int D_{\nu,\sigma}(E_{\sigma}^{\nu}) (\nabla_{\mathbf{k}} E_{\mathbf{k},\sigma}^{\nu}) f(E_{\sigma}^{\nu}) dE_{\sigma}^{\nu} \\ &= \frac{1}{(2\pi)^d} \sum_{\sigma, \nu} \sigma \int dE_{\sigma}^{\nu} f(E_{\sigma}^{\nu}) \int \mathbf{n} dl = 0 \end{aligned} \quad (\text{A22})$$

with $\mathbf{n} = \nabla_{\mathbf{k}} E_{\mathbf{k},\sigma}^{\nu} / |\nabla_{\mathbf{k}} E_{\mathbf{k},\sigma}^{\nu}|$. The integral over the closed constant-energy surface vanishes $\int \mathbf{n} dl = 0$, resulting in the vanishing global spin current.

APPENDIX B: EXISTENCE OF THE PARTIAL SPIN CURRENT

Here, we discuss the existence of the partial spin current in spin-triplet excitonic insulator states. First, we make the Bloch-like argument for the partial spin current [defined in Eq. (A9)] as an application of the method given in Appendix A. Next, we make the argument based on the discrete lattice symmetries.

1. Argument based on the Bloch-like theorem

Introducing the operator defined as

$$\hat{W} = \exp \left\{ i \frac{\pi}{2} \sum_{j,\sigma} (\hat{c}_{j,\sigma}^\dagger \hat{f}_{j,\sigma}^\dagger) \tau^z \begin{pmatrix} \hat{c}_{j,\sigma} \\ \hat{f}_{j,\sigma} \end{pmatrix} \right\}, \quad (\text{B1})$$

we find that the fermion creation and annihilation operators for the c - and f -band electrons are transformed as

$$\hat{W}^\dagger \hat{c}_{j,\sigma} \hat{W} = i \hat{c}_{j,\sigma}, \quad (\text{B2})$$

$$\hat{W}^\dagger \hat{c}_{j,\sigma}^\dagger \hat{W} = -i \hat{c}_{j,\sigma}^\dagger, \quad (\text{B3})$$

$$\hat{W}^\dagger \hat{f}_{j,\sigma} \hat{W} = -i \hat{f}_{j,\sigma}, \quad (\text{B4})$$

$$\hat{W}^\dagger \hat{f}_{j,\sigma}^\dagger \hat{W} = i \hat{f}_{j,\sigma}^\dagger. \quad (\text{B5})$$

Thus, using this operator \hat{W} and the twist operator defined in Eq. (A6), we obtain

$$\begin{aligned} \frac{1}{L^d} (\hat{U}(\boldsymbol{\varphi}) \hat{W})^\dagger [\hat{\mathcal{H}}, (\hat{U}(\boldsymbol{\varphi}) \hat{W})] \\ = \frac{1}{L^d} \sum_{\mathbf{k}, \sigma} (\hat{c}_{\mathbf{k},\sigma}^\dagger \hat{f}_{\mathbf{k},\sigma}^\dagger) \tau^z [\mathcal{H}_{\sigma}(\mathbf{k}), \tau^z] \begin{pmatrix} \hat{c}_{\mathbf{k},\sigma} \\ \hat{f}_{\mathbf{k},\sigma} \end{pmatrix} \\ + 2\boldsymbol{\varphi} \cdot \hat{\mathbf{J}}^z + \mathcal{O}(L^{-2}), \end{aligned} \quad (\text{B6})$$

where we note that the first and second terms of the right-hand side are of the orders 1 and L^{-1} , respectively, if we assume that the bulk partial spin current exists. However, unless the commutator $[\mathcal{H}_{\sigma}(\mathbf{k}), \tau_z]$ is zero, the straightforward Bloch-like argument cannot be applied to the present case. In other words, because the first term is larger than the second one, we do not obtain the contradiction to the passivity of the thermal equilibrium states. Thus, in general, the partial spin current is not prohibited by the Bloch-like argument as long as there is the interorbital hybridization satisfying $[\hat{W}, \hat{\mathcal{H}}] \neq 0$. In this

sense, vanishing of the expectation value of the first term is a sufficient condition to prohibit the partial spin current. It should be noted that this condition is already broken in systems with the cross-hopping terms. However, the partial spin current does not appear in the normal phases, which is due to the other conditions associated with the lattice symmetries. As discussed below, the partial spin current emerges as a result of the “inversion” symmetry breaking in the excitonic phases.

2. Argument based on the discrete lattice symmetries

Now, let us prove the existence of the partial spin current from the viewpoint of the symmetries that are broken in the excitonic phases. Our strategy is based on the following two assumptions: (i) The ground state of our system is unique. (ii) There is no symmetry operation \hat{g} that anticommutes with the current operator \hat{J}_τ . These two assumptions are naturally applicable to our mean-field solutions obtained as the stationary points of the free energy. The relevance of these assumptions may be confirmed as follows: If there is at least one symmetry operation \hat{g} that anticommutes with the current operator $\{\hat{g}, \hat{J}_\tau\} = 0$, we obtain

$$0 = \langle \psi | \hat{g}^{-1} \{ \hat{J}_\tau, \hat{g} \} | \psi \rangle = 2 \langle \psi | \hat{J}_\tau | \psi \rangle, \quad (\text{B7})$$

where we use the uniqueness of the ground state, i.e., $\hat{g} |\Psi\rangle = e^{i\theta} |\Psi\rangle$ except for an arbitrary phase θ . Thus, we find that the

partial spin current is absent as long as the conditions (i) and (ii) are satisfied.

Next, let us examine the symmetries of our two-band Hubbard model. For simplicity, we consider the symmetries of the one body part of the Hamiltonian only and treat the interaction terms within the mean-field approximation. It is, however, not difficult to extend our argument to the interacting systems. As discussed in the main text, we have two types of the cross-hopping integrals, i.e., either with *even* parity (*s* type) or with *odd* parity (*p* type), where the latter has a sign change $\mathbf{k} \rightarrow -\mathbf{k}$ for the spatial inversion. The mean-field Hamiltonian transforms under the time-reversal symmetry operation (\mathcal{T}) or under the space-inversion symmetry operation (\mathcal{P}) as

$$\mathcal{T}\mathcal{H}(\mathbf{k})\mathcal{T}^{-1} = \mathcal{H}(-\mathbf{k}), \quad (\text{B8})$$

$$\mathcal{P}\mathcal{H}(\mathbf{k})\mathcal{P}^{-1} = \mathcal{H}(-\mathbf{k}), \quad (\text{B9})$$

where we note that \mathcal{P} is a unitary operator satisfying $\mathcal{P}^2 = 1$ while \mathcal{T} is an antiunitary operator containing the complex conjugate operation \mathcal{K} .¹ In our system, there are several candidates for these symmetry operations, which depend on both the parity of the cross-hopping term $l \in \{s, p\}$ and the phase of the excitonic order parameter $\phi \in \{0, \frac{\pi}{2}\}$. To see this explicitly, it is instructive to rewrite our mean-field Hamiltonian using the Pauli matrices as

$$\mathcal{H}_{\text{MF}}(\mathbf{k}) = \varepsilon'_+(\mathbf{k}) I_2 \otimes I_2 + \varepsilon'_-(\mathbf{k}) \tau^z \otimes I_2 + \begin{cases} \gamma_+(\mathbf{k}) \tau^x \otimes I_2 + \Delta_0 \tau^x \otimes \sigma^z, & (l, \phi) = (s, 0) \\ \gamma_+(\mathbf{k}) \tau^x \otimes I_2 + \Delta_\pi \tau^y \otimes \sigma^z, & (l, \phi) = (s, \frac{\pi}{2}) \\ \gamma_-(\mathbf{k}) \tau^y \otimes I_2 + \Delta_0 \tau^x \otimes \sigma^z, & (l, \phi) = (p, 0) \\ \gamma_-(\mathbf{k}) \tau^y \otimes I_2 + \Delta_\pi \tau^y \otimes \sigma^z, & (l, \phi) = (p, \frac{\pi}{2}) \end{cases} \quad (\text{B10})$$

where

$$2\varepsilon'_\pm(\mathbf{k}) = \varepsilon'_c(\mathbf{k}) \pm \varepsilon'_f(\mathbf{k}), \quad (\text{B11})$$

$$\gamma_+(\mathbf{k}) = 2 \sum_\tau V_\tau \cos k_\tau, \quad (\text{B12})$$

$$\gamma_-(\mathbf{k}) = 2 \sum_\tau V_\tau \sin k_\tau, \quad (\text{B13})$$

$$2\Delta_\phi = -U' |\Phi_0^l| e^{-i\phi}, \quad (\text{B14})$$

and \otimes denotes the tensor product of two matrices. τ^α and σ^α denote the Pauli matrices for the orbital and spin degrees of freedom, respectively. We note that $\gamma_-(\mathbf{k})$ is an odd function with respect to the inversion $\mathbf{k} \rightarrow -\mathbf{k}$. Then, if we note the relations $\{\sigma^a, \sigma^b\} = \{\tau^a, \tau^b\} = 2\delta_{ab}$ and $\{\tau^y, \mathcal{K}\} = \{\sigma^y, \mathcal{K}\} = 0$, we can easily write down the time-reversal \mathcal{T} and space inversion \mathcal{P} symmetries such that Eqs. (B8) and (B9) are satisfied. In fact, we can choose $\mathcal{T} = I_2 \otimes \sigma^x \mathcal{K}$ and

$\mathcal{P} = \tau^z \otimes \sigma^x$ for $(l, \phi) = (p, \frac{\pi}{2})$. For other (l, ϕ) , we can also choose \mathcal{T} and \mathcal{P} in the same manner.

Then, let us examine whether our mean-field Hamiltonian has the time-reversal \mathcal{T} or space-inversion \mathcal{P} symmetry that satisfies the condition (ii) given above. Using the mean-field Hamiltonian, the global and partial spin currents in Eqs. (A6) and (A9) can be rewritten, respectively, as

$$\mathcal{J}_\tau^z(\mathbf{k}) = \partial_\tau \varepsilon'_+(\mathbf{k}) I_2 \otimes \sigma^z + \partial_\tau \varepsilon'_-(\mathbf{k}) \tau^z \otimes \sigma^z + \begin{cases} \partial_\tau \gamma_+(\mathbf{k}) \tau^x \otimes \sigma^z & (l = s) \\ \partial_\tau \gamma_-(\mathbf{k}) \tau^y \otimes \sigma^z & (l = p) \end{cases} \quad (\text{B15})$$

$$\mathcal{J}_\tau^{l,z}(\mathbf{k}) = \partial_\tau \varepsilon'_+(\mathbf{k}) I_2 \otimes \sigma^z + \partial_\tau \varepsilon'_-(\mathbf{k}) \tau^z \otimes \sigma^z - \begin{cases} \partial_\tau \gamma_+(\mathbf{k}) \tau^x \otimes \sigma^z & (l = s) \\ \partial_\tau \gamma_-(\mathbf{k}) \tau^y \otimes \sigma^z & (l = p) \end{cases} \quad (\text{B16})$$

where we use the following notations:

$$\hat{\mathcal{O}} = \sum_{\mathbf{k}} \hat{\mathbf{c}}_{\mathbf{k}}^\dagger \mathcal{O}(\mathbf{k}) \hat{\mathbf{c}}_{\mathbf{k}}, \quad (\text{B17})$$

$$\hat{\mathbf{c}}_{\mathbf{k}} = (\hat{c}_{\mathbf{k},\uparrow}, \hat{f}_{\mathbf{k},\uparrow}, \hat{c}_{\mathbf{k},\downarrow}, \hat{f}_{\mathbf{k},\downarrow})^T, \quad (\text{B18})$$

$$\hat{\mathbf{c}}_{\mathbf{k}}^\dagger = (\hat{c}_{\mathbf{k},\uparrow}^\dagger, \hat{f}_{\mathbf{k},\uparrow}^\dagger, \hat{c}_{\mathbf{k},\downarrow}^\dagger, \hat{f}_{\mathbf{k},\downarrow}^\dagger). \quad (\text{B19})$$

¹Note that we use a general definition Eq. (B8) of the time-reversal symmetry operation in this Appendix; another definition, which uses the antiunitary operator that changes the signs of \mathbf{k} and spin, does not satisfy the condition (ii).

TABLE I. The time-reversal and space-inversion symmetries for the mean-field Hamiltonian with the indexes (l, ϕ) . ω and $\omega\mathcal{K}$ (\cdot^{-}) denote the system with (without) time-reversal symmetry $\mathcal{T} = \omega\mathcal{K}$ or space-inversion symmetry $\mathcal{P} = \omega$. Here, ω is the unitary matrix defined as $\omega = e^{i\phi I_2 \otimes \sigma^z} = \cos \phi I_2 \otimes I_2 + i \sin \phi I_2 \otimes \sigma^z$. Note that the other time-reversal or space-inversion symmetries, which anti-commute with the spin current operators, do not exist except for $\mathcal{T} = \omega\mathcal{K}$ and $\mathcal{P} = \omega$.

	global		partial	
	\mathcal{T}	\mathcal{P}	\mathcal{T}	\mathcal{P}
$(l, \phi) = (s, 0)$	$\omega\mathcal{K}$	ω	$\omega\mathcal{K}$	ω
$(l, \phi) = (s, \frac{\pi}{2})$	-	ω	-	ω
$(l, \phi) = (p, 0)$	$\omega\mathcal{K}$	-	$\omega\mathcal{K}$	-
$(l, \phi) = (p, \frac{\pi}{2})$	-	-	-	-

By a straightforward calculation, we obtain the time-reversal symmetry \mathcal{T} and space-inversion symmetry \mathcal{P} that satisfy the relations $\mathcal{T}\hat{J}_\tau^z(\mathbf{k})\mathcal{T}^{-1} = -\hat{J}_\tau^z(-\mathbf{k})$ and $\mathcal{P}\hat{J}_\tau^z(\mathbf{k})\mathcal{P}^{-1} = -\hat{J}_\tau^z(-\mathbf{k})$, which correspond to the anticommutation relation for the partial spin current operator \hat{J}_τ^z , as shown in Table I.

In particular, if $(l, \phi) = (p, \pi/2)$, we find that there is no corresponding time-reversal \mathcal{T} or space-inversion \mathcal{P} symmetries in the system. In other words, because the mean-field Hamiltonian does not satisfy the condition (ii), the global

and partial spin currents are allowed by the symmetries \mathcal{T} and \mathcal{P} . However, the global spin current is prohibited by the Bloch theorem, so that only the partial spin current is allowed. Moreover, such symmetry breakings in the excitonic phase may lead to the asymmetry of the band structures, resulting in the k -space spin textures. In this sense, the partial spin current is a signature of the absence of the time-reversal \mathcal{T} and space-inversion \mathcal{P} symmetries in the system. It should be noted, however, that we do not deny the possible existence of the other symmetries that satisfy the conditions (i) and (ii). In fact, the model with the f -type cross hopping has the threefold rotational symmetry C_3 . Then, even if both the time-reversal \mathcal{T} and space-inversion \mathcal{P} symmetries are broken in the excitonic phase, the partial spin currents are canceled out due to the C_3 symmetry.

Finally, let us make a remark on our derivation of the partial spin currents. In this appendix, we use two approaches to prove the existence of the partial spin current. However, we should note that the arguments given in both of these two approaches are not the necessary condition, but they are the sufficient condition for the absence of the partial spin current. In other words, the existence of the partial spin currents is allowed only if the system has the cross hopping satisfying $[\hat{W}, \hat{\mathcal{H}}] \neq 0$ and does not satisfy the conditions (i) and (ii). Thus, if the system does not have the cross hopping satisfying $[\hat{W}, \hat{\mathcal{H}}] \neq 0$, the partial spin currents are prohibited by the Bloch-like argument, irrespective of whether condition (i) and (ii) are satisfied.

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