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Topological aspects of the quantum spin-Hall effect in graphene: Z_2 topological order and spin Chern number

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For generic time-reversal-invariant systems with spin-orbit couplings, we clarify a close relationship between the Z_2 topological order and the spin Chern number (SChN) in the quantum spin-Hall effect. It turns out that a global gauge transformation connects sectors with different SChNs (even integers) modulo 4, which implies that the SChN and Z_2 topological orders yield the same classification. We present a method of computing the SChN and demonstrate it in single and double planes of graphene.

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Topological orders[1,2] play a crucial role in the classification of various phases in low-dimensional systems. The integer quantum Hall effect (IQHE) is one of the most typical examples,[3,4] in which the quantized Hall conductance is given by a topological invariant, the Chern number (ChN), due to the Berry potential induced in the Brillouin zone. Such a topological feature should be more fundamental, since it has a close relationship with the parity anomaly of Dirac fermions.[5–7]

Recently, the spin-Hall effect[8–11] has been attracting much current interest as a new device of so-called spintronics. In particular, Kane and Mele[12,13] have found a new class of insulator showing the quantum spin-Hall (QSH) effect[14–16] which should be realized in graphene with spin-orbit couplings. They have pointed out[13] that the QSH state can be specified by a Z_2 topological order which is inherent in time-reversal- ($\mathcal{T}$-) invariant systems. This study is of fundamental importance, since the Z_2 order is involved with the Z_2 anomaly of Majorana fermions.[17,18]

On the other hand, Sheng *et al.*[19] have recently computed the spin-Hall conductance by imposing a spin-dependent twisted boundary condition (BC), generalizing the idea of Niu *et al.*[2,20] They have shown that it is given by a ChN which is referred to as SChN below. This is very natural, since the QSH effect is a spin-related version of the IQHE. The SChN for graphene computed by Sheng *et al.* indeed has a good correspondence with the classification by Z_2. A more general BC has been also discussed by Qi *et al.*[21] However, the ChN is specified by the set of integers Z, not by Z_2. Although the studies by Sheng *et al.*[19] suggest a close relationship between two topological orders, natural questions arise: How does the concept Z_2 enter into the classification by ChNs or, otherwise, does the SChN carry additional information?

In this Rapid Communication, we clarify the relationship for the generic $\mathcal{T}$-invariant systems. We show that while the two sectors in the Z_2 classification are separated by topological changes due to *bulk gap-closing phenomena*, each of these sectors is further divided into many sectors by *boundary-induced topological changes* in the SChN classification. The latter is an artifact which is due to broken translational invariance and broken $\mathcal{T}$ invariance at the boundary. Therefore, the different SChN in each sector of Z_2 describe the same topologically ordered states of the bulk.

Consider generic electron systems on a lattice with $\mathcal{T}$ symmetry, described by the Hamiltonian H. Denote the electron creation operator at the jth site as $c_j^\dagger=(c_{\uparrow j}^\dagger,c_{\downarrow j}^\dagger)$. Then, the $\mathcal{T}$ transformation is defined by $c_j\to\mathcal{T}c_j$ with $\mathcal{T}\equiv i\sigma^2K$, where the Pauli matrix σ^2 operates the spin space and K stands for the complex conjugation operator. Let $\mathcal{H}(k)$ be the Fourier-transformed Hamiltonian defined by $H=\Sigma_k c^\dagger(k)\mathcal{H}(k)c(k)$ and let $|n(k)\rangle$ be an eigenstate of $\mathcal{H}(k)$. Assume that the ground state is composed of an M-dimensional multiplet of degenerate single-particle states which is a generalized noninteracting Fermi sea.[2] Kane and Mele[13] have found that the $\mathcal{T}$-invariant systems have two kinds of important states belonging to "even" subspace and "odd" subspace: The states in the even subspace have the property that $|n(k)\rangle$ and $\mathcal{T}|n(k)\rangle$ are identical, which occurs when $\mathcal{T}\mathcal{H}(k)\mathcal{T}^{-1}=\mathcal{H}(k)$. By definition, the states at $k=(0,0)$, $(0,\pi)$, $(\pi,0)$, and (π,π) always belong to this subspace. The odd subspace has the property that the multiplet $|n(k)\rangle$ is orthogonal to the multiplet $\mathcal{T}|n(k)\rangle$. These special subspaces can be detected by the Pfaffian $p_{\rm KM}(k)\equiv \mathrm{pf}\langle n(k)|\mathcal{T}|m(k)\rangle$. Namely, $p_{\rm KM}(k)=1$ in the even subspace and 0 in the odd subspace. Kane and Mele (KM) have claimed that the number of zeros of $p_{\rm KM}(k)$ which always appears as $\mathcal{T}$ pairs $\pm k^*$ with opposite vorticities is a topological invariant for $\mathcal{T}$-invariant systems. Specifically, if the number of zeros in half the Brillouin zone is 1 (0) mod 2, the ground state is in the QSH (insulating) phase.

We now turn to the SChN proposed by Sheng *et al.*[19] According to their formulation, we impose spin-dependent (-independent) twisted BC along the 1- (2-) direction:

$$c_{j+L_1\hat{1}}=e^{i\theta_1\sigma^3}c_j,\quad c_{j+L_2\hat{2}}=e^{i\theta_2}c_j, \tag{1}$$

where a set of integers $j\equiv(j_1,j_2)$ specifies the site and $\hat{1}$ and $\hat{2}$ stand for the unit vectors in the 1- and 2-directions, respectively. Let $\mathcal{H}(\theta)$ denote the twisted Hamiltonian, and let $|n(\theta)\rangle$ be corresponding eigenstate. The torus spanned by θ is referred to as twist space. It follows from Eq. (1) that $\mathcal{T}$ transformation induces $\mathcal{T}\mathcal{H}(\theta_1,\theta_2)\mathcal{T}^{-1}=\mathcal{H}(\theta_1,-\theta_2)$, and therefore we can always choose $|n(\theta_1,-\theta_2)\rangle=\mathcal{T}|n(\theta_1,\theta_2)\rangle$ except for $\theta_2=0,\pi$. The states on the *lines* $\theta_2=0,\pi$ belong to the even subspace. The BC (1) enables us to define the SChN, but the cost we have to pay is broken translational invariance as well as broken $\mathcal{T}$ invariance at the boundary. The former implies that while the twist into the j_2 direction just shifts the momentum $k_2\to k_2+\theta_2/L_2$ after a gauge transformation (GT), the twist into the j_1 direction cannot be described by such a shift of k_1. The latter may be important to computing the SChN, since experimentally observed spin accumulation at the boundaries of samples[10,11] is also due to broken $\mathcal{T}$ invariance.

Let us define a Pfaffian for the present twisted system as a function of the twist angles:

$$p(\theta)\equiv \mathrm{pf}\langle n(\theta)|\mathcal{T}|m(\theta)\rangle,\quad n,m=1,\ldots,M, \tag{2}$$

where M (even) is a number of one-particle states below the Fermi energy. Here, we assume that these states are separated from others by a finite gap. Since the lines $\theta_2=0,\pi$ belong to the even subspace, the zeros of the Pfaffian in the $\theta_2>0$ or <0 twist space can move only among the same half twist space keeping their vorticities and never cross the $\theta_2=0,\pi$ lines. Therefore, only one $\mathcal{T}$ pair of zeros cannot be annihilated, like those of the KM Pfaffian $p_{\rm KM}(k)$. Furthermore, the two zeros in the same half twist space are never annihilated unless they have opposite vorticities. This is a crucial difference between the KM Pfaffian and the twist Pfaffian. The number of zeros in the twist Pfaffian may be classified by even integers.

Are these Pfaffians topologically different quantities? The answer is no. To show this, let us consider a global GT $c_j\to g(\varphi)c_j$, where

$$g(\varphi)\equiv e^{i\sigma^2\varphi}=\cos\varphi+i\sigma^2\sin\varphi. \tag{3}$$

This GT replaces the the Pauli matrices in the spin-orbit couplings into $g^{\rm t}(\varphi)\sigma g(\varphi)=(\cos 2\varphi\sigma^1-\sin 2\varphi\sigma^3,\sigma^2,\cos 2\varphi\sigma^3+\sin 2\varphi\sigma^1)$. On the other hand, since Eq. (3) is an orthogonal transformation, the one-parameter family of transformed Hamiltonian, denoted by H^φ or $\mathcal{H}^\varphi(\theta)$ below, is equivalent. The Pfaffian (2) is also invariant. Therefore, when we are interested in the bulk properties, we can deal with any Hamiltonian H^φ. So far we have discussed the bulk properties. However, if we consider finite periodic systems like Eq. (1), a family of the Hamiltonian H^φ behaves as different models. It follows from Eq. (1) that the GT (3) is commutative with $e^{i\theta_2}$, but *not* with $e^{i\theta_1\sigma^3}$. This tells us that the spin-dependent twisted BC is not invariant under the GT (3) and breaks the gauge equivalence of the Hamiltonian H^φ which the bulk systems should have.

To understand this, the following alternative consideration may be useful: If we want to study the bulk properties of $\mathcal{T}$-invariant systems, we can start with any of H^φ. For one H^φ with φ fixed, let us impose the twisted BC (1). After that, we can make the GT (3) back to H^0. Then, we can deal with the same Hamiltonian H^0, but with a gauge-dependent twisted BC for the 1-direction:

$$c_{j+L_1\hat{1}}=e^{i\theta_1(\cos 2\varphi\sigma^3-\sin 2\varphi\sigma^1)}c_j. \tag{4}$$

Namely, the gauge equivalence is broken only by the BC in the 1-direction. Now, imagine a situation that at $\varphi=0$ the Pfaffian (2) has one $\mathcal{T}$ pair of zeros. We denote them as $(\theta_1^*,\pm\theta_2^*)$ with vorticity $\pm m$. Let us change φ smoothly from 0 to $\pi/2$. Then, it follows from Eq. (4) that at $\varphi=\pi/2$ the coordinate of the torus is changed from (θ_1,θ_2) into $(-\theta_1,\theta_2)$ and, therefore, we find the zeros at $(-\theta_1^*,\pm\theta_2^*)$ with vorticity $\mp m$. Namely, the zero in the $\theta_2>0$ (<0) space moves into the $\theta_2<0$ (>0) space, and thus the zeros can move in the whole twist space like those of the KM Pfaffian. During the process, there should occur a topological change, but it is attributed to the boundary—i.e., an artifact of broken translational invariance—and a number of the zeros of the twist Pfaffian should be also classified by Z_2, by taking into account the GT (3).

Using this Pfaffian, we next show that its zeros can be detectable by computing the SChN. The SChN[19] is defined by $c_{\rm s}=\frac{1}{2\pi i}\int d^2\theta F_{12}(\theta)$, where $F_{12}(\theta)\equiv\partial_1A_2(\theta)-\partial_2A_1(\theta)$ is the field strength due to the U(1) part of the (non-Abelian) Berry potential,[2] $A_\mu(\theta)\equiv \mathrm{tr}\langle n(\theta)|\partial_\mu|m(\theta)\rangle$, with $\partial_\mu=\partial/\partial\theta_\mu$. First, we will show the relationship between the zeros of the twist Pfaffian and the SChN $c_{\rm s}$. For the time being, we fix φ. The degenerate ground state as the M-dimensional multiplet has a local U(M) gauge degree of freedom, $|n(\theta)\rangle\to\Sigma_m|m(\theta)\rangle V_{mn}(\theta)$, where $V(\theta)$ is a unitary matrix.[2] Let us denote $V(\theta)=e^{i\alpha(\theta)/M}\tilde{V}(\theta)$, where $\det\tilde{V}(k)=1$. This transformation induces $A_\mu(\theta)\to A_\mu(\theta)+i\partial_\mu\alpha(\theta)$ to the Berry potential. If one can make a gauge-fixing globally over the whole twist space, the ChN is proved to be zero. Only if the global gauge-fixing is impossible can the ChN be nonzero.

Among various kinds of gauge fixing, we can use the gauge that $p(\theta)$ *is real positive*, because $p(\theta)\to p(\theta)\det V(\theta)=p(\theta)e^{i\alpha(\theta)}$. This rule can fix the gauge of the Berry potential except for $p(\theta)=0$. Therefore, nontrivial SChN is due to an obstruction[22] to the smooth gauge fixing by the twist Pfaffian. This correspondence also proves that *the SChN is an even integer*, since the Pfaffian (2) always has the $\mathcal{T}$ pair zeros and since $F_{12}(\theta_1,-\theta_2)=F_{12}(\theta_1,\theta_2)$.

Let us now change φ. At $\varphi=0$, we obtain some integer $c_{\rm s}$. Remember that at $\varphi=\pi/2$, the coordinate of the torus is changed into $(-\theta_1,\theta_2)$. Therefore, we have a mapping $c_{\rm s}\to -c_{\rm s}$ for $(\theta_1,\theta_2)\to(-\theta_1,\theta_2)$. As in the case of the Pfaffian (2), we expect topological changes along the mapping. However, as stressed, these changes are accompanied by *no gap closing in the bulk spectrum*, just induced by the symmetry-breaking *boundary* term which is an artifact to define the ChN. Therefore, the states with $\pm c_{\rm s}$ should belong to an equivalent topological sector. Since the minimum nonzero SChN is 2, we expect $c_{\rm s}$ mod 4 (if we define the SChN in half the twist space, mod 2) to classify the topological sectors.

So far we have discussed the Z_2 characteristics of the SChN $c_{\rm s}$. We next present several examples. To this end, we employ an efficient method of computing ChNs proposed in Ref. 23 based on recent developments in lattice gauge theories.[24] We first discretize the twist space $[0,2\pi]\otimes[0,2\pi]$ into a square lattice such that $\theta_\mu=2\pi j_\mu/N_\mu$, where $j_\mu=1,\ldots,N_\mu$.[25] We denote the sites on this lattice as θ_ℓ with $\ell=1,2,\ldots,N_1N_2$. We next define a U(1) link variable associated with the ground-state multiplet of dimension M,

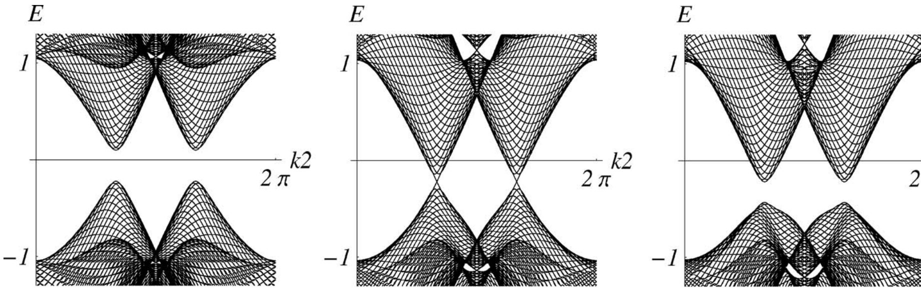

FIG. 1. Spectrum for $\theta_1=0$ as a function of k_2. Parameters used are $V_{\rm so}=0.1t$, $v_{\rm s}=0.3t$, and $V_{\rm R}=0.1t$ (left), $V_{\rm R}=0.225207t$ (middle), and $V_{\rm R}=0.3t$ (right).

$U_\mu(\theta_\ell)=|\det \boldsymbol{U}_\mu(\theta_\ell)|^{-1}\det \boldsymbol{U}_\mu(\theta_\ell)$, where $\boldsymbol{U}_\mu(\theta_\ell)_{mn}=\langle m(\theta_\ell)|n(\theta_\ell+\hat{\mu})\rangle$ with $n,m=1,\ldots,M$ denotes the (non-Abelian) Berry link variable. Here, $\hat{\mu}$ is the vector in μ direction with $|\hat{\mu}|=2\pi/N_\mu$. Next define the lattice field strength $F_{12}(\theta_\ell)=\ln U_1(\theta_\ell)U_2(\theta_\ell+\hat{1})U_1^{-1}(\theta_\ell+\hat{2})U_2^{-1}(\theta_\ell)$, where we choose the branch of the logarithm as $|F_{12}(\theta_\ell)|<\pi$. Finally, the manifestly *gauge invariant* lattice SChN is obtained:

$$c_{\rm s}=\frac{1}{2\pi i}\sum_\ell F_{12}(\theta_\ell). \tag{5}$$

As shown in Ref. 23, the SChN thus defined is strictly *integral*. To see this, let us introduce a lattice gauge potential $A_\mu(\theta_\ell)=\ln U_\mu(\theta_\ell)$ which is also defined in $|A_\mu(\theta_\ell)|<\pi$. Note that this field is periodic, $A_\mu(\theta_\ell+N_\mu)=A_\mu(\theta_\ell)$. Then, we readily find $F_{12}(\theta_\ell)=\Delta_1A_2(\theta_\ell)-\Delta_2A_1(\theta_\ell)+2\pi i n_{12}(\theta_\ell)$, where Δ_μ stands for the difference operator and $n_{12}(\theta_\ell)$ is a local *integral* field which is referred to as the n-field. Finally, we reach $c_{\rm s}=\Sigma_\ell n_{12}(\theta_\ell)$. This completes the proof that the SChN is integral. While the n-field depends on a gauge, the sum is invariant. For the $\mathcal{T}$-invariant systems, *the Pfaffian (2) is very useful for the gauge fixing* also for the lattice computation. In the continuum theory, we have stressed that the zeros of the Pfaffian play a central role in the Z_2 classification. Since such zeros occur at several specific points in the twist space, it is very hard to search them numerically.

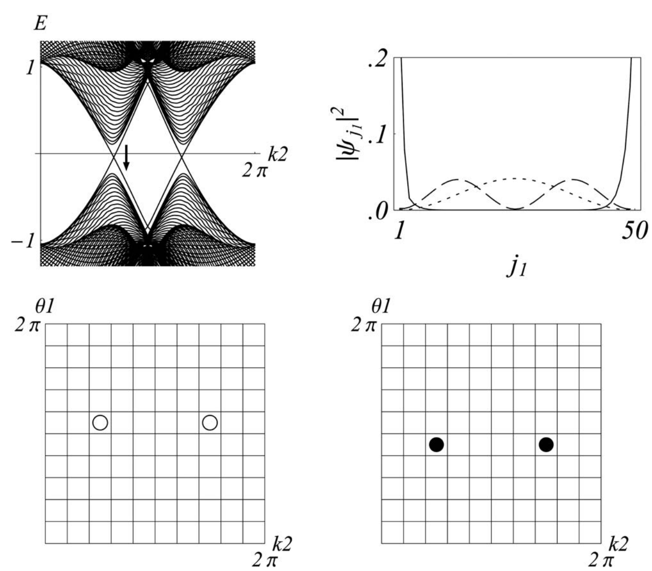

FIG. 2. Upper left: spectrum for nonzero $\varphi=\pi/4$ as a function of k_2 at $\theta_1=\pi/2$. Other parameters are the same as those of the left in Fig. 1. Upper right: the amplitude $|\psi_{j_1}|^2$ of the wave functions at $k_2=0.8\pi$ indicated by arrow. The solid, dotted, and dashed lines correspond to the first, second, and third states from the zero energy into negative energy, respectively. Lower left and right: the n-field configuration corresponding to the left in Fig. 1. The left (right) is at $\varphi=0$ $(\pi/2)$. The white (black) circle denotes $n=1(-1)$, while the blank means $n=0$. We used the meshes $N_1=N_2=10$.

Contrary to this, we can detect the zeros in the lattice approach as follows: Suppose that we obtain the exact SChN using Eq. (5) with sufficiently large N_μ. Since the lattice SChN is topological (integral), which implies that even if we slightly change the lattice (e.g., change the lattice size or infinitesimally shift the lattice), the SChN remains unchanged. Next, let us compute the n-field in the gauge that *the Pfaffian is real positive*. If the zeros of the Pfaffian happen to locate on sites of the present lattice, we cannot make gauge fixing. Even in such cases we can always avoid the zeros of the Pfaffian by redefining the lattice with the SChN kept unchanged. Thus we can always compute the well-defined n-field configuration. If the SChN is nonzero, there exist nonzero n-fields anywhere in the twist space. These nonzero n-fields occur in general near the zeros of the Pfaffian: Thus, without searching them in the continuum twist space, *we can find the zeros by the nonzero n-fields on a lattice*.

Now let us study a graphene model[12,13,19]

$$H=-t\sum_{\langle i,j\rangle}c_i^\dagger c_j+\frac{2i}{\sqrt{3}}V_{\rm so}\sum_{\langle\langle i,j\rangle\rangle}c_i^\dagger\boldsymbol{\sigma}\cdot(\boldsymbol{d}_{kj}\times\boldsymbol{d}_{ik})c_j$$
$$+iV_{\rm R}\sum_{\langle i,j\rangle}c_i^\dagger(\boldsymbol{\sigma}\times\boldsymbol{d}_{ij})^3c_j+v_{\rm s}\sum_j\ \mathrm{sgn}\,j c_j^\dagger c_j. \tag{6}$$

Analyzing the KM Pfaffian, Kane and Mele[12] have derived the Phase diagram: It is in the QSH phase for $|6\sqrt{3}V_{\rm so}-v_{\rm s}|>\sqrt{v_{\rm s}^2+9V_{\rm R}^2}$ and in the insulating phase otherwise. Sheng *et al.*[19] have computed the SChN $c_{\rm s}=2$ in the QSH phase and 0 in the insulating phase.

For numerical computations, it is convenient to use the momentum k_2 instead of θ_2 (Ref. 19) because of the translational invariance along this direction even with the BC (1). First, we show in Fig. 1 the spectrum at $\theta_1=0$ as a function of k_2. The left belongs to the QSH phase with $c_{\rm s}=2$, whereas the right to the insulating phase with $c_{\rm s}=0$. This topological change is due to the gap closing in the *bulk* spectrum, as shown in the middle figure in Fig. 1. Therefore, the phase with $c_{\rm s}=2$ is topologically distinguishable from the phase with $c_{\rm s}=0$.

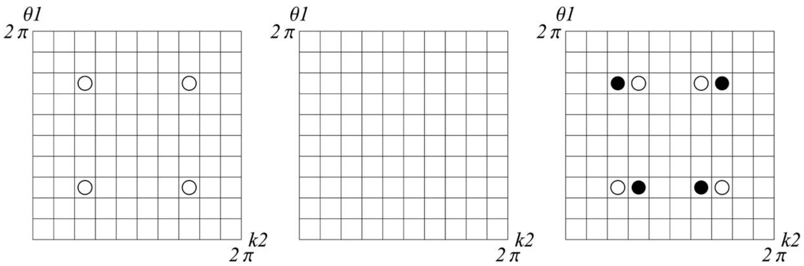

FIG. 3. The n-field configuration for $\gamma_1=0.1t$. Other parameters are same as those of the left in Fig. 1. Left: $\varphi_1=0$ and $\varphi_2=0$ ($c_s=4$). Middle: $\varphi_1=\pi/2$ and $\varphi_2=0$ ($c_s=0$). Right: $\varphi_1=\pi/4$ and $\varphi_2=-\pi/4$ ($c_s=0$). In the case $\varphi_1=\pi/2$ and $\varphi_2=\pi/2$ we have the same figure as the left but with black circles ($c_s=-4$). We used the meshes $N_1=N_2=10$.

Contrary to this, how about the phases with $c_s=\pm 2$? As we have mentioned, the phase with c_s changes into $-c_s$ when we vary φ from 0 to $\pi/2$. In this process, *boundary*-induced topological changes must occur. We show in Fig. 2 the spectrum cut at $\theta_1=\pi/2$ for $\varphi=\pi/4$. We indeed observe a gap closing at finite θ_1, and the SChN $c_s=2$ for $0\leqslant\varphi<\pi/4$ is changed into $c_s=-2$ for $\pi/4<\varphi\leqslant\pi/2$. As stressed, this change is attributed to the boundary (edge states in Fig. 2): Because of the spin-dependent twisted BC, some states can be pinned around $j_1=1$ and L_1 lines. We refer to such midgap states as edge states. The wave function denoted by the solid line in Fig. 2 is indeed localized around $j_1=1$ and $L_1=50$, not to the bulk, and we conclude that the phase $c_s=\pm 2$ is classified as the same QSH phase. These SChNs $c_s=\pm 2$ are well visualized by the n-field. In Fig. 2, we also show the n-field for $\varphi=0$ and $\pi/2$ cases in the QSH phase. The points of the nonzero n-field are closely related with the positions of the Pfaffian zeros.

Next, let us study a bilayer graphene. Suppose that we have two decoupled sheets of graphene described by H^{φ_i} with $i=1,2$ whose lattices include A, B sites and $\tilde{A}$, $\tilde{B}$ sites, respectively. For simplicity, we take into account only the interlayer coupling γ_1 between $\tilde{A}$ and B (Ref. 26): $V_{12}=\gamma_1\Sigma_j c^\dagger_{1\tilde{A},j}c_{2B,j}+\text{H.c.}$, where $i=1,2$ in $c_{i,j}$ indicate the ith sheet. Now make GT (3) separately for each sheet to obtain the same H^0 as Eq. (6). Then, we have an identical bilayer system $H^0\otimes H^0$ coupled by $V_{12}=\gamma_1\Sigma_j c^\dagger_{1\tilde{A},j}g(\varphi_1)g^{\text{t}}(\varphi_2)c_{2B,j}+\text{H.c.}$ with two independent BCs $c_{i,j+L_1\hat{1}}=e^{i\theta_1(\cos 2\varphi_i\sigma^3+\sin 2\varphi_i\sigma^1)}c_{i,j}$.

For the same parameters as those of the left in Fig. 1, the SChN is, of course, $c_s=2+2=4$ in the limit $\gamma_1=0$. This SChN remains unchanged for small but finite interlayer coupling γ_1. However, taking into account the GT $g(\varphi_i)$, it changes. In Fig. 3, we show examples of the n-field for $\gamma_1=0.1t$. We have the SChNs 4, 0, and -4 (see the figure caption): All of them are denoted as $c_s=0$ mod 4, which belong to the insulating phase.[27] A detail analysis of this model including the interlayer coupling γ_3 will be published elsewhere.

Finally, we mention that Fu and Kane[28] and Moore and Balents[29] have recently discussed the relationship between the Z_2 order and the SChN and reached a similar conclusion. The Z_2 classification in 3D has been also discussed in Refs. 29–31.

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