

Chern numbers in two-dimensional systems with spiral boundary conditions

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(Received 3 January 2024; revised 8 July 2024; accepted 7 August 2024; published 23 August 2024)

We discuss methods for calculating Chern numbers of two-dimensional lattice systems using spiral boundary conditions, which sweep all lattice sites in one-dimensional order. Specifically, we establish the one-dimensional representation of Fukui-Hatsugai-Suzuki's method, based on lattice gauge theory, and the Coh-Vanderbilt's method, which relates to electronic polarization. The essential point of this discussion is that the insertion of flux into the extended one-dimensional chain generates an effective current in the perpendicular direction. These methods are valuable not only for a unified understanding of topological physics in different dimensions but also for numerical calculations.

DOI: [10.1103/PhysRevB.110.075144](https://doi.org/10.1103/PhysRevB.110.075144)

I. INTRODUCTION

For over a decade, there has been extensive research on topological phases and transitions in the context of topological insulators [1–7]. Topological insulators exhibit energy gaps in the bulk and gapless edge (surface) states in two (three) dimensions. The concept of topology has been further extended to include topological superconductors, Kitaev systems, non-Hermitian skin effects, and other related phenomena [8–10].

On the other hand, the study of topological phases and transitions in one-dimensional (1D) quantum spin systems has been ongoing since the 1970s. For instance, the dimer-Néel transition in a spin-1/2 frustrated anisotropic Heisenberg chain and the successive dimerization observed in Haldane gap systems are interpreted as transitions between different gapped phases that possess distinct topological properties [11–14].

In this paper, we present a unified study of topological phases and transitions in various systems and dimensions using the concept of electronic polarization and related concepts [15–18]. In 1D lattice electron systems, we introduce polarization operator (or twist operator) U defined as the exponential of the position operator, and consider its expectation value in the ground state $|\Psi_0\rangle$,

$$z = \langle \Psi_0 | U | \Psi_0 \rangle, \quad U = \exp \left(i \frac{2\pi}{L} \sum_{j=1}^L j n_j \right). \quad (1)$$

Here, L represents the number of sites and n_j is the electron number operator at the j th site. Resta established a relationship between z and electronic polarization, given by $\lim_{L \rightarrow \infty} (e/2\pi) \text{Im} \ln z$ [16]. The signs of z provide information about the system's topology, such as the presence of charge or spin-density waves and edge states [19,20]. Furthermore, the condition $z = 0$ can be utilized to detect phase transition points.

The same quantity as in Eq. (1) was also introduced in the Lieb-Schultz-Mattis (LSM) theorem for 1D quantum systems [21–25]. In the LSM theorem, Eq. (1) appears as an overlap

between the ground state and a variational excited state. According to the theorem, an energy gap above nondegenerate ground state is possible for $z \neq 0$ with $L \rightarrow \infty$.

Thus the property of z has been well studied for 1D systems. However, its application to higher-dimensional systems is not fully discussed. In our preceding paper [26], we have extended the twist operator in Eq. (1) to two-dimensional (2D) systems using spiral boundary conditions (SBCs) that encompass all lattice sites in one-dimensional order as illustrated in Fig. 1. These boundary conditions have been utilized to extend the LSM theorem to higher dimensions [27–29], eliminating unphysical limitations on the system size [30]. By calculating z with SBCs, we have examined the 2D Wilson-Dirac model [31,32] and identified topological transition points as $z = 0$.

However, the aforementioned extension does not account for transverse response, so that it does not include the information of the Chern number. Therefore, z needs to be modified to incorporate the flux effect, which is perpendicular to the twist direction. For conventional periodic boundary conditions (PBCs), this extension was carried out by Coh and Vanderbilt for the Haldane model [33]. On the other hand, Fukui, Hatsugai, and Suzuki proposed a method to calculate the Chern number based on the lattice gauge theory [34]. Therefore, we aim to elucidate the relationship between the Coh-Vanderbilt's method and the Fukui-Hatsugai-Suzuki's method. Subsequently, we derive the formalism of electronic polarization with SBCs to identify the system's topology by Chern numbers.

This paper is organized as follows. In Sec. II, we provide a review of the two methods for calculating Chern numbers in lattice systems. Next, in Sec. III, we discuss the justification of twist operators with SBCs and establish the correspondence between wave numbers in conventional PBCs and those in the SBCs. In Sec. IV, we employ the two methods with SBCs to calculate Chern numbers in several models. Finally, we present a summary and discussion in Sec. V. In the Appendix, we examine the Chern numbers obtained by the two methods in the continuum limits. Throughout this paper, we set the lattice constant a and the reduced Planck constant \hbar to unity.

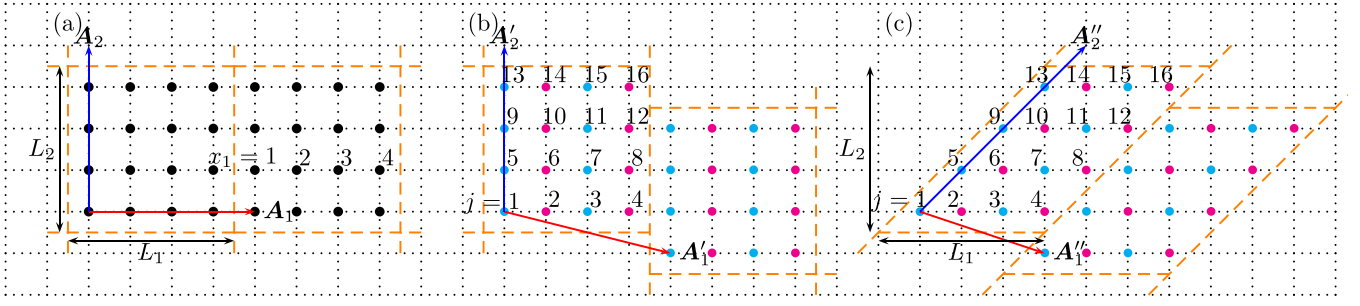


FIG. 1. Several boundary conditions for 2D square lattices with $L_1 \times L_2$ sites. (a) Conventional periodic boundary conditions (PBCs), (b) spiral boundary conditions (SBCs) for $(\pi, 0)$ charge order, and (c) SBCs for (π, π) order. For the systems with SBCs, the lattice sites are labeled as extended 1D chains.

II. CHERN NUMBER

In this section, we will review two methods for calculating the Chern number in 2D lattice systems: the Fukui-Hatsugai-Suzuki (FHS)'s method and the Coh-Vanderbilt (CV)'s method. The CV's method is specifically related to the electronic polarization.

A. Fukui-Hatsugai-Suzuki's method

A method for calculating the Chern number in lattice systems has been proposed by Fukui, Hatsugai, and Suzuki [34]. In this method, we define the following function as an overlap between neighboring two-wave vectors:

$$V_{k, k+\hat{k}_\mu}^{(n)} = \langle u_n(\mathbf{k}) | u_n(\mathbf{k} + \hat{k}_\mu) \rangle, \quad (2)$$

where $|u_n(\mathbf{k})\rangle$ is the Bloch state of the n th band, and $\hat{k}_\mu = \hat{x}_\mu 2\pi/L_\mu$ with \hat{x}_μ being a unit vector along μ direction. Hereafter, we omit the band indices for simplicity, and assume the contribution from the occupied bands. We further define the following product on a plaquette as shown in Fig. 2:

$$Z(\mathbf{k}) = V_{k, k+\hat{k}_1} V_{k+\hat{k}_1, k+\hat{k}_1+\hat{k}_2} V_{k+\hat{k}_1+\hat{k}_2, k+\hat{k}_2} V_{k+\hat{k}_2, k}, \quad (3a)$$

$$F_{12}(\mathbf{k}) = \ln Z(\mathbf{k}), \quad (3b)$$

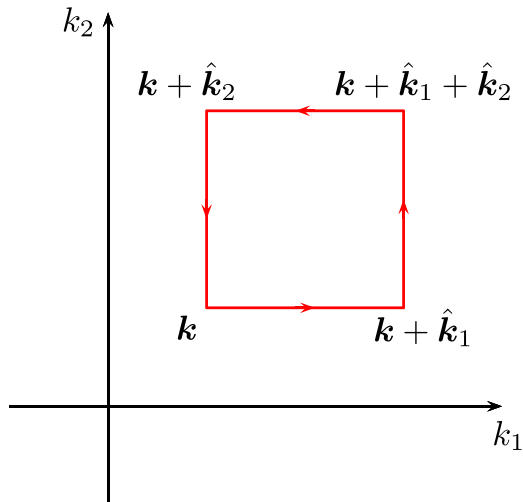


FIG. 2. Path along a plaquette for the Fukui-Hatsugai-Suzuki's method.

where we determine the principal branch by restricting the region of $F_{12}(\mathbf{k})$ as

$$-\pi < -i F_{12}(\mathbf{k}) \leq \pi. \quad (4)$$

Note that (2) and (3b) are related to the link variable and the Wilson loop, respectively in the lattice gauge theory. Then the Chern number is given as

$$\nu = -\frac{1}{2\pi i} \sum_{\mathbf{k}} F_{12}(\mathbf{k}). \quad (5)$$

The continuum representation is given in Appendix.

B. Coh-Vanderbilt's method

On the other hand, Coh and Vanderbilt related the Chern number and the electronic polarization by flux insertion [33]. Later, this method has been discussed in details by Kang, Lee, and Cho [35]. In this method, the Chern number is given by the relations

$$z(\phi_2) = \langle \Psi_0(0, \phi_2) | U_1 | \Psi_0(0, \phi_2) \rangle \quad (6a)$$

$$= -\prod_{\mathbf{k}} V_{k+\frac{\phi_2}{2\pi}\hat{k}_2, k+\frac{\phi_2}{2\pi}\hat{k}_2-\hat{k}_1}, \quad (6b)$$

$$\nu = -\frac{\partial}{\partial \phi_2} \text{Im} \ln z(\phi_2), \quad (6c)$$

and the polarization operator along μ direction is

$$U_\mu = \exp\left(i \frac{2\pi}{L_\mu} \sum_r x_\mu n_r\right). \quad (7)$$

This is the twist operator introduced in the LSM theorem for $d \geq 2$ [27,28]. $|\Psi_0(\phi_1, \phi_2)\rangle$ is the many-body ground state as a function of the flux ϕ_μ . The Chern number ν is quantized in the thermodynamic limit.

As discussed in Appendix, the Chern number in the continuum limit is given by different ‘‘gauges’’ of the Berry connection as that of FHS's method. Whereas the gauge of FHS's method is like the ‘‘symmetric gauge’’, that of CV's method corresponds to the ‘‘Landau gauge.’’ However, we can modify the CV's method so that the Chern number is given by ‘‘symmetric gauge.’’ For example, we define the polarization as follows:

$$z(\phi) = \langle \Psi_0(\phi, \phi) | U_1 U_2^{-1} | \Psi_0(\phi, \phi) \rangle \quad (8)$$

$$= -\prod_{\mathbf{k}} V_{k+\frac{\phi}{2\pi}(\hat{k}_1+\hat{k}_2), k+\frac{\phi}{2\pi}(\hat{k}_1+\hat{k}_2)-\hat{k}_1+\hat{k}_2}. \quad (9)$$

For $L_1 = L_2$ this gives the same representation as that of FHS's method in the continuum limit.

III. SPIRAL BOUNDARY CONDITIONS

For 2D systems, the exponential position operator with SBCs is given by

$$U_{\text{SBC}} = \exp \left(i \sum_{j=1}^L \frac{2\pi j n_j}{L} \right), \quad L = L_1 L_2, \quad (10)$$

where j is the site number of the extended 1D chain, which sweeps all lattice sites in 1D order as shown in Fig. 1(b). On the other hand, for conventional PBCs as in Fig. 1(a), there are two operators as Eq. (7). In this section, we discuss the relationship between U_{SBC} and U_μ for 2D systems with PBCs, and how the wave number \mathbf{k} appearing in Sec. II should be replaced for SBCs.

A. Definition of spiral boundary conditions

In order to consider the flux insertion to the system with SBCs, we reinterpret the twist operators in the Oshikawa's argument (7). First, we consider the primitive vectors in the real space and the reciprocal lattice space of 2D systems as

$$\mathbf{A}_1 = (L_1, 0), \quad \mathbf{B}_1 = 2\pi \left(\frac{1}{L_1}, 0 \right), \quad (11a)$$

$$\mathbf{A}_2 = (0, L_2), \quad \mathbf{B}_2 = 2\pi \left(0, \frac{1}{L_2} \right). \quad (11b)$$

Then these vectors satisfy the relation

$$\mathbf{A}_\mu \cdot \mathbf{B}_\nu = 2\pi \delta_{\mu,\nu}. \quad (12)$$

The twist operator (7) is written using the above primitive vectors in the reciprocal lattice space as

$$U_\mu = \exp \left(i \sum_r \mathbf{B}_\mu \cdot \mathbf{r} n_r \right). \quad (13)$$

Next, we choose the primitive vectors for SBCs as shown in Fig. 1(b) so that they satisfy the relation (12). Then we have

$$\mathbf{A}'_1 = (L_1, -1), \quad \mathbf{B}'_1 = 2\pi \left(\frac{1}{L_1}, 0 \right), \quad (14a)$$

$$\mathbf{A}'_2 = (0, L_2), \quad \mathbf{B}'_2 = 2\pi \left(\frac{1}{L_1 L_2}, \frac{1}{L_2} \right). \quad (14b)$$

The twist operators in 2D systems with SBCs are introduced as

$$U'_\mu = \exp \left(i \sum_r \mathbf{B}'_\mu \cdot \mathbf{r} n_r \right). \quad (15)$$

For $\mu = 1$, because the relation $\mathbf{B}'_1 = \mathbf{B}_1$ holds, U'_1 is the same operator as U_1 with SBCs. In order to represent U_1 in SBCs, we use the following relation:

$$\frac{2\pi j n_j}{L_1} = \frac{2\pi x_1 n_r}{L_1} \pmod{2\pi}. \quad (16)$$

For $\mu = 2$, the exponent part of the twist operator is confirmed as that of SBCs as

$$\sum_r \mathbf{B}'_2 \cdot \mathbf{r} n_r = \sum_{i_1=1}^{L_1} \sum_{i_2=0}^{L_2-1} 2\pi \frac{i_1 + i_2 L_1}{L_1 L_2} n_{(i_1, i_2)} \quad (17)$$

$$= \sum_{j=1}^L \frac{2\pi}{L} j n_j, \quad (18)$$

where $L = L_1 L_2$ and $j = i_1 + i_2 L_1$. Thus the twist operators for SBCs are identified as

$$U'_1 = \exp \left(i \sum_{j=1}^L \frac{2\pi j n_j}{L_1} \right) = (U_{\text{SBC}})^{L_2}, \quad (19a)$$

$$U'_2 = U_{\text{SBC}}. \quad (19b)$$

These correspondences mean that the flux insertion for the extended 1D chain of SBCs gives rise an effective current along y direction, while U'_1 causes a current only to x direction because of the relation (16).

In the same way, the primitive vectors of the system with SBCs for (π, π) order illustrated in Fig. 1(c), are identified as

$$\mathbf{A}'_1 = (L_1 - 1, -1), \quad \mathbf{B}'_1 = \frac{2\pi}{L_1 L_2 + L_1 - L_2} (L_2, -L_1), \quad (20a)$$

$$\mathbf{A}'_2 = (L_1, L_2), \quad \mathbf{B}'_2 = \frac{2\pi}{L_1 L_2 + L_1 - L_2} (1, L_1 - 1). \quad (20b)$$

Then, the exponential position operators in these SBCs U'_j for the isotropic case $L_1 = L_2$ are related as

$$U''_1 = U_1 U_2^{-1}, \quad U''_2 = U_{\text{SBC}}. \quad (21)$$

Since we are not interested in charge orders in this paper, we will not use these boundary conditions.

B. Redefinition of Coh-Vanderbilt's method

In the Coh-Vanderbilt method, we need to apply flux to the system to generate a current in the vertical direction of the twist operator for calculating the Chern number. However, since the flux is continuum number, we cannot distinguish whether the direction of the flux is along \mathbf{B}'_1 or \mathbf{B}'_2 . On the other hand, roles of twist operators for each directions are apparently distinguished as in Eq. (19). Therefore, we apply the flux to \mathbf{B}'_2 direction, which is along the extended 1D chain, and turn our attention to the response to \mathbf{B}'_1 direction.

It follows from Eq. (19) that the expectation value of the twist operator with flux (6a) for the system with SBCs is redefined as

$$z'(\phi) = \langle \Psi'_0(\phi) | U'_1 | \Psi'_0(\phi) \rangle, \quad (22)$$

where $|\Psi'_0(\phi)\rangle$ is the many-body wave function of the ground state with flux ϕ . The flux ϕ is imposed to the extended 1D chain with $L = L_1 L_2$ sites. From Eq. (6), the following relation is satisfied:

$$z'(\phi) = e^{-i\nu\phi} z'(0). \quad (23)$$

If we consider the expectation value of U'_2 as

$$z'_2(\phi) = \langle \Psi'_0(\phi) | U'_2 | \Psi'_0(\phi) \rangle, \quad (24)$$

we can not detect the Chern number, because the applied current by the flux and its response are in the parallel directions and there is no perpendicular component in the response.

C. Correspondence of wave numbers

Now we discuss the correspondence of the wave numbers defined in 2D PBCs with those of SBCs. Let us consider a tight-binding model defined on a 2D square lattice. When we apply SBCs to this system, the hopping term is written as

$$\begin{aligned} \mathcal{H} &= -t \sum_{j=1}^L [(c_j^\dagger c_{j+1} + \text{H.c.}) + (c_j^\dagger c_{j+\Lambda} + \text{H.c.})] \\ &= -2t \sum_k [\cos k + \cos \Lambda k] c_k^\dagger c_k, \end{aligned} \quad (25)$$

where c_j^\dagger (c_j) is a creation (annihilation) operator at j th site of the extended 1D chain with $L \equiv L_1 L_2$ sites, and Λ is a parameter depending on the number of lattice sites in x direction. As shown in Fig. 1, this parameter is related to ways to label the sites of extended 1D chain and $\Lambda \in \mathbb{Z}$. For SBCs for $(\pi, 0)$ order $\Lambda = L_1$ while those for (π, π) order, $\Lambda = L_1 - 1$. In the present case, we are not interested in charge orders, so that we choose SBCs for $(\pi, 0)$ order for simplicity. The Fourier transformation of the extended 1D chain is given by

$$c_k = \frac{1}{\sqrt{L}} \sum_{j=1}^L e^{-ikx_j} c_j. \quad (26)$$

Then the 2D wave vectors are replaced as the 1D wave number by

$$\mathbf{k} = (k_x, k_y) \rightarrow (k, L_1 k), \quad (27a)$$

$$k = \frac{2\pi}{L} n, \quad n = 0, 1, 2, \dots, L-1. \quad (27b)$$

When we apply the flux ϕ to the system, the Hamiltonian (25) is modified by the following replacements:

$$c_j \rightarrow c_j e^{-i\phi x_j/L}, \quad k \rightarrow k + \phi/L. \quad (28)$$

The dispersion relations of these systems with different boundary conditions are completely different. In the case of SBCs, there are many oscillations resulting from the long-range hopping. However, physical properties of these systems in the thermodynamic limit become the same. This is confirmed, for example, by analytical calculation of the density of states [36].

Next we consider the unit wave numbers \hat{k}_μ ($\mu = 1, 2$) appearing in Sec. II. According to the results of \mathbf{B}'_μ given in Eq. (14), there are following relations:

$$\hat{k}_1 = (\hat{k}_1, 0) \rightarrow (L_2 \hat{k}, 0), \quad (29a)$$

$$\hat{k}_2 = (0, \hat{k}_2) \rightarrow (\hat{k}, L_1 \hat{k}), \quad (29b)$$

where

$$\hat{k}_\mu = \frac{2\pi}{L_\mu}, \quad \hat{k} = \frac{2\pi}{L}. \quad (30)$$

Then $Z(\mathbf{k})$ defined by Eq. (3a) and z by Eq. (6b) are replaced as

$$\begin{aligned} Z(\mathbf{k}) &\rightarrow V_{(k, L_1 k), (k+L_2 \hat{k}, L_1 k)} V_{(k+L_2 \hat{k}, L_1 k), (k+L_2 \hat{k} + \hat{k}, L_1 k + L_1 \hat{k})} \\ &\quad \times V_{(k+L_2 \hat{k} + \hat{k}, L_1 k + L_1 \hat{k}), (k + \hat{k}, L_1 k + L_1 \hat{k})} V_{(k + \hat{k}, L_1 k + L_1 \hat{k}), (k, L_1 k)}, \end{aligned} \quad (31)$$

$$z'(\phi) \rightarrow - \prod_k V_{(k + \frac{\phi}{L}, L_1 k + \frac{\phi}{L_2}), (k + \frac{\phi}{L} - L_2 \hat{k}, L_1 k + \frac{\phi}{L_2})}. \quad (32)$$

IV. RESULTS

We demonstrate the above discussions in representative models for Chern insulators: the Wilson-Dirac model and the Haldane model.

A. Wilson-Dirac model

As a fundamental model to describe 2D Chern insulators, we consider the Wilson-Dirac model [31,32],

$$\begin{aligned} \mathcal{H} &= \frac{-it}{2} \sum_{j, \mu=x, y} (c_j^\dagger \tau_\mu c_{j+\hat{\mu}} - \text{H.c.}) + (M - B) \sum_j c_j^\dagger \tau_3 c_j \\ &\quad + \frac{B}{2} \sum_{j, \mu=x, y} (c_j^\dagger \tau_3 c_{j+\hat{\mu}} + \text{H.c.}). \end{aligned} \quad (33)$$

The Fourier representation of this model becomes

$$\mathcal{H} = \sum_{\mathbf{k}, \alpha, \beta} c_{\mathbf{k}, \alpha}^\dagger H_{\alpha\beta}(\mathbf{k}) c_{\mathbf{k}, \beta}, \quad (34a)$$

$$H(\mathbf{k}) = t \sum_{\mu=x, y} \sin k_\mu \tau_\mu + \left[M - B \sum_{\mu=x, y} (1 - \cos k_\mu) \right] \tau_z, \quad (34b)$$

where $t = 1$ is the hopping amplitude, M is the mass, B is the coefficient of the Wilson term, $c_{\mathbf{k}, \alpha}$ is the annihilation operator of a fermion with a 2D wave number, $\alpha, \beta \in \{1, 2\}$ are orbital indices, and τ_μ are the Pauli matrices. The energy eigenvalue is given by

$$\varepsilon_k^2 = t^2 (\sin^2 k_x + \sin^2 k_y) + \{M - B(2 - \cos k_x - \cos k_y)\}^2. \quad (35)$$

This system with positive M is a trivial insulator for $B < M/4$, and a topological insulator with $\nu = 1$ for $M/4 \leq B \leq M/2$ and that with $\nu = -1$ for $M/2 \leq B$. Topological phase transition occurs at $B = M/4$ and $M/2$ [37]. These transition points can be identified by vanishing of the bulk energy gap $\varepsilon_k = 0$. The sign of ν is interchanged for negative M . In the continuum version of the model, the Hall conductivity is calculated as [38]

$$\sigma_{xy} = -\frac{e^2}{2h} [\text{sgn}(M) + \text{sgn}(B)]. \quad (36)$$

Therefore the system is a topological (trivial) insulator for $MB > 0$ ($MB < 0$), so that the sign of σ_{xy} is interchanged depending on the sign of M for fixed B . This is consistent with the lattice model.

As shown in Fig. 3, the Chern number of the WD model obtained by the FHS method and the CV method with

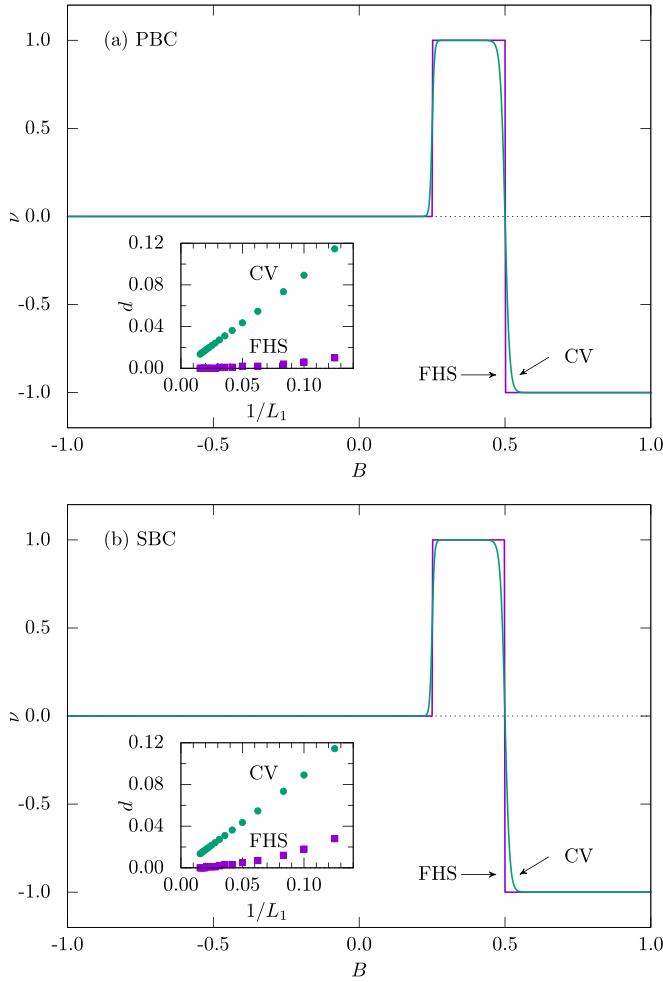


FIG. 3. Chern numbers of the 2D WD model in $L = 64 \times 64$ sites at $M = 1$ with conventional (a) PBCs and (b) SBCs, calculated by Fukui-Hatsugai-Suzuki's (FHS) method and Coh-Vanderbilt's (CV) method. Topological regions are $1/4 \leq B \leq 1/2$ with $\nu = 1$ and $1/2 \leq B$ with $\nu = -1$. Insets show the size dependence of the displacement of the Chern number from the exact value.

conventional PBCs and SBCs. The finite-size effect of the FHS method tends to be smaller than that of the CV method, and that of the conventional PBCs tends to be smaller than the SBCs. This tendency is observed by the following displacement

$$d = \int_{B_{\min}}^{B_{\max}} dB [v(L) - v(\infty)]^2, \quad (37)$$

where we have set $B_{\min} = 0$ and $B_{\max} = 1$, shown in the insets of Fig. 3.

Figure 4(a) shows $z'(\phi)$, the ground-state expectation values of the twist operator U_1' in SBCs. According to the results, $z'(0)$ does not change the sign. On the other hand, $z'(\pi)$ changes the sign in the topological regions $M/4 < B$ with the Chern number $\nu = \pm 1$, as a consequence of the relation (23). We can also identify the topological regions by calculating the ratio of the expectation values of U_1' with and without flux $z'(\pi)/z'(0)$ as shown in Fig. 4(b).

In case we consider the expectation value of U_{SBC} as (24), it has the opposite sign in the second topological region

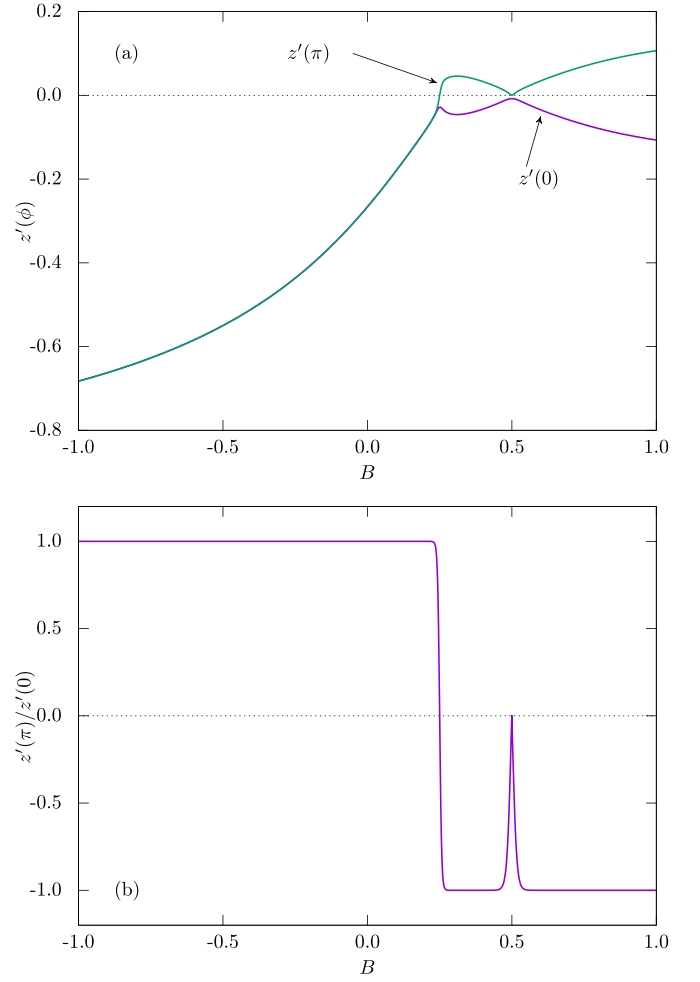


FIG. 4. (a) Expectation values of the twist operator U_1' with and without flux, $z'(0)$ and $z'(\pi)$. (b) The ratio of the expectation values $z'(\pi)/z'(0)$. There is no sign change for $z'(0)$, while $z'(\pi)$ has the opposite sign in the topological regions. These results are calculated for the systems with $M = 1$ and $L = 64 \times 64$ sites.

$M/2 < B$, and that with different SBCs, as shown in Fig. 1(c), it has opposite sign in the both topological regions $M/4 < B$. These results are already discussed in Ref. [26].

B. Haldane model

As another fundamental model for a Chern insulator, we consider the Haldane model [1] describing the fermions on a honeycomb lattice with a hopping amplitude $t = 1$, an alternating potential M , and a next-nearest-neighbor hopping κ ,

$$\mathcal{H} = t \sum_{\langle ij \rangle} c_i^\dagger c_j + M \sum_i \eta_i c_i^\dagger c_i + i \frac{\kappa}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle} v_{ij} c_i^\dagger c_j, \quad (38)$$

where c_i^\dagger (c_i) is a creation (annihilation) operator at site i (spin indices are omitted). $\langle ij \rangle$ and $\langle\langle ij \rangle\rangle$, denote a nearest and a next-nearest pair, respectively. $\eta_i = 1$ ($\eta_i = -1$) for A (B) sublattice, and $v_{ij} = (2/\sqrt{3})(\mathbf{c}_1 \times \mathbf{c}_2)_z = \pm 1$, where \mathbf{c}_1 and \mathbf{c}_2 are primitive vectors along the two bonds on which the electron hops from a site j to i , as shown in Fig. 5.

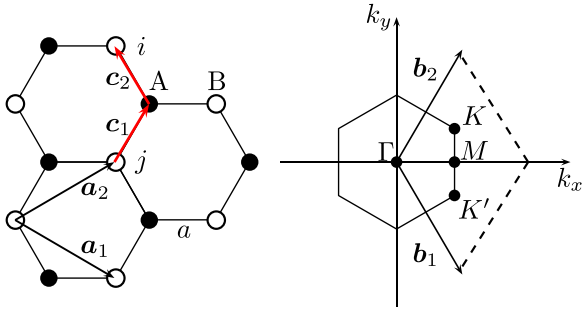


FIG. 5. Primitive vectors \mathbf{a}_i and reciprocal lattice vectors \mathbf{b}_i of the honeycomb lattice. \mathbf{c}_i is the primitive vectors along the two bonds on which the electron hops from a site j to i .

For the honeycomb lattice, the primitive vectors are

$$\mathbf{a}_1 = \frac{a}{2}(3, -\sqrt{3}), \quad \mathbf{a}_2 = \frac{a}{2}(3, \sqrt{3}). \quad (39)$$

Then the reciprocal lattice vectors are chosen as

$$\mathbf{b}_1 = \frac{2\pi}{3a}(1, -\sqrt{3}), \quad \mathbf{b}_2 = \frac{2\pi}{3a}(1, \sqrt{3}), \quad (40)$$

by the relation

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}. \quad (41)$$

The wave numbers are given in these bases as

$$\mathbf{k} = k_1 \mathbf{b}_1 + k_2 \mathbf{b}_2, \quad (42)$$

where $k_i \in [0, 2\pi]$.

The Hamiltonian in the momentum space has the following form:

$$H(\mathbf{k}) = \sum_i d_i(\mathbf{k}) \tau_i, \quad (43)$$

with the energy

$$\varepsilon(\mathbf{k}) = \pm \sqrt{\sum_i d_i^2(\mathbf{k})}. \quad (44)$$

The parameters in Hamiltonian are given as follows:

$$d_1 = t[\cos(\mathbf{k} \cdot \mathbf{a}_1) + \cos(\mathbf{k} \cdot \mathbf{a}_2) + 1], \quad (45a)$$

$$d_2 = t[\sin(\mathbf{k} \cdot \mathbf{a}_1) + \sin(\mathbf{k} \cdot \mathbf{a}_2)], \quad (45b)$$

$$d_3 = M - \frac{2\kappa}{3\sqrt{3}}[\sin(\mathbf{k} \cdot \mathbf{a}_1) - \sin(\mathbf{k} \cdot \mathbf{a}_2) - \sin(\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2))]. \quad (45c)$$

Thus we can calculate the Chern number as in the same way of the square lattice systems, by using the wave vector as $\mathbf{k} = (k_1, k_2)$.

In order to consider honeycomb lattices with SBCs as shown in Fig. 6, it is convenient to consider chirality of carbon nanotubes [39] defined as

$$\mathbf{C} = n\mathbf{a}_1 + m\mathbf{a}_2 \equiv (n, m). \quad (46)$$

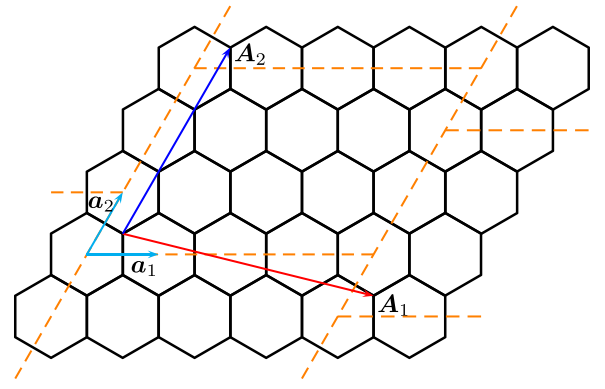


FIG. 6. Spiral boundary conditions (SBCs) for a honeycomb lattice with $L_1 \times L_2$ hexagons and $2L_1L_2$ sites. The vectors \mathbf{A}_i are defined as $\mathbf{A}_1 = L_1\mathbf{a}_1 - \mathbf{a}_2$ and $\mathbf{A}_2 = L_2\mathbf{a}_2$ with L_i being integers.

The discussion for the square lattices in Sec. III corresponds to the honeycomb lattices with $L_1 \times L_2$ hexagons with $2L_1L_2$ sites and chirality $(L_1, -1)$.

Then the Hall conductivity of the system at the charge neutrality point becomes

$$\sigma_{xy} = -\frac{e^2}{h} \text{sgn}(\kappa) \theta(|\kappa| - |M|). \quad (47)$$

This means that the system is a Chern insulator for $|\kappa| > |M|$ with $\nu = \pm 1$ and a trivial insulator for $|\kappa| < |M|$ with $\nu = 0$.

Figure 7 shows the Chern number of the Haldane model obtained by the FHS method and the CV method with conventional PBCs and SBCs. Finite-size effect of the FHS method tends to be smaller than that of the CV method. These tendencies are same for those of the WD model, and are shown in the insets of Fig. 7, where the displacement of Eq. (37) are calculated for $\kappa_{\min} = 0$ and $\kappa_{\max} = 1$.

Figure 8(a) shows the ground-state expectation values of the twist operators in SBCs without flux. The result of $z'(0)$ has large finite-size effects with oscillations, so that it is difficult to characterize the insulating states and the electronic polarization. This behavior is considered to be an effect of the next-nearest-neighbor-hopping process. However, the ratio of $z'(\phi)$ with and without flux $z'(\pi)/z'(0)$ well characterizes the topologies of the system as shown in Fig. 8(b). For this quantity, the calculation should be done so that the anomaly is canceled as

$$\frac{z(\pi)}{z(0)} = \prod_{\mathbf{k}} \frac{V_{\mathbf{k} + \frac{1}{2}\hat{k}_2, \mathbf{k} + \frac{1}{2}\hat{k}_2 - \hat{k}_1}}{V_{\mathbf{k}, \mathbf{k} - \hat{k}_1}}. \quad (48)$$

V. SUMMARY AND DISCUSSION

In summary, we have explored the relationship between electronic polarization and the Chern number in 2D systems with SBCs. Initially, we examined two methods for calculating Chern numbers in 2D lattice systems: Fukui-Hatsugai-Suzuki's method and Coh-Vanderbilt's method. Subsequently, we introduced twist operators in 2D systems with SBCs and redefined the aforementioned methods using the wave numbers of the extended 1D chain. The crucial aspect of this discussion is that flux insertion into the extended

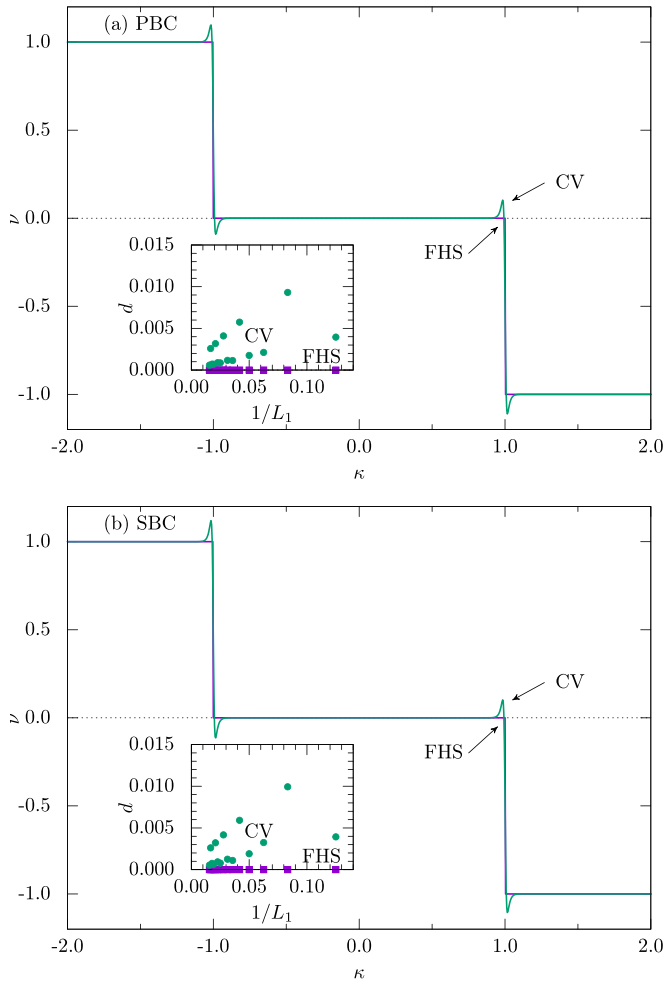


FIG. 7. Chern numbers of the Haldane model in $L = 64 \times 64$ sites at $M = 1$ with conventional (a) PBCs and (b) SBCs, calculated by Fukui-Hatsugai-Suzuki's (FHS) method and Coh-Vanderbilt's (CV) method. Topological regions are $\kappa \leq -1$ with $\nu = 1$ and $1 \leq \kappa$ with $\nu = -1$. Insets show the size dependence of the displacement of the Chern number from the exact value.

1D chain generates an effective current along the y direction, and the twist operator detects the response to the x direction. Finally, we illustrated the above discussions in representative models for Chern insulators, such as the Wilson-Dirac model and the Haldane model, demonstrating that the calculation of Chern numbers and the detection of topological phases are achievable using methods with SBCs.

The relationship between topological states in 1D and those in 2D with a Chern number is considered as follows: As mentioned in Sec. I, the signs of z classify 1D gapped states. In some cases, such as the Su-Schrieffer-Heeger model [40,41], an insulating state with localized edge electrons emerges. If we then consider creating a 2D system by connecting these 1D edge states with spiral boundary conditions (SBCs), an insulating state with edge current may appear in response to applied flux. This state represents a 2D topological state with a Chern number.

As an extension of the argument presented in this paper, we may consider SBCs in general dimensions. According to

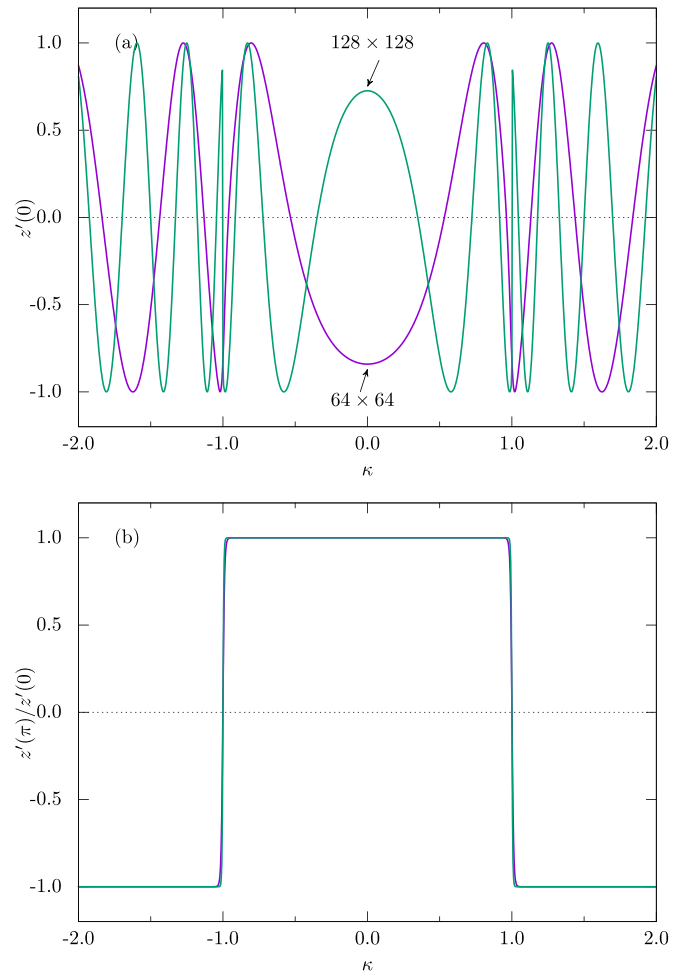


FIG. 8. (a) Expectation values of twist operators U'_1 without flux $z'(0)$. (b) The ratio of the expectation values of U'_1 with and without flux $z'(\pi)/z'(0)$ calculated in the systems with $L = 64 \times 64$ and $L = 128 \times 128$.

the discussion in Sec. III, the twist operators in d -dimensional systems are generalized as follows:

$$U'_\mu = \exp \left(i \sum_{j=1}^L \frac{2\pi j n_j}{\prod_{k=1}^{\mu} L_k} \right), \quad L = \prod_{k=1}^d L_k. \quad (49)$$

By utilizing these operators and incorporating flux insertions, we may identify d -dimensional topological phases and higher-order topological states.

The present method with SBCs is expected to be applicable to numerical calculations, such as the density matrix renormalization group method. For systems in more than 2D, finite-size scaling is not as straightforward as in 1D systems because increasing the number of lattice sites cannot be done linearly while maintaining the symmetry of the unit systems. However, in systems with SBCs, we can increase the lattice size linearly, enabling finite-size scaling similar to 1D systems [36,42,43]. We anticipate that the present method will prove useful for the numerical analysis of topological systems with electron-electron interactions.

ACKNOWLEDGMENTS

M.N. acknowledges the research fellow position of the Institute of Industrial Science, The University of Tokyo. M.N. is supported partly by MEXT/JSPS KAKENHI Grant No. JP20K03769. The authors thank S. Nishimoto and H. Watanabe for helpful discussions.

APPENDIX: CONTINUUM LIMIT

In this section, we discuss the continuum limits of the formulas for the Chern number given by the Fukui-Hatsugai-Suzuki's method and by the Coh-Vanderbilt's method for lattice systems, to compare the Thouless-Kohmoto-Nightingale-den Nijs (TKNN) formula.

1. TKNN formula

Let us consider a 2D system. When the system is translationally invariant, the Hamiltonian satisfies the following eigenvalue equation in term of the Bloch state,

$$H(\mathbf{k})|u_n(\mathbf{k})\rangle = E_n(\mathbf{k})|u_n(\mathbf{k})\rangle, \quad (\text{A1})$$

where $|u_n(\mathbf{k})\rangle$ is the Bloch eigenstate of the n th band, and normalized as $\langle u_n(\mathbf{k})|u_m(\mathbf{k})\rangle = \delta_{n,m}$. The Berry connection of the n th band is defined as

$$\mathbf{A}^{(n)}(\mathbf{k}) = i\langle u_n(\mathbf{k})|\nabla_{\mathbf{k}}u_n(\mathbf{k})\rangle. \quad (\text{A2})$$

Then the Berry curvature is given as

$$\mathbf{B}^{(n)}(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathbf{A}^{(n)}(\mathbf{k}). \quad (\text{A3})$$

The Berry connection and the Berry curvature correspond to the vector potential and the magnetic field in the electrodynamics, respectively.

The Chern number for the n th band ν_n is given by the Berry curvature as follows:

$$\begin{aligned} \nu_n &= \frac{1}{2\pi} \iint_{\text{BZ}} d^2\mathbf{k} [\mathbf{B}^{(n)}(\mathbf{k})]_z \\ &= \frac{1}{2\pi} \oint_{\partial\text{BZ}} d\mathbf{k} \cdot \mathbf{A}^{(n)}(\mathbf{k}), \end{aligned} \quad (\text{A4})$$

where BZ means the first Brillouin zone. Then the Chern number ν is given by the summation of ν_n over the occupied bands, and the Hall conductivity is related to the Chern number as follows:

$$\sigma_{xy} = -\nu \frac{e^2}{h}, \quad \nu = \sum_{n \in \text{occupied}} \nu_n. \quad (\text{A5})$$

This is so-called TKNN formula [44–47]. Hereafter, we omit the band indices for simplicity, and assume the contribution from the occupied bands.

2. Fukui-Hatsugai-Suzuki's method

Now we show that the Chern numbers in lattice systems are related to those defined in the continuous Brillouin zone (A4) in the continuum limit. By the Taylor expansion $V_{\mathbf{k},\mathbf{k}+\hat{k}_\mu}$ defined by Eq. (2) in the continuum limit becomes

$$V_{\mathbf{k},\mathbf{k}+\hat{k}_\mu} \simeq 1 - i\frac{2\pi}{L_\mu} A_\mu(\mathbf{k}), \quad (\text{A6})$$

where $A_\mu(\mathbf{k})$ is the Berry connection defined in (A2). Similarly, we get

$$\begin{aligned} V_{\mathbf{k}+\hat{k}_\mu,\mathbf{k}+\hat{k}_\mu+\hat{k}_\nu} &\simeq 1 - i\frac{2\pi}{L_\nu} A_\nu(\mathbf{k} + \hat{k}_\mu) \\ &\simeq 1 - i\frac{2\pi}{L_\nu} A_\nu(\mathbf{k}) - i\frac{(2\pi)^2}{L_\mu L_\nu} \partial_\mu A_\nu(\mathbf{k}), \end{aligned} \quad (\text{A7})$$

where $\mu \neq \nu$, and we have abbreviated as $\partial_\nu = \partial_{k_\nu}$. Next, $F_{12}(\mathbf{k})$ defined by Eq. (3) becomes

$$\begin{aligned} F_{12}(\mathbf{k}) &\simeq \ln \left[\left(1 - i\frac{2\pi}{L_1} A_1 \right) \left(1 - i\frac{2\pi}{L_2} A_2 - i\frac{(2\pi)^2}{L_1 L_2} \partial_1 A_2 \right) \right. \\ &\quad \left. \times \left(1 + i\frac{2\pi}{L_1} A_1 + i\frac{(2\pi)^2}{L_1 L_2} \partial_2 A_1 \right) \left(1 + i\frac{2\pi}{L_2} A_2 \right) \right] \\ &\simeq \ln \left[1 - i\frac{(2\pi)^2}{L_1 L_2} (\partial_1 A_2 - \partial_2 A_1) \right] \\ &\simeq -i\frac{(2\pi)^2}{L_1 L_2} (\partial_1 A_2 - \partial_2 A_1), \end{aligned} \quad (\text{A8})$$

so that the Chern number in lattice systems (5) becomes

$$\nu \simeq \frac{1}{2\pi} \iint d^2\mathbf{k} [\partial_1 A_2(\mathbf{k}) - \partial_2 A_1(\mathbf{k})]. \quad (\text{A9})$$

This coincides with the TKNN formula (A4).

3. Coh-Vanderbilt's method

The relations of the Coh-Vanderbilt's (CV's) method (6) are confirmed by the following calculations,

$$\begin{aligned} &\prod_{\mathbf{k}} \left\langle u \left(k_1, k_2 + \frac{\phi_2}{L_2} \right) \middle| u \left(k_1 - \frac{2\pi}{L_1}, k_2 + \frac{\phi_2}{L_2} \right) \right\rangle \\ &\simeq \prod_{\mathbf{k}} \left(1 - \frac{2\pi}{L_1} \left\langle u \left(k_1, k_2 + \frac{\phi_2}{L_2} \right) \middle| \partial_1 u \left(k_1, k_2 + \frac{\phi_2}{L_2} \right) \right\rangle \right) \\ &\simeq \exp \left[i\frac{L_2}{2\pi} \iint d^2\mathbf{k} A_1 \left(k_1, k_2 + \frac{\phi_2}{L_2} \right) \right] \\ &\simeq \exp \left[i\frac{L_2}{2\pi} \iint d^2\mathbf{k} A_1(k_1, k_2) \right] \\ &\quad \times \exp \left[i\phi_2 \underbrace{\frac{1}{2\pi} \iint d^2\mathbf{k} \partial_2 A_1(k_1, k_2)}_{-\nu} \right]. \end{aligned} \quad (\text{A10})$$

In this case, the Chern number in the continuum limit is given by the Berry connection, which has the same structure of the ‘‘Landau gauge’’, whereas the Chern number given by the FHS's method corresponds to the ‘‘symmetric gauge.’’ Thus we get the relation

$$z(0, \phi_2) = z(0, 0)e^{-i\phi_2 \nu}. \quad (\text{A11})$$

Similarly, we get

$$\langle \Psi_0(\phi_1, 0) | U_2 | \Psi_0(\phi_1, 0) \rangle \sim z(0, 0)e^{i\phi_1 \nu}. \quad (\text{A12})$$

Thus we have shown that the relationship between $z(\phi_2)$ and the Chern number ν are given by Eq. (6c).

Furthermore, we can modify the CV's method so that the Chern number is given by the "symmetric gauge." For this purpose, we define the polarization as

$$\begin{aligned} z(\phi_1, \phi_2) &= \langle \Psi_0(\phi_1, \phi_2) | U_1 U_2^{-1} | \Psi_0(\phi_1, \phi_2) \rangle \\ &= - \prod_k \left\langle u \left(k_1 + \frac{\phi_1}{L_1}, k_2 + \frac{\phi_2}{L_2} \right) \middle| u \left(k_1 + \frac{\phi_1 - 2\pi}{L_1}, k_2 + \frac{\phi_2 + 2\pi}{L_2} \right) \right\rangle. \end{aligned} \quad (\text{A13})$$

In the thermodynamic limit $L_\mu \gg 1$, the Taylor expansion gives

$$\begin{aligned} z(0, 0) &= - \prod_k \left\langle u(k_1, k_2) \middle| u \left(k_1 - \frac{2\pi}{L_1}, k_2 + \frac{2\pi}{L_2} \right) \right\rangle \\ &\simeq - \exp \left[i \iint d^2\mathbf{k} \left\{ \frac{L_2}{2\pi} A_1(k_1, k_2) - \frac{L_1}{2\pi} A_2(k_1, k_2) \right\} \right], \end{aligned} \quad (\text{A14})$$

where $A_\mu(k_1, k_2)$ is a component of the Berry connection defined in Eq. (A2). Therefore Eq. (A13) becomes

$$\begin{aligned} z(\phi_1, \phi_2) &= - \exp \left[i \iint d^2\mathbf{k} \left\{ \frac{L_2}{2\pi} A_1 \left(k_1 + \frac{\phi_1}{L_1}, k_2 + \frac{\phi_2}{L_2} \right) - \frac{L_1}{2\pi} A_2 \left(k_1 + \frac{\phi_1}{L_1}, k_2 + \frac{\phi_2}{L_2} \right) \right\} \right] \\ &= z(0, 0) \exp \left[i \iint d^2\mathbf{k} \left\{ \frac{L_2}{L_1} \frac{\phi_1}{2\pi} \partial_1 A_1(\mathbf{k}) + \frac{\phi_2}{2\pi} \partial_2 A_1(\mathbf{k}) - \frac{\phi_1}{2\pi} \partial_1 A_2(\mathbf{k}) - \frac{L_1}{L_2} \frac{\phi_2}{2\pi} \partial_2 A_2(\mathbf{k}) \right\} \right] \\ &\simeq z(0, 0) \exp \left[-i \frac{\phi}{2\pi} \iint d^2\mathbf{k} (\partial_1 A_2(\mathbf{k}) - \partial_2 A_1(\mathbf{k})) \right], \quad (\phi = \phi_1 = \phi_2, L_1 = L_2) \\ &= z(0, 0) \exp(-i\phi \nu). \end{aligned} \quad (\text{A15})$$

Thus we have obtained the Chern number given by the "symmetric gauge."

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