Flow of unitary matrices: Real-space winding numbers in one and three dimensions

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The notion of the flow introduced by Kitaev is a manifestly topological formulation of the winding number on a real lattice. First, we show in this paper that the flow is quite useful for practical numerical computations for systems without translational invariance. Second, we extend it to three dimensions. Namely, we derive a formula of the flow on a three-dimensional lattice, which corresponds to the conventional winding number when systems have translational invariance.

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I. INTRODUCTION

Topological classification of states in condensed matter physics [1–6] has been extended to various systems that are not necessarily so regular. For example, topologically protected edge modes were reported in geophysics as well as biophysics [7,8]. In real circumstances such systems are far from regular, which does not allow to calculate the Berry curvature as a function of the wave vectors. Nevertheless, topological protection ensures robustness of the topological edge states. Accordingly, direct computational schemes of topological invariants for various irregular systems have become increasingly important.

For disordered and/or interacting systems, there are many attempts at computing topological invariants in real spaces. One way is the use of the twisted boundary conditions, where twist angles play a role of the wave vectors [9]. However, note that the integration of the Berry curvature over the twist angles has no clear physical reason: Topological numbers should be basically attributed to fixed boundary conditions. Indeed, in the case of the Chern number, if one uses the discretized plaquette method [10] for a sufficiently large system, just one plaquette, in principle, reproduces the correct Chern number [11]. The merit of this method is that it is always integral, and for clean noninteracting systems, it reduces to the topological invariants based on the Berry curvatures. Another way is based on the direct real-space representations of topological invariants [12–23]. The Zak phase is the typical example of them [24], which is also the basis of the quantum mechanical theory of electric polarization in crystalline insulators [25,26]. However, the topological nature of them seems unclear at first sight.

In this paper, we restrict our discussions to winding numbers of unitary matrices in odd dimensions, which are topological invariants characterizing half-filled ground states of systems with chiral symmetry. As mentioned above, real-space representations of topological invariants are more or less based on the quantum mechanical position operators. However, Kitaev [12] has proposed a quite useful notion, the *flow* of the unitary matrices. This is equivalent to the Zak-like representation by the use of the position operators if the systems have translational symmetry. Moreover, the flow in one dimension is manifestly topological. The purpose of the paper is firstly to show the usefulness of the flow also in the practical computations, and secondly to present the three-dimensional extension of the flow. Recently, a method of computing a winding number in a discretized wave-vector space in three dimensions has been proposed in Ref. [27]. The three-dimensional flow in this paper is an alternative discrete formulation of the three-dimensional winding number.

II. FLOW OF UNITARY MATRICES IN ONE DIMENSION

In condensed matter physics, topological invariants are defined on the torus (the Brillouin zone) spanned by the continuum wave vector, which implies that corresponding real spaces are composed of infinite lattices. Indeed, the flow introduced by Kitaev is basically defined by unitary matrices U_{ij} specified by site indices i, j running from $-\infty$ to $+\infty$. In other words, only for infinite dimensional matrices, the flow is topological. Practically, this feature is rather problematic, especially for numerical computations for finite size systems, since the flow vanishes trivially. Keeping these points in mind, we review in this section the flow of unitary matrices introduced by Kitaev [12], using the Su-Schrieffer-Heeger (SSH) model [28] as a typical example, stressing why the flow vanishes for finite systems, and how to overcome this difficulty for numerical calculations using finite systems.

Before proceeding, let us fix our notation of unitary matrices often denoted as U_{ij}. The indices i, j stand for the lattice sites of unit cells, often referred to simply as sites, and if the systems have any n internal degrees of freedom such as orbitals, U_{ij} is a $n \times n$ matrix specified by i, j. The symbol tr means the trace over the internal degrees of freedom, whereas Tr stands for the trace including sites $\mathrm{Tr}\, U = \sum_i \mathrm{tr}\, U_{ii}$.

A. SSH model

Let us start with the generalized SSH model described by the Hamiltonian on an infinite lattice:

$$\hat{H} = (\boldsymbol{c}_A^\dagger, \boldsymbol{c}_B^\dagger)\begin{pmatrix} & \Delta \\ \Delta^\dagger & \end{pmatrix}\begin{pmatrix} \boldsymbol{c}_A \\ \boldsymbol{c}_B \end{pmatrix}, \tag{1}$$

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where $\boldsymbol{c}_A^\dagger = (\ldots, c_{A,-1}^\dagger, c_{A,0}^\dagger, c_{A,1}^\dagger, c_{A,2}^\dagger, \ldots)$, and likewise for $\boldsymbol{c}_B$, and the hopping matrix Δ is defined by

$$\Delta = \begin{pmatrix} \ddots & & & & & & & \\ & t_1 & & & & & & \\ & t_2 & t_1 & & & & & \\ & t_3 & t_2 & t_1 & & & & \\ & & t_3 & t_2 & t_1 & & & \\ & & & t_3 & t_2 & t_1 & & \\ & & & & t_3 & t_2 & t_1 & \\ & & & & & & & \ddots \end{pmatrix}. \tag{2}$$

The basic symmetry of the Hamiltonian Eq. (1) is chiral symmetry. In addition, the model possesses time-reversal symmetry, so that the model belongs to class BDI [1–4]. The half-filled ground state is topologically characterized by the winding number of the Fourier-transformed matrix Δ. Note that t_3 is a specific hopping for a nontrivial high winding number [16,21]. For the bulk system without disorder, the Fourier transformation gives $\Delta = t_1 + t_2 e^{ik} + t_3 e^{2ik}$. Now, let us try to calculate the winding number in the lattice space, using the flow of Kitaev. To this end, let us unitarize the matrix Δ by using the singular value decomposition $\Delta = VGW^\dagger$ such that

$$U = VW^\dagger. \tag{3}$$

We separate the one-dimensional lattice sites specifying the positions of the unit cells as follows: Let j be the label of the unit cell. Then, let us separate them into two regions, say, $j \geqslant 0$ and $j < 0$, and let us call them region $A = 1$ and 2, respectively. Now, according to Kitaev [12], we introduce the flow of U as

$$\mathcal{F}_1(U) = \sum_{j\geqslant 0, k<0} \mathrm{tr}(U_{kj}^\dagger U_{jk} - U_{jk}^\dagger U_{kj}), \tag{4}$$

where in the present SSH model, tr is needless. Let us define the projector onto region 1 as $\Pi_1 \equiv \Pi$, where $\Pi_{ij} = \delta_{ij}$ for $i \geqslant 0$ and $\Pi_{ij} = 0$ otherwise, and the projector onto region 2 as $\Pi_2 \equiv \mathbb{1} - \Pi$. Then, the flow can be written as

$$\mathcal{F}_1(U) = \mathrm{Tr}(\epsilon^{AB} U^\dagger \Pi_A U \Pi_B) = \mathrm{Tr}(U^\dagger \Pi U - \Pi) = \mathrm{Tr} U^\dagger [\Pi, U]. \tag{5}$$

When a system has translational invariance, this reduces to Eqs. (A3) and (A5),

$$\mathcal{F}_1(U) = \mathcal{W}_1(U) \equiv \frac{i}{2\pi} \int dq \, \mathrm{tr}\, U_q^\dagger \partial_q U_q, \tag{6}$$

where $\mathcal{W}_1(U)$ is the conventional winding number of the unitary matrix U defined in the Fourier space. In the present case of the SSH model, U_q is just a single complex number, so that the trace in Eq. (6) is not necessary. Without translational symmetry, the winding number $\mathcal{W}_1$ cannot be defined, whereas the flow $\mathcal{F}_1$ is well defined.

For an infinite system, two matrices inside Tr in Eq. (5) are infinite dimensional, so that the Tr operation should be carried out after the subtraction of the two matrices. It should be noted that $U^\dagger \Pi U$ is a projector having 0 or 1 eigenvalues. Thus, $\mathcal{F}_1$ is integer valued. Moreover, it is manifestly topological, since even if a unit cell in region 1 is assigned to region 2, i.e., even if the regions 1 and 2 are deformed, the flow is invariant as Kitaev showed [12]. (See also Appendix C.) While the flow counts the difference of eigenvalue 1 between $U^\dagger \Pi U$ and Π, we can give an alternative formulation which counts the difference of 0's, as presented in Appendix B. This may be a kind of the index theorem.

As proposed by Kitaev, the above trace can be evaluated as if it were for finite dimensional matrices, when one introduces the truncation projector $\Pi^{(L)}$

$$\mathcal{F}_1 = \mathrm{Tr}\Pi^{(L)} U^\dagger \Pi U - \mathrm{Tr}\Pi^{(L)}\Pi, \tag{7}$$

where

$$\Pi_{ij}^{(L)} = \begin{cases} \delta_{ij} & (-L \leqslant i \leqslant L-1) \\ 0 & (\text{otherwise}) \end{cases}. \tag{8}$$

This formula may be useful for practical numerical applications, although it spoils the integer nature of $\mathcal{F}_1$. Below, let us show some examples.

1. Topological phase

The topological phase of the conventional SSH model ($t_3 = 0$) is adiabatically deformed to the model with $t_1 = 0$ and $t_2 = 1$ [29]. In this case, Δ is already a unitary matrix without using the singular value decomposition Eq. (3), and we find for $U = \Delta$,

$$U^\dagger \Pi U = \left(\begin{array}{cccc|cccc} \ddots & & & & & & & \\ & 0 & & & & & & \\ & & 0 & & & & & \\ & & & 1 & & & & \\ \hline & & & & 1 & & & \\ & & & & & 1 & & \\ & & & & & & 1 & \\ & & & & & & & \ddots \end{array}\right) \equiv \mathrm{diag}(\ldots, 0, 0, 1|1, 1, 1, \ldots),$$
$$\Pi = \mathrm{diag}(\ldots, 0, 0, 0|1, 1, 1, \ldots), \tag{9}$$

where the straight lines in the matrix stand for the boundaries separated by $\Pi_{1,2}$. Thus, we have $\mathcal{F}_1 = 1$. This is very sharp contrast to the trivial phase below in Sec. II A 2. One knows that Δ in this case actually moves a particle to its neighbor. Although nothing can be found in $U^\dagger U = \mathbb{1}$, the boundary introduced by the projector Π in between $U^\dagger$ and U reveals the flow just at the boundary, as can be seen in Eq. (9). It would be a kind of the bulk-edge correspondence.

2. Trivial phase

Let us set $t_2 = 0$ and $t_1 = 1$. Then, $\Delta = \mathbb{1}$ is a unitary matrix. In this case, $U^\dagger \Pi U = \Pi$. Thus, we have $\mathcal{F}_1 = 0$.

B. Finite systems with the periodic boundary condition

For numerical calculations, we inevitably use finite systems. With the periodic boundary condition, Δ in Eq. (2)

becomes

$$\Delta = \begin{pmatrix} t_1 & & & & & t_3 & t_2 \\ t_2 & t_1 & & & & & t_3 \\ t_3 & t_2 & t_1 & & & & \\ & & & \ddots & & & \\ & & & t_2 & t_1 & & \\ & & & t_3 & t_2 & t_1 & \\ & & & & t_3 & t_2 & t_1 \end{pmatrix}. \tag{10}$$

Let us assume that the number of the unit cells of the SSH model is finite, $2N$. The matrix Δ is then $2N \times 2N$ matrix. Let us separate the sites into two sets $0 \leqslant j \leqslant N-1$ and $-N \leqslant j \leqslant -1$, called region 1 and 2, respectively, and introduce corresponding projectors $\Pi_1 \equiv \Pi$ and $\Pi_2 \equiv \mathbb{1} - \Pi$, similarly in the infinite system.

1. Topological phase

As in the case of the infinite lattice, the matrix U with winding number 1 is adiabatically deformed into

$$U = \begin{pmatrix} 0 & & & & & & 1 \\ 1 & 0 & & & & & \\ & 1 & 0 & & & & \\ & & & \ddots & & & \\ & & & & 0 & & \\ & & & & 1 & 0 & \\ & & & & & 1 & 0 \end{pmatrix}. \tag{11}$$

The top right matrix element $U_{-N,N-1} = 1$ is due to the periodic boundary condition. This matrix U is unitary, and we have

$$U^\dagger \Pi U = \mathrm{diag}(0, 0, \dots, 0, 1|1, 1, \dots, 1, 0). \tag{12}$$

The finite-size effect is manifest as the matrix element $(U^\dagger \Pi U)_{N-1,N-1} = 0$ (the last 0 in the above): For the infinite one-dimensional (1D) chain, the projector Π chooses the space $j \geqslant 0$ which has only one boundary at $j = 0$, whereas in the periodic chain, the projector gives rise to two boundaries. Since the flow occurs at one direction, a positive flow at one boundary induces a negative flow at the other boundary, implying vanishing total flow. Therefore, we have $\mathcal{F}_1 = 0$ for the finite-size system even for the SSH model in the topological phase. This is also expected from the conventional identity associated with the trace, $\mathrm{Tr} U^\dagger \Pi U = \mathrm{Tr} U U^\dagger \Pi = \mathrm{Tr}\Pi$ holds for finite-dimensional matrices. Nevertheless, the truncation projector $\Pi^{(L)}$ in Eq. (8) is useful, in practice, even for finite systems. Namely, we have for Eq. (12)

$$\mathcal{F}_1 = \mathrm{Tr}\Pi^{(L)}(U^\dagger \Pi U - \Pi) = 1, \tag{13}$$

where $\Pi^{(L)}$ is defined by Eq. (8), if one chooses L as $1 \leqslant L \leqslant N-1$. This truncation projector removes the flow at an artificial boundary due to finite-size effects.

In Fig. 1, we show the flow as a function of the truncation size L near the SSH transition point $t_1 = t_2$ ($t_3 = 0$). It turns out that the flow does not so strongly depend on L, and the size $L \sim N/2$ may be suitable to reproduce the correct topological transition.

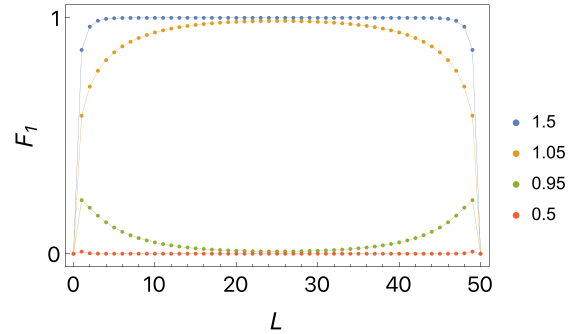

FIG. 1. The flow Eq. (13) as a function of the truncation size L for the finite unitary matrix Eq. (10) under the periodic boundary condition with $t_2 = 1.5, 1.05, 0.95, 0.5$. The other parameters $t_1 = 1$ and $t_3 = 0$ and the system size $2N = 100$ are fixed. $\mathcal{F}_1 = 0$ at $L = N$ reflects the fact that finite-size systems always show the trivial flow without the truncation.

C. Application to the SSH model with disorder

As an example of the calculation of the flow, we examine the generalized SSH model studied in Refs. [16,21], which gives topological transition due to disorder. We set

$$t_{1,j} = 0 + \delta t_{1,j}, \quad t_{2,j} = 1 + \delta t_{2,j}, \quad t_3 = -2, \tag{14}$$

where $\delta t_{1,j} \in [-W/2, W/2]$ and $\delta t_{2,j} \in [-W/4, W/4]$ are random parameters. In Fig. 2, we show the flow $\mathcal{F}_1$ as a function of the disorder strength for the generalized SSH model. It turns out that the flow can reveal the topological transitions quantitatively, and thus the truncation scheme works around the transition points of dirty systems. As discussed in Ref. [16], the sequential topological transition $\mathcal{F}_1 = 2 \to 1 \to 0$ shows that the present model can be characterized by the winding numbers rather than the polarizations (the Berry phase) with Z_2 nature. Although it may be difficult to find the model in the real materials, the metamaterial such as topoelectrical circuits could give an experimental platform for observing the sequential topological transitions.

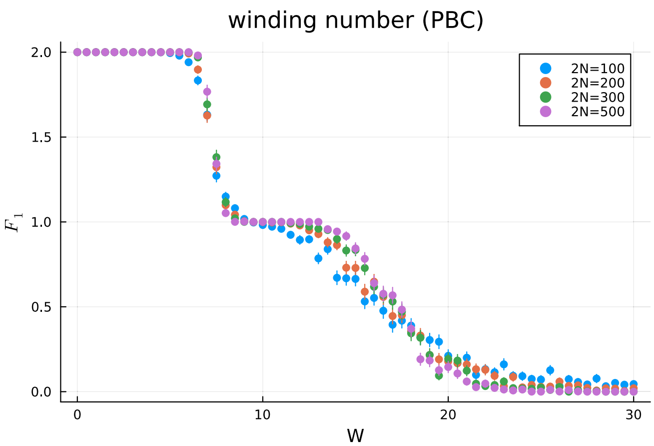

FIG. 2. The flow as a function of the disorder strength W of the generalized SSH model with size $2N = 100$, 200, 300, and 500 averaged over 100 ensembles.

III. FLOW IN THREE DIMENSIONS

The flow introduced by Kitaev is basically for one dimension, but the same idea leads to the Chern number in two dimensions, which is represented by the projectors to the occupied states on a lattice [12]. In this section, we further generalize the flow to three dimensions, and derive the real-space winding number on a three dimensional lattice.

A. Winding number

Let U_q be a unitary matrix as a function of the wave vector $q=(q_x,q_y,q_z)$. Then, the winding number of U_q is defined by

$$\mathcal{W}_3(U)=\frac{1}{24\pi^2}\int d^3q\epsilon^{\mu\nu\rho}\mathrm{tr}(U^\dagger\partial_\mu UU^\dagger\partial_\nu UU^\dagger\partial_\rho U), \quad (15)$$

where $\partial_\mu\equiv\partial_{q_\mu}$. On a lattice, the site dependence of the matrix U is generically denoted as U_{jk}, where $j=(j_x,j_y,j_z)$ and k label two sites. In the present case with translational invariance, we assume $U_{jk}=U_{j-k}$. Then, U_{j-k} is related with U_q via the Fourier transformation

$$U_{j-k}=\int_{-\pi}^{\pi}\frac{d^3q}{(2\pi)^3}e^{iq\cdot(j-k)}U_q. \quad (16)$$

Using Eq. (A5), the winding number Eq. (15) can be rewritten in the real space as

$$\mathcal{W}_3(U)=\frac{\pi i}{3}\mathrm{tr}(\epsilon^{\mu\nu\rho}U^\dagger[X_\mu,U]U^\dagger[X_\nu,U]U^\dagger[X_\rho,U]), \quad (17)$$

where $X_{\mu,ij}=i_\mu\delta_{ij}$ is the position operator. Equation (A3) further leads to

$$\begin{aligned}\mathcal{W}_3(U)&=\frac{\pi i}{3}\mathrm{Tr}(\epsilon^{\mu\nu\rho}U^\dagger[\Pi_\mu,U]U^\dagger[\Pi_\nu,U]U^\dagger[\Pi_\rho,U])\\&=-\frac{\pi i}{3}\mathrm{Tr}(\epsilon^{\mu\nu\rho}U^\dagger\Pi_\mu U\Pi_\nu U^\dagger\Pi_\rho U)\\&\equiv-\frac{\pi i}{3}w_3(U,\Pi_x,\Pi_y,\Pi_z), \quad (18)\end{aligned}$$

where Π_μ is the projector onto the non-negative μ direction, $(\Pi_\mu)_{jk}=\delta_{jk}$ for $j_\mu\geqslant 0$ and $=0$ otherwise.

B. Flow

Let us separate the three-dimensional lattice spanned by $j=(j_x,j_y,j_z)$ into four regions denoted by $A=1,2,3,4$ and introduce corresponding projectors Π_A. For example, we can choose each region such that $j_x\geqslant 0$, $j_y\geqslant 0$, $j_z<0$ $(A=1)$, $j_x<0$, $j_y\geqslant 0$, $j_z<0$ $(A=2)$, $j_z\geqslant 0$ $(A=3)$, and $j_y<0$, $j_z<0$ $(A=4)$. We assume $\Pi_A\Pi_B=\delta_{AB}\Pi_A$ and $\sum_A\Pi_A=\mathbb{1}$ with $A=1,2,3,4$, for simplicity. Define the flow by

$$\mathcal{F}_3(U)=-2\pi i\mathrm{Tr}(\epsilon^{ABCD}U^\dagger\Pi_A U\Pi_B U^\dagger\Pi_C U\Pi_D). \quad (19)$$

This may be a generalized definition of the flow Eq. (5) to three dimensions. Using $\Pi_4=1-(\Pi_1+\Pi_2+\Pi_3)$, we have

$$\begin{aligned}\mathcal{F}_3(U)&=-2\pi i\mathrm{Tr}(\epsilon^{ABC}U^\dagger\Pi_A U\Pi_B U^\dagger\Pi_C U),\\&\equiv-2\pi i f_3(U,\Pi_1,\Pi_2,\Pi_3), \quad (20)\end{aligned}$$

where A,B,C are restricted to $A,B,C=1,2,3$. What is important here is that any two regions among 1,2,3, and 4 share not only lines but also finite areas around generic contact point of all the regions 1,2,3, and 4. Then, the flow is kept unchanged under the deformation of the regions, as shown in Appendix C. In this sense, we claim that the flow defined above is manifestly topological.

So far we have defined the winding number Eq. (18) and the flow Eq. (20) in three dimensions. Next, we have to consider the relationship between w_3 and f_3. The projector Π_x is divided into

$$\Pi_x=\sum_{i,j=\pm}\Pi_{+ij}, \quad (21)$$

where Π_{+++} is the projector onto $j_x\geqslant 0$, $j_y\geqslant 0$, and $j_z\geqslant 0$, Π_{++-} is the projector onto $j_x\geqslant 0$, $j_y\geqslant 0$, but $j_z<0$, and so on. Then, we obtain

$$w_3(U,\Pi_x,\Pi_y,\Pi_z)=\sum_{i,j,k,l,m,n=\pm}w_3(U,\Pi_{+ij},\Pi_{k+l},\Pi_{mn+}). \quad (22)$$

In this summation, contributions are three kinds, $\pm f_3/2$ and zero. To be concrete, let us assign the vector $v_{ijk}=(i,j,k)^T$ for Π_{ijk}, where $\pm$ in Π_{ijk} mean ± 1 in (i,j,k), and calculate the determinant $\det(v_{+ij},v_{k+l},v_{mn+})$. If it vanishes, corresponding w_3 vanishes. For nonzero determinant, let us define the sign of the determinant s. Then, we have $w_3(\Pi_{+ij},\Pi_{k+l},\Pi_{mn+})=s\,f_3/2$. Exceptions are the cases where three regions spanned by three projectors Π_{+ij}, Π_{k+l}, and Π_{mn+} separate the remaining region into two disconnected regions such as Π_{++-}, Π_{-++}, and Π_{+-+}. These are vanishing, even though the determinants are finite. Thus, in the summation above, there are 15 positive-sign terms and 3 negative-sign terms which give finite contributions. We finally reach

$$w_3(U,\Pi_x,\Pi_y,\Pi_z)=6f_3(U,\Pi_1,\Pi_2,\Pi_3), \quad (23)$$

from which it follows

$$\mathcal{F}_3(U)=\mathcal{W}_3(U). \quad (24)$$

As in the one-dimensional case of Eq. (6), it turns out that the winding number in three dimensions $\mathcal{W}_3$ can be represented by the flow $\mathcal{F}_3$ defined on the real lattice space. Note that the flow Eq. (20) is well defined in the absence of translational symmetry. As in the case of one dimension, for numerical computations using finite-size systems, the flow in three dimensions also vanishes trivially. Nevertheless, as discussed in Sec. II B, the truncation scheme enables to obtain an approximate winding number. Namely,

$$\mathcal{F}_3(U)=-2\pi i\mathrm{Tr}(\epsilon^{ABC}\Pi^{(L)}U^\dagger\Pi_A U\Pi_B U^\dagger\Pi_C U) \quad (25)$$

is useful for numerical computations, where for simplicity, we assume the truncation projector $\Pi^{(L)}$ as

$$\Pi^{(L)}_{ij}=\begin{cases}\delta_{ij} & (-L\leqslant i_x,i_y,i_z\leqslant L-1)\\ 0 & (\text{otherwise})\end{cases} \quad (26)$$

for a finite lattice system, $-N\leqslant i_x,i_y,i_z\leqslant N-1$.

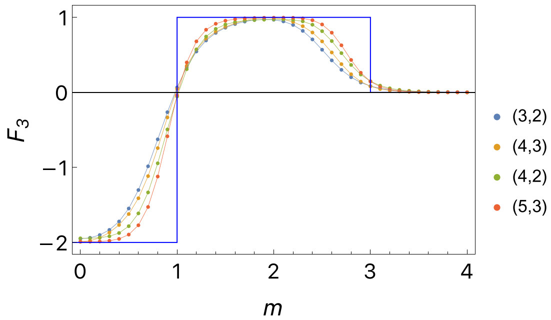

FIG. 3. The flow $\mathcal{F}_3$ for $(N, L) =$ (3, 2), (4,3), (4,2), and (5,2) systems. The blue straight lines show the exact winding numbers $\mathcal{W}_3 = -2, 1, 0$ for $|m| < 1$, $1 < |m| < 3$, and $3 < |m|$, respectively, where we have set $t = b = 1$.

C. Application to the Wilson-Dirac model

Recently, Shiozaki examined the Dirac operator on the lattice for his discrete formula of the winding number [27]. Let us compute the flow of the same model to check the validity of Eq. (24). To this end, let us start with the Wilson-Dirac model, a typical model of a topological insulator with chiral symmetry in three dimensions, described by the following Hamiltonian represented by the wave vector

$$H = t\gamma^\mu \sin k_\mu + \gamma^4\left(m + b\sum_\mu \cos k_\mu\right). \tag{27}$$

For the γ matrices defined by $\gamma^\mu = \sigma^1 \otimes \sigma^\mu$ for $\mu = 1, 2, 3$ and $\gamma^4 = \sigma^2 \otimes \sigma^0$, where σ^0 stands for the unit matrix, it turns out that this model has time-reversal symmetry described by $T = K\sigma^1 \otimes i\sigma^2$, where K denotes the complex conjugation, as well as chiral symmetry described by $C = \sigma^3 \otimes \sigma^0$, and hence, the model belongs to class DIII [1–4]. Thus, the topological property of the half-filled ground state for this model is specified basically by the winding number $\mathcal{W}_3$ in Eq. (15). With the choice of the γ matrices above, the Hamiltonian is represented as

$$H = \begin{pmatrix} & D \\ D^\dagger & \end{pmatrix}. \tag{28}$$

Here, the so-called Wilson-Dirac operator D is defined by

$$\begin{aligned} D &= t\sigma^\mu \sin k_\mu - i\sigma^0\left(m + b\sum_\mu \cos k_\mu\right) \\ &= \frac{t}{2i}\sigma^\mu(\delta_\mu - \delta^*_\mu) - i\sigma^0\left[m + \frac{b}{2}\sum_\mu(\delta_\mu + \delta^*_\mu)\right]. \end{aligned} \tag{29}$$

The second line above is the operator represented on the real lattice denoted by the forward and backward shift operators to the μ direction, $\delta_\mu f_j = f_{j+\hat{\mu}}$ and $\delta^*_\mu f_j = f_{j-\hat{\mu}}$, where j stands for a lattice site and $\hat{\mu}$ is the unit vector toward μ direction.

It is known that there appear three phases with winding number −2, 1, and 0, depending on the parameters of the model, obtained by the direct computation of the winding number. Comparing this exact result, let us check the validity of the three-dimensional flow derived in Sec. III B. In Fig. 3, we show numerical results of the flow $\mathcal{F}_3$ calculated for D in Eq. (29) represented in the real lattice space. Here, we have firstly unitarized the operator D by the use of the singular value decomposition, as in Eq. (3), and next computed the three-dimensional flow $\mathcal{F}_3$ given by Eq. (20). Contrary to the case of one dimension, the number of lattice sites to each direction are very limited. Indeed, the system sizes demonstrated in Fig. 3 are from 6^3 to 10^3. Nevertheless, it turns out that the exact winding number is qualitatively reproduced as a function of m. In particular, in the middle of each phase apart from phase boundaries, the flow is saturated at the exact winding number.

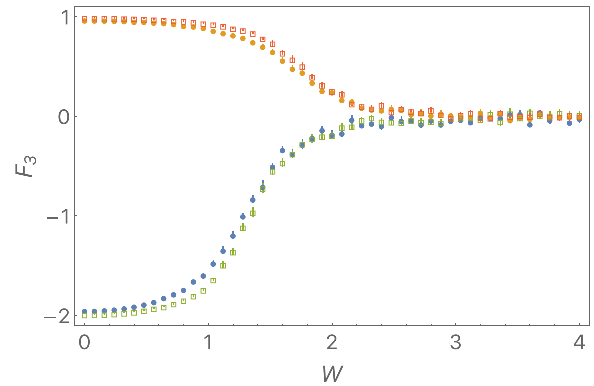

FIG. 4. The flow $\mathcal{F}_3$ as a function of the disorder strength W for $(N, L) = (3, 2)$ (circles) and (4,2) (squares) systems averaged over 10 ensembles. Upper two data are for $m = 2$, whereas the lower two are for $m = 0$.

Let us introduce disorder into this model and compute the flow $\mathcal{F}_3$, instead of the winding number $\mathcal{W}_3$, to see whether topological transitions occur, since $\mathcal{W}_3$ is no longer well defined due to broken translational symmetry. It should be noted here that due to the limited system size, the flow is not very exact, especially near the phase boundary. We replace the hopping parameters t and b into site-dependent ones t_j and b_j and set

$$t_j = 1 + \delta t_j, \quad b_j = 1 + \delta b_j, \tag{30}$$

where $\delta t_j \in [-W, W]$ and $\delta b_j \in [-W, W]$ are random parameters. In Fig. 4, the flow $\mathcal{F}_3$ is shown as a function of the disorder strength W. In both cases $m = 0$ and 2, the transition from topological to trivial phases are observed, but the analysis of detailed behavior of the transition may need more large systems. Experimentally, the Wilson-Dirac model can be implemented by the topoelectrical circuits on the hyperbolic lattice. Indeed, the four-dimensional Wilson-Dirac model has been realized on the hyperbolic {8, 8} lattice and the second Chern number has been observed [30]. Freezing one direction of such a circuit, one can obtain the three-dimensional circuit corresponding to the Wilson-Dirac model denoted by Eqs. (28) and (29).

IV. SUMMARY AND DISCUSSIONS

The flow of a unitary matrix introduced by Kitaev is a manifestly topological formulation of the winding number represented on a real lattice. Applying to a disordered model with topological transitions, we showed that the flow is quite useful for numerical computations with a suitable truncation scheme. We also extended the notion of the flow into three dimensions. In such a three-dimensional formulation, our formula reproduces a qualitative feature of the winding number for the Wilson-Dirac operator. However, to reveal the quantitative properties, e.g., a topological transition of a dirty system, requires numerical ingenuity.

ACKNOWLEDGMENT

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APPENDIX A: PROJECTORS AND POSITION OPERATORS

Let i denote a site on a lattice. For the time being, we consider the one-dimensional case. Let θ_i be the discrete step function defined by $\theta_i = 1$ for $i \geqslant 0$ and $\theta_i = 0$ for $i < 0$. Then, the projection operator can be written as $\Pi_{ij} = \theta_i\delta_{ij}$. Let X be the position operator defined by $X_{ij} = i\delta_{ij}$. Let A_{ij} and B_{ij} be matrices which depend on the i and j sites. Then, we have

$$[\Pi, B]_{ij} = (\theta_i - \theta_j)B_{ij}, \;\; [X, B]_{ij} = (i - j)B_{ij}. \tag{A1}$$

Thus,

$$\begin{aligned}(A[\Pi, B])_{ij} &= \sum_k A_{ik}(\theta_k - \theta_j)B_{kj},\\ (A[X, B])_{ij} &= \sum_k A_{ik}(k - j)B_{kj}.\end{aligned} \tag{A2}$$

For a system with translational invariance, we assume $A_{ij} = A_{i-j}$. Let Tr be the trace over the matrix A_{ij} as well as over the site i, i.e., $\mathrm{Tr}A = \sum_i \mathrm{tr}A_{ii}$. Then,

$$\begin{aligned}\mathrm{Tr}(A[\Pi, B]) &= \sum_{i,k} \mathrm{tr}A_{i-k}(\theta_k - \theta_i)B_{k-i}\\ &= \sum_{i,k} \mathrm{tr}A_{-k}(\theta_{i+k} - \theta_i)B_k\\ &= \sum_k \mathrm{tr}A_{-k}kB_k = \mathrm{tr}(A[X, B]),\end{aligned} \tag{A3}$$

where we have used $\sum_i(\theta_{i+j} - \theta_{i+k}) = j - k$. Note that the last equation does not depend on i for translational invariance, as can be seen from Eq. (A2) in the case of $i = j$.

Translational invariance also enables to make the Fourier transformation

$$A_j = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{iqj} A_q. \tag{A4}$$

It follows that

$$\mathrm{tr}(A[X, B]) = \frac{i}{2\pi} \int_{-\pi}^{\pi} dq \mathrm{tr}A_q\partial_q B_q. \tag{A5}$$

The above Π-X correspondence, Eq. (A3) is valid only in the case of the trace of matrices including a single commutator of Π and X. In the three-dimensional case, the winding number has three commutators of X_μ and Π_μ, but they are different directions. Therefore, Eq. (A3) can be applied.

APPENDIX B: THE FLOW REPRESENTED BY ZERO MODES

Given a unitary matrix, we can define a Hermitian matrix in doubly extended space. In this section, we show that the flow has an intimate relationship with the zero modes of such a Hermitian matrix. It may be a kind of the index theorem.

From a unitary matrix Eq. (3), let us define the Hermitian operator (or the SSH-like Hamiltonian but with the projector) as

$$H = \begin{pmatrix} & \Pi U\\ U^\dagger\Pi & \end{pmatrix} = \begin{pmatrix} \Pi & \\ & \mathbb{1}\end{pmatrix}\begin{pmatrix} & U\\ U^\dagger & \end{pmatrix}\begin{pmatrix} \Pi & \\ & \mathbb{1}\end{pmatrix}. \tag{B1}$$

For a while, we consider the infinite system in Sec. II B. This operator H has chiral symmetry

$$\Gamma H\Gamma^{-1} = -H, \quad \Gamma \equiv \begin{pmatrix} \mathbb{1} & \\ & -\mathbb{1}\end{pmatrix}, \tag{B2}$$

where $\mathbb{1}$ stands for the identity matrix in the space of U. Note that

$$H^2 = \begin{pmatrix} \Pi & \\ & U^\dagger\Pi U\end{pmatrix}. \tag{B3}$$

Then, the flow Eq. (5) can be written by

$$\mathcal{F}_1 = -\widetilde{\mathrm{Tr}}\,\Gamma H^2, \tag{B4}$$

where $\widetilde{\mathrm{Tr}}$ stands for the trace in the extended space. Using $\widetilde{\mathrm{Tr}}\,\Gamma = 0$, we have

$$\mathcal{F}_1 = \widetilde{\mathrm{Tr}}\,\Gamma(1 - H^2). \tag{B5}$$

The operator H has eigenvalues ± 1 and 0. Let φ_n ($n = 1, 2, \ldots,$) be the wave function of H with eigenvalues 1. Then, because of chiral symmetry, the wave functions with eigenvalue -1 denoted by φ_{-n} can be given by $\varphi_{-n} = \Gamma\varphi_n$ ($n = 1, 2, \ldots$). Namely, the ± 1 energy states are always paired. Let φ_{0m} ($m = 1, 2, \ldots$) be the wave function of H with eigenvalue 0. Such zero-energy states can be chosen as the eigenstates of Γ. Therefore, the zero modes are classified as $\varphi_{0m}^\pm$, where $\Gamma\varphi_{0m}^\pm = \pm\varphi_{0m}^\pm$. To be concrete, they are solutions of

$$U^\dagger\Pi\varphi_{0m}^+ = 0, \quad \Pi U\varphi_{0m}^- = 0. \tag{B6}$$

Using the eigenfunctions, the flow can be expressed as

$$\mathcal{F}_1 = \sum_m \varphi_{0m}^\dagger\Gamma\varphi_{0m} = \#(+) - \#(-). \tag{B7}$$

Namely, the flow is just the difference of the numbers of the zero modes of H. However, note that this is just a formal result, since $\#(\pm)$ are, respectively, infinite. Therefore, some regularization should be needed. Moreover, the flow vanishes for finite systems.

For practical purposes, the truncation scheme mentioned in the text is also useful:

$$\begin{aligned}\mathcal{F}_1 &= \widetilde{\mathrm{Tr}}\,\Gamma\widetilde{\Pi}^{(L)}(1 - H^2)\\ &= \sum_m \varphi_{0m}\Gamma\widetilde{\Pi}^{(L)}\varphi_{0m}\\ &= \sum_m \varphi_{0m}^+\widetilde{\Pi}^{(L)}\varphi_{0m}^+ - \sum_m \varphi_{0m}^-\widetilde{\Pi}^{(L)}\varphi_{0m}^-,\end{aligned} \tag{B8}$$

where $\widetilde{\Pi}^{(L)} \equiv \mathrm{diag}(\Pi^{(L)}, \Pi^{(L)})$ stands for the projector $\Pi^{(L)}$ extended to the doubled space of H. This formula is valid for finite systems.

APPENDIX C: FLOW AS A TOPOLOGICAL INVARIANCE

We show that the flow is manifestly topological. To begin with, let us start in the case of one dimension to fix our notations. In this Appendix C, a unitary matrix U is denoted as $U_{i_1 i_2}$, where i_a specifies the number of the unit cell as well as the number of internal degrees of freedom inside the unit cell such as $i_a = (i, s)$. Then, according to Kitaev, let us define the current

$$f_{i_1 i_2} \equiv U^\dagger_{i_1 i_2} U_{i_2 i_1} - U^\dagger_{i_2 i_1} U_{i_1 i_2} = \epsilon^{ab} U^\dagger_{i_a i_b} U_{i_b i_a}, \tag{C1}$$

where $a, b = 1, 2$ are implicitly summed in the last equality. Note that

$$f_{i_1 i_2} = -f_{i_2 i_1}. \tag{C2}$$

The current is conserved: For a fixed i_1, we have

$$\sum_{i_2} f_{i_1 i_2} = \sum_{i_2} \left(U^\dagger_{i_1 i_2} U_{i_2 i_1} - U^\dagger_{i_2 i_1} U_{i_1 i_2} \right) = 1 - 1 = 0, \tag{C3}$$

where the sum over $i_2 = (i, s)$ means the sum over i and s, and we have used the fact that U is unitary. The flow in Eqs. (4) or (5) is given by

$$\mathcal{F}_1(U) = \sum_{i_1 \in 1} \sum_{i_2 \in 2} f_{i_1 i_2}. \tag{C4}$$

Now let us pick up a specific site $i_0 \in 1$, and define the new region $1'$ excluding i_0, i.e., $1 = 1' + i_0$. Then, the above flow can be written as

$$\mathcal{F}_1(U) = \sum_{i_1 \in 1'} \sum_{i_2 \in 2} f_{i_1 i_2} + \sum_{i_2 \in 2} f_{i_0 i_2}. \tag{C5}$$

If one reassigns i_0 to region 2, the flow changes into

$$\mathcal{F}'_1(U) = \sum_{i_1 \in 1'} \sum_{i_2 \in 2} f_{i_1 i_2} + \sum_{i_1 \in 1'} f_{i_1 i_0}. \tag{C6}$$

The difference is

$$\begin{aligned} \mathcal{F}_1 - \mathcal{F}'_1 &= \sum_{i_2 \in 2} f_{i_0 i_2} - \sum_{i_1 \in 1'} f_{i_1 i_0} \\ &= \sum_{i_2 \in 2} f_{i_0 i_2} + \sum_{i_1 \in 1'} f_{i_0 i_1} + f_{i_0 i_0} \\ &= \sum_{i_2} f_{i_0 i_2} = 0, \end{aligned} \tag{C7}$$

where we have used Eqs. (C2) and (C3). Thus, the flow is invariant under the reassignment of a site into another region. In the three-dimensional case, the invariance of flow can also be shown in parallel with the one-dimensional case. Let us define a current in three dimensions

$$f_{i_1 i_2 i_3 i_4} = \epsilon^{abcd} U^\dagger_{i_a i_b} U_{i_b i_c} U^\dagger_{i_c i_d} U_{i_d i_a}, \tag{C8}$$

where i_a $(a = 1, 2, 3, 4)$ specifies a site in three dimensions. By definition, $f_{i_1 i_2 i_3 i_4}$ is antisymmetric in all four indices i_a. We first show that the current is conserved at each site:

$$\begin{aligned} \sum_{i_4} f_{i_1 i_2 i_3 i_4} &= \epsilon^{abc} \big[U^\dagger_{i_a i_b} U_{i_b i_c} U^\dagger_{i_c i_4} U_{i_4 i_a} - U^\dagger_{i_a i_b} U_{i_b i_4} U^\dagger_{i_4 i_c} U_{i_c i_a} \\ &\quad + U^\dagger_{i_a i_4} U_{i_4 i_b} U^\dagger_{i_b i_c} U_{i_c i_a} - U^\dagger_{i_4 i_a} U_{i_a i_b} U^\dagger_{i_b i_c} U_{i_c i_4} \big] \\ &= \epsilon^{abc} \big[U^\dagger_{i_a i_b} U_{i_b i_a} \delta_{i_a i_c} - U^\dagger_{i_a i_b} U_{i_b i_a} \delta_{i_b i_c} \\ &\quad + U^\dagger_{i_a i_c} U_{i_c i_a} \delta_{i_a i_b} - U^\dagger_{i_b i_a} U_{i_a i_b} \delta_{i_a i_c} \big] \\ &= \epsilon^{abc} \delta_{i_a i_c} \big[U^\dagger_{i_a i_b} U_{i_b i_a} + U^\dagger_{i_b i_a} U_{i_a i_b} \\ &\quad - U^\dagger_{i_a i_b} U_{i_b i_a} - U^\dagger_{i_b i_a} U_{i_a i_b} \big] \\ &= 0, \end{aligned} \tag{C9}$$

where a, b, c are restricted to 1,2,3, and repeated i_4 in the unitary matrices are implicitly summed. Using the current, we can write the flow $\mathcal{F}_3$ such that

$$\mathcal{F}_3(U) = 2\pi i \sum_{i_1 \in 1} \sum_{i_2 \in 2} \sum_{i_3 \in 3} \sum_{i_4 \in 4} f_{i_1 i_2 i_3 i_4}, \tag{C10}$$

where 1,2,3,4 stand for the regions in the three-dimensional lattice introduce above Eq. (19).

Next, let us show that the flow Eq. (C10) is topological, since the flow is invariant even if a site in a region is assigned to another region, implying that the flow does not depend on the detailed shapes of regions 1,2,3, and 4. Let $i_0 \in 1$ be a site in region 1, and let $1'$ be the set of sites in region 1 except for i_0, i.e., $1 = i_0 + 1'$. Then,

$$\mathcal{F}_3 = 2\pi i f_{1234} \equiv 2\pi i \big(f_{1'234} + f_{i_0 234} \big), \tag{C11}$$

where $f_{1ijk} = \sum_{l \in 1} f_{lijk}$, and so on. Let us assign i_0 in region 2. Then, the flow becomes

$$\mathcal{F}'_3 = 2\pi i \big(f_{1'234} + f_{1' i_0 34} \big). \tag{C12}$$

The difference is

$$\mathcal{F}_3 - \mathcal{F}'_3 = 2\pi i \big(f_{i_0 234} - f_{1' i_0 34} \big) \quad = 2\pi i \big(f_{i_0 234} + f_{i_0 1' 34} \big). \tag{C13}$$

On the other hand, the conservation of the current Eq. (C9) can be written as

$$f_{1' jkl} + f_{i_0 jkl} + f_{2jkl} + f_{3jkl} + f_{4jkl} = 0, \tag{C14}$$

for fixed j, k, l, when $i_0 \in 1$. Sum over $j \in 3$ and $k \in 4$ in the above conservation law yields

$$\begin{aligned} 0 &= f_{1' 34 l} + f_{i_0 34 l} + f_{234 l} + f_{334 l} + f_{434 l} \\ &= f_{1' 34 l} + f_{i_0 34 l} + f_{234 l}. \end{aligned} \tag{C15}$$

Setting $l = i_0$, we have

$$0 = f_{1' 34 i_0} + f_{i_0 34 i_0} + f_{234 i_0} = f_{1' 34 i_0} + f_{234 i_0}. \tag{C16}$$

It follows from Eq. (C13) that $\mathcal{F}_3 = \mathcal{F}'_3$.

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