Topological Invariants and Ground-State Wave functions of Topological Insulators on a Torus

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We define topological invariants in terms of the ground-state wave functions on a torus. This approach leads to precisely defined formulas for the Hall conductance in four dimensions and the topological magnetoelectric θ term in three dimensions, and their generalizations in higher dimensions. They are valid in the presence of arbitrary many-body interactions and disorder. These topological invariants systematically generalize the two-dimensional Niu-Thouless-Wu formula and will be useful in numerical calculations of disordered topological insulators and strongly correlated topological insulators, especially fractional topological insulators.

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I. INTRODUCTION

Topological insulators are among the major recent developments in condensed matter physics [1–3]. The physics of topological insulators started with noninteracting systems [4–15], for which simple and calculable topological invariants have been invaluable tools. More recently, it became clear that the interplay between topology and many-body interactions is a still-richer field [16–59]; therefore, it is highly desirable to develop topological invariants that are valid in the presence of strong interactions.

The root state of three-(spatial)-dimensional (3D) and two-(spatial)-dimensional (2D) topological insulators with time-reversal symmetry is the four-(spatial)-dimensional (4D) quantum Hall (QH) state [11,60] from which the topological field theory of 3D and 2D insulators can be obtained by the procedure of "dimensional reduction" [11]. The electromagnetic effective action of the 4D QH effect reads [3,61]

$$S_{\rm eff} = \frac{\sigma_{4D}}{24\pi^2}\int dt d^4x \epsilon^{\mu\nu\rho\sigma\tau} A_\mu \partial_\nu A_\rho \partial_\sigma A_\tau, \tag{1}$$

where we have adopted the units in which the electric charge e, the Planck constant h, and the light velocity c are all unity. The coefficient $\sigma_{\rm 4D}$ is referred to as the "4D Hall conductance" (or the 4D Hall coefficient). Physically, the 4D QH effect has the nonlinear topological electromagnetic response [11] $j^\mu = \frac{\delta S_{\rm eff}}{\delta A_\mu} = \frac{\sigma_{\rm 4D}}{8\pi^2}\epsilon^{\mu\nu\rho\sigma\tau}\partial_\nu A_\rho \partial_\sigma A_\tau$ in the bulk, which is described naturally by the Chern-Simons effective action. If a nontrivial 4D QH insulator is cut open in one direction, there are $|\sigma_{\rm 4D}|$ copies of 3D chiral-fermion (Weyl-fermion) modes localized at the boundary. These boundary modes are close analogues of the 1D chiral edge states [62,63] of 2D QH. In fact, the QH effect can be generalized to all even spatial dimensions, whose boundary modes are chiral fermions in odd spatial dimensions.

In the noninteracting limit, the explicit formula for $\sigma_{\rm 4D}$ has been obtained by Qi, Hughes, and Zhang as [11]

$$\sigma_{\rm 4D} = c_2 \equiv \frac{1}{32\pi^2}\int d^4k \epsilon^{ijkl} {\rm Tr} f_{ij} f_{kl}, \tag{2}$$

where f_{ij} is the non-Abelian Berry curvature defined in terms of the noninteracting Bloch states [64].

Now, a natural question arises: Can we find a formula for $\sigma_{\rm 4D}$ that is precisely defined in the presence of arbitrary interaction and disorder? Such a formula, if it exists, will be especially desirable for the investigation of fractional quantum Hall states in 4D. More importantly, it may also shed light on strongly interacting topological insulators in lower dimensions.

The same question also arises for the 3D topological insulators, whose effective topological response theory is given by [11]

$$\begin{aligned} S_{\rm eff} &= \frac{1}{8\pi^2}\int dt d^3x \epsilon^{ijkl}\theta \partial_i A_j \partial_k A_l \\ &= \frac{1}{4\pi^2}\int dt d^3x \theta \mathbf{E}\cdot\mathbf{B}. \end{aligned} \tag{3}$$

This topological effective action describes the quantized topological magnetoelectric effect, in which an electric field induces a magnetization with a universal constant of proportionality [11].

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In the noninteracting limit, θ has a simple expression [11,65,66]

$$\theta = \frac{1}{4\pi}\int d^3k\epsilon^{ijk}\mathrm{Tr}\left\{\left[\partial_i a_j(k) + \frac{2}{3}ia_i(k)a_j(k))\right]a_k(k)\right\}, \tag{4}$$

which is a 3D Chern-Simons term. In the presence of time-reversal symmetry, this Chern-Simons term is quantized and has been shown to be equivalent [66] to the Z_2 topological invariant [12]. The natural question is as follows: Is there a formula for θ that is valid in the presence of an arbitrary interaction and disorder? From the experimentalist's perspective, this question is more urgent than the 4D QH case because many 3D topological insulators have been realized in experiments, and the electron-electron interaction has been playing a more important role.

To partially answer these questions, interacting topological invariants expressed in terms of Green's functions at zero frequency (namely, the "topological Hamiltonian" [67]) for interacting insulators have been proposed [68–70], which provide an efficient approach for topological invariants of various topological insulators and superconductors (see, e.g., Refs. [40,50–56,71–75] for applications). However, there are several shortcomings of this approach. First, it cannot be directly applied to disordered systems in which the momentum **k** in the single-particle Green's function is not a good quantum number [76]. Second, it is unclear whether or not that approach will fail for some fractional topological states.

In Ref. [77], Niu, Thouless, and Wu found, for the 2D QH, a topological invariant (the first Chern number) expressed in terms of the ground-state wave function, which is valid in the presence of an arbitrary interaction and disorder. To search for the general formulas for $\sigma_{4\mathrm{D}}$ in 4D and θ in 3D, a hopeful approach is to generalize their formulas to higher dimensions. However, as we will see later, the most straightforward 4D generalization of their formulas, namely, the generalization of the 2D phase twisting (θ_1, θ_2) to the 4D phase twisting $(\theta_1, \theta_2, \theta_3, \theta_4)$ [see Eq. (30)], cannot produce the 4D Hall conductance $\sigma_{4\mathrm{D}}$. Because of this difficulty, it is unclear how this approach can be generalized to higher-dimensional topological states.

In this paper, we propose general topological invariants for higher-dimensional topological insulators in terms of ground-state wave functions. The boundary conditions adopted here are not the same as the standard one used in Ref. [77], which is a pure gauge with vanishing field strength. Using these new boundary conditions (see Secs. II and VIII, we obtain for $\sigma_{4\mathrm{D}}$ and θ simple formulas expressed in terms of the ground-state wave function on a torus [see Eqs. (12,29,41,44), etc]. We also generalize these formulas to higher dimensions [see Eq. (24), etc]. These topological invariants are valid in the presence of an arbitrary interaction and disorder; thus, they can be applied to topological states with strong disorders and strongly correlated topological states including fractionalized states. Unexpectedly, the generalized formula for σ_{4D} appears not as a second Chern number but as the difference between two first Chern numbers [Eqs. (12,29)]. Similarly, the formula for θ does not appear as a Chern-Simons term but as the difference between two winding numbers [Eqs. (41,44)].

The rest of this paper is organized as follows. In Sec. II, we study the 4D QH and define the topological invariant for integer QH in 4D. In Sec. III, we test this topological invariant in two noninteracting models. We then generalize the 4D topological invariant to higher-dimensional QH effects in Sec. IV. In Sec. V, we present the topological invariants for fractional quantum Hall effects. A different boundary condition is investigated in Sec. VI, which leads to a 4D topological invariant unrelated to the 4D Hall conductance. The next two sections, namely, Secs. VII and VIII, are devoted to 1D and 3D θ terms, respectively.

II. THE 4D HALL COEFFICIENTS $\sigma_{4\mathrm{D}}$ EXPRESSED IN TERMS OF THE GROUND-STATE WAVE FUNCTION

In this section, we describe the topological invariant defined in terms of the ground-state wave function of a 4D insulator on a torus with generalized twisted boundary conditions. For simplicity, in this section, we assume that the ground state is unique, while the cases with ground-state degeneracy will be studied in Sec. V. We take the system to be a 4D torus with circumference L_1, L_2, L_3, L_4 along the x_1, x_2, x_3, x_4, directions, respectively. We take the generalized twisted boundary condition parametrized by $(\theta_1, \theta_2, \phi)$ as follows [78]. First, for $i = 1, 2$,

$$\begin{aligned}\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k + L_i\hat{\mathbf{x}}_i, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi)\\ = \exp(i\theta_i)\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi),\end{aligned} \tag{5}$$

where $\mathbf{r}_k$ is the coordinate of the kth particle (other arguments such as spin are not shown here for simplicity of notation), N is the total particle number, and $\hat{\mathbf{x}}_i$ is the unit vector along the x_i direction. This condition is the same as the one adopted in Ref. [77]. Second,

$$\begin{aligned}\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k + L_3\hat{\mathbf{x}}_3, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi)\\ = \exp\left(-i\phi\frac{x_4}{L_4}\right)\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi).\end{aligned} \tag{6}$$

Since $x_4 \equiv x_4 + L_4$ on the torus, the flux ϕ has to be quantized as $n\phi_0$, where the unit flux $\phi_0 \equiv 2\pi$, and n is an integer. Lastly,

$$\begin{aligned}\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k + L_4\hat{\mathbf{x}}_4, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi)\\ = \Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi).\end{aligned} \tag{7}$$

Physically, these twisted boundary conditions tell us that there is a gauge potential $A_i = \theta_i/L_i$ along the $x_i (i = 1, 2)$ direction and a gauge potential $A_3 = -\phi \frac{x_4}{L_3 L_4}$ along the x_3 direction; in other words, there is a magnetic flux ϕ inside any 2D torus T_{34} whose coordinates are (X_1, X_2, x_3, x_4) with fixed (X_1, X_2).

Before proceeding to our central results, let us briefly outline the motivations of the boundary conditions given in Eqs. (5), (6), and (7). The first motivation is that the $(\theta_1, \theta_2, \theta_3, \theta_4)$ boundary condition [see Sec. VI] does not produce the 4D Hall conductance. The second motivation is the intuitive relation between the 4D Hall effect and the 2D Hall effect. In Eq. (1), if we take A_3, A_4 to be independent of x_0, x_1, x_2, and at the same time take A_0, A_1, A_2 to be independent of x_3, x_4, then there is a "dimensional reduction" [79] of the 4D Chern-Simons term to the 2D Chern-Simons term: $\sigma_{4D}\epsilon^{\mu\nu\rho\sigma\tau}A_\mu\partial_\nu A_\rho \partial_\sigma A_\tau \to \sigma_{4D} B_{34}\epsilon^{\mu\nu\rho}A_\mu\partial_\nu A_\rho$ (up to a numerical factor), where $B_{34} \equiv \partial_3 A_4 - \partial_4 A_3$, and the indices μ, ν, ρ in "$\epsilon^{\mu\nu\rho}$" take the values 0, 1, 2. According to this argument, in our boundary conditions given in Eqs. (5,6), and (7), we have taken $\partial_3 A_4 - \partial_4 A_3 = \phi/L_3 L_4$; thus, we have the dimensional reduction $\sigma_{4D}\epsilon^{\mu\nu\rho\sigma\tau}A_\mu\partial_\nu A_\rho\partial_\sigma A_\tau \to \sigma_{4D}\phi\epsilon^{\mu\nu\rho}A_\mu\partial_\nu A_\rho$. Intuitively, we have the evident identity

$$\frac{\partial}{\partial\phi}(\sigma_{4D}\phi\epsilon^{\mu\nu\rho}A_\mu\partial_\nu A_\rho) = \sigma_{4D}\epsilon^{\mu\nu\rho}A_\mu\partial_\nu A_\rho. \tag{8}$$

Since the right-hand side of this equation is a 2D Chern-Simons term, it seems that we can calculate σ_{4D} using well-known results of 2D quantum Hall effects. In practice, however, it is impossible to take the derivative with respect to ϕ because ϕ is quantized; i.e., ϕ takes only discrete values. To resolve this difficulty, we will take a difference instead of a derivative (see below).

Now our task is to formulate these intuitive arguments as a precise mathematical framework. We can define the Berry connection

$$a_i(\theta_1, \theta_2, \phi) = -i\langle\Psi(\theta_1, \theta_2, \phi)|\partial_{\theta_i}|\Psi(\theta_1, \theta_2, \phi)\rangle \tag{9}$$

and the Berry curvature

$$F_{ij}(\theta_1, \theta_2, \phi) = \frac{\partial a_j}{\partial\theta_i} - \frac{\partial a_i}{\partial\theta_j}, \tag{10}$$

from which we can define a first Chern number

$$C(\phi) = \frac{1}{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 F_{12}(\theta_1, \theta_2, \phi), \tag{11}$$

where we have chosen the notation "C" instead of "C_1" to distinguish C from the first Chern number appearing in the 2D quantum Hall effects [77].

With these preparations, the general formula for σ_{4D} appearing in Eq. (1) is proposed as

$$\sigma_{4D} = C(\phi_0) - C(0). \tag{12}$$

The first term is the Chern number with a unit flux $\phi_0 \equiv 2\pi$ in T_{34}, and the second term is the Chern number without this flux; in other words, Eq. (12) measures the jump of the first Chern number after inserting a flux ϕ_0 in T_{34}. The necessity of the second term $C(0)$ in Eq. (12) can be easily appreciated in a noninteracting model [see Eq. (19)], to be presented in Sec. III. It is also useful to note that $C(0)$ may be zero if the ground state has certain symmetries. For instance, if there is time-reversal symmetry, we have $C(0) = 0$ and $\sigma_{4D} = C(\phi_0)$.

Equation (12) is expressed in terms of the Berry phase of ground-state wave functions on a torus, which is well defined in the presence of an arbitrary interaction and disorder [80]. Equation (12) can also be written equivalently as

$$\sigma_{4D} = \frac{1}{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 [F_{12}(\theta_1, \theta_2, \phi_0) - F_{12}(\theta_1, \theta_2, 0)]. \tag{13}$$

Equations (12) and (13) are among the central equations of the present paper.

Several remarks about Eq. (12) are in order. The noninteracting topological invariant for the 2D quantum Hall effect, namely, the Thouless-Kohmoto-Nightingale-den Nijs (TKNN) invariant [81], is expressed as the first Chern number in the Brillouin zone. The Niu-Thouless-Wu formula [77], as a generalization of the TKNN invariant, is again a first Chern number. Given the second Chern number in Eq. (2) for the 4D noninteracting quantum Hall effect, we may try to express the 4D Hall coefficient σ_{4D} as a second Chern number on a certain parameter space, for an interacting system. However, this attempt turns out to be unfruitful. Instead, the topological invariant defined in Eq. (12), which gives σ_{4D}, is the difference between two first Chern numbers.

Let us conclude this section with a side remark that the Laughlin's gauge argument [82] can also be generalized to 4D QH. The boundary conditions in the x_3, x_4, direction are the same as given by Eqs. (6) and (7), but the system is open along the x_2 direction. When we do the adiabatic evolution $\theta_1 \to \theta_1 + 2\pi$, the charge transferred from the boundary $x_2 = 0$ to $x_2 = L_2$ is denoted as $\Delta Q(\phi)$. The Hall conductance is given as $\sigma_{4D} = \Delta Q(\phi_0) - \Delta Q(0)$.

III. THE NONINTERACTING LIMIT: TWO SIMPLE MODELS

In this section, we will check in two simple noninteracting models [Eqs. (14) and (19)] that Eq. (12) gives the same result as Eq. (2), as should be the case in the noninteracting limit. Incorporating well-known results of topological classification of noninteracting insulators, we will show that Eq. (12) reduces to Eq. (2) for all noninteracting 4D insulators.

First, let us consider a noninteracting Hamiltonian for 4D QH [11],

$$h(\mathbf{k}) = v\sum_{i=1}^{4} \sin k_i\Gamma^i + M(\mathbf{k})\Gamma^0, \tag{14}$$

where $M(\mathbf{k}) = m + 4 - \sum_{i=1}^{4} \cos k_i$, v and m are parameters of the Hamiltonian, and $k_i \in [0, 2\pi]$ is the ith momentum of the free Bloch state (the lattice constant has been taken as unity). Here, the Gamma matrices satisfy the identities $\{\Gamma^\mu, \Gamma^\nu\} = 2\delta^{\mu\nu}$. For our convenience, we choose the representation $\Gamma^1 = \tau^1$, $\Gamma^2 = \tau^2$, $\Gamma^3 = \tau^3\sigma^1$, $\Gamma^4 = \tau^3\sigma^2$, $\Gamma^0 = \tau^3\sigma^3$.

Instead of solving the model numerically in real space, which is less illuminating for our purpose, let us perform the calculation in the limit where $|m|$ is significantly smaller than unity. In this limit, we can keep only the $\mathbf{k}$-linear terms near $\mathbf{k} = 0$, and the Dirac Hamiltonian reads

$$h(\mathbf{k}) \approx v(k_1\tau^1 + k_2\tau^2) + \tau^3(vk_3\sigma^1 + vk_4\sigma^2 + m\sigma^3). \tag{15}$$

In the presence of twisted boundary conditions, the momenta should be replaced by $k_i \to -iD_i = -i(\partial_i - A_i)$. Let us calculate the first term $C(\phi_0)$ of Eq. (12) for the Dirac Hamiltonian in Eq. (15). In this linear-$\mathbf{k}$ limit, we can first solve the Hamiltonian $h'(k_3, k_4) = vk_3\sigma^1 + vk_4\sigma^2 + m\sigma^3$, whose eigenvalues read [83]

$$E_0 = m, \quad E_{n\pm} = \pm\sqrt{m^2 + 2nBv^2}(n = 1, 2, \cdots), \tag{16}$$

where $B = \phi_0/L_3L_4$. The corresponding eigenwavefunctions are $(\psi_0, 0)^T$ and $(\psi_n, \pm\psi_{n-1})^T$, where ψ_n is the wave function of the nth Landau level of Schrodinger particles [83], whose precise forms do not concern us here. It is useful to note that when $m = 0$, the existence of the zero mode E_0 is guaranteed by the Atiyah-Singer index theorem. Inputting the eigenvalues given in Eq. (16) into the second set of parentheses in Eq. (15), we have the 2D Hamiltonians

$$h_0 = v(k_1\tau^1 + k_2\tau^2) + m\tau^3;$$
$$h_{n\pm} = v(k_1\tau^1 + k_2\tau^2) + E_{n\pm}\tau^3(n = 1, 2, \cdots). \tag{17}$$

The value of $C(\phi_0)$ can be obtained as the summation of the first Chern number of h_0 and $h_{n\pm}$, namely, $\frac{1}{2}[\mathrm{sgn}(E_0) + \sum_n\sum_{\alpha=\pm}\mathrm{sgn}(E_{n\alpha})] = \frac{1}{2}\mathrm{sgn}(m)$, thanks to the fact that the ground-state wave functions are a Slate determinant of Bloch states in the noninteracting cases. In this calculation, we have not been careful about the high-energy regularization; thus, we can only assert that $C(\phi_0) = \frac{1}{2}\mathrm{sgn}(m) + \text{constant}$. Since we require $C(\phi_0) = 0$ as $m \to +\infty$, we have $C(\phi_0) = \frac{1}{2}[\mathrm{sgn}(m) - 1]$. Similarly, we can obtain $C(0) = 0$; therefore, we have

$$\sigma_{4D} = C(\phi_0) - C(0) = \frac{1}{2}[\mathrm{sgn}(m) - 1], \tag{18}$$

which is the same as c_2 obtained [11] from Eq. (2) (see also Ref. [84] for calculations for a different model using charge pumping).

Let us move to the second noninteracting model, which will explain the reason why we must include the second term $C(0)$ in Eq. (12). The simple model has the free Hamiltonian

$$h(\mathbf{k}) = v(\sin k_1\tau^1 + \sin k_2\tau^2) + (m + 2 - \cos k_1 - \cos k_2)\tau^3, \tag{19}$$

which is independent of k_3 and k_4. If we take $m = -0.1$, then it is obvious that both $C(\phi_0)$ and $C(0)$ are nonzero; however, they are equal, and therefore $\sigma_{4D} = C(\phi_0) - C(0) = 0$. From Eq. (2), it is obvious that we have $\sigma_{4D} = c_2 = 0$; therefore, Eqs. (12) and (2) produce the same result in this example.

Although we have only explicitly checked that Eq. (12) reduces to Eq. (2) in Dirac models, it is possible to make a more general statement that Eq. (12) is always equivalent to Eq. (2) in the noninteracting limit. In fact, as has been shown in Refs. [15,85], there is a Dirac-Hamiltonian representative in each class of the 4D QH insulators, which means that any noninteracting Hamiltonian for the 4D insulator can always be smoothly connected to a Dirac Hamiltonian. Therefore, equivalence between Eqs. (12) and (2) in the Dirac model implies their equivalence for all noninteracting Hamiltonians. In the presence of interactions, however, Eq. (2) loses definition, while Eq. (12) remains useful.

IV. QUANTUM HALL EFFECT IN $d = 2l + 2$ SPATIAL DIMENSIONS

Equation (12) can be generalized to $d = 2l + 2$ spatial dimensions. The boundary conditions for the (x_1, x_2) direction given in Eq. (5) are unchanged, while the boundary conditions for other directions are defined as

$$\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k + L_{2j+1}\hat{\mathbf{x}}_{2j+1}, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi_1, \cdots, \phi_l) = \exp\left(-i\phi_j\frac{x_{2j+2}}{L_{2j+2}}\right)\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi_1, \cdots, \phi_l) \tag{20}$$

and

$$\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k + L_{2j+2}\hat{\mathbf{x}}_{2j+2}, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi_1, \cdots, \phi_l) = \Psi(\mathbf{r}_1, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N; \theta_1, \theta_2, \phi_1, \cdots, \phi_l) \tag{21}$$

for $j = 1, 2, \cdots l$. Physically, these conditions means that there is a flux ϕ_j in the 2D torus $T_{2j+1,2j+2}$. We can define the Berry connection

$$a_i(\theta_1,\theta_2,\phi_1,\cdots,\phi_l) = -i\langle\Psi(\theta_1,\theta_2,\phi_1,\cdots,\phi_l)|\partial_{\theta_i}|\Psi(\theta_1,\theta_2,\phi_1,\cdots,\phi_l)\rangle \tag{22}$$

for $i = 1$, 2, and a first Chern number

$$C(\phi_1,\cdots,\phi_l) = \frac{1}{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 F_{12}(\theta_1,\theta_2,\phi_1,\cdots,\phi_l). \tag{23}$$

Now, the d-dimensional Hall conductance is given by

$$\sigma_d = \sum_{\phi_1,\cdots,\phi_l=\phi_0,0} (-1)^{\sum_i \delta(\phi_i,0)} C(\phi_1,\cdots,\phi_l) = C(\phi_0,\cdots,\phi_0,\phi_0) - C(\phi_0,\cdots,\phi_0,0) + \cdots - C(0,\cdots,0,0), \tag{24}$$

where the delta function satisfies $\delta(\phi_i, 0) = 1$ when $\phi_i = 0$, and $\delta(\phi_i, 0) = 0$ when $\phi_i = \phi_0 \equiv 2\pi$. When $d = 4$ (i.e., $l = 1$), Eq. (24) reduces to Eq. (12). The original Niu-Thouless-Wu formula is also a special case of Eq. (24) with $d = 2$ (i.e., $l = 0$).

V. FRACTIONAL QUANTUM HALL EFFECTS

One of the main motivations for introducing the topological invariant in Eq. (12) is its potential applications in fractional quantum Hall states. Before moving to higher dimensions, let us first present a review of the Niu-Thouless-Wu formula of 2D fractional QH. As has been known in Ref. [77], fractional quantization of 2D Hall conductance is possible if the ground states are degenerate on a 2D torus.

In 2D, the standard boundary condition is given [77] by Eq. (5) except that the argument ϕ is absent. Suppose that a 2D fractional quantum Hall system has p-fold degenerate ground states $|\Psi_1(\theta_1,\theta_2)\rangle, \cdots, |\Psi_p(\theta_1,\theta_2)\rangle$ [86]. The Hall conductance is given by an average over these degenerate ground states as [77] (recall that we have taken the units $e = h = c = 1$)

$$\begin{aligned}\sigma_{2D} &= \frac{1}{p}\frac{1}{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 \sum_{\alpha=1}^{p} [\langle\partial_{\theta_1}\Psi_\alpha|\partial_{\theta_2}\Psi_\alpha\rangle - \langle\partial_{\theta_2}\Psi_\alpha|\partial_{\theta_1}\Psi_\alpha\rangle] \\ &= \frac{1}{p}\frac{1}{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 \mathrm{Tr}F_{12}(\theta_1,\theta_2) \\ &= \bar{C}_1,\end{aligned} \tag{25}$$

where the matrix elements of the non-Abelian Berry curvature F_{ij} read $F_{ij}^{\alpha\beta} = \partial_i a_j^{\alpha\beta} - \partial_j a_i^{\alpha\beta} + i[a_i, a_j]^{\alpha\beta}$, in which $a_i^{\alpha\beta} = -i\langle\Psi_\alpha(\theta_1,\theta_2)|\partial_{\theta_i}|\Psi_\beta(\theta_1,\theta_2)\rangle$ is the non-Abelian Berry connection. The average Chern number $\bar{C}_1 \equiv \frac{1}{p}C_1 \equiv \frac{1}{p}\frac{1}{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 \mathrm{Tr}F_{12}(\theta_1,\theta_2)$, where C_1 is the standard definition of the first Chern number [87] of the $U(p)$ fiber bundle. Note that the $i[a_i, a_j]$ term in F_{ij} vanishes after the tracing. It is a mathematical fact that the first Chern number C_1 is quantized as an integer; therefore, the Hall conductance is quantized as a rational number with denominator p.

Equation (25) can be rewritten as [77]

$$\sigma_{2D} = \frac{1}{p}\frac{1}{2\pi i}\int_0^{2\pi p} d\theta_1 \int_0^{2\pi} d\theta_2 [\langle\partial_{\theta_1}\Psi_1|\partial_{\theta_2}\Psi_1\rangle - \langle\partial_{\theta_2}\Psi_1|\partial_{\theta_1}\Psi_1\rangle], \tag{26}$$

where we have picked up a ground state Ψ_1 from the degenerate ground state $\Psi_1, \cdots, \Psi_p$. The parameter space has been enlarged to $(0 < \theta_1 < 2\pi p, 0 < \theta_2 < 2\pi)$.

Now, let us move to higher dimensions. For a 4D fractional QH system, suppose that the ground states are p-fold degenerate on the 4D torus T^4 with boundary conditions described in Sec. II; in other words, the ground states form a $U(p)$ bundle over the 2D torus with coordinates (θ_1, θ_2) (note that ϕ is fixed) [88]. We can define the Berry connection $a_i^{\alpha\beta}(\theta_1,\theta_2,\phi) = -i\langle\Psi_\alpha(\theta_1,\theta_2,\phi)|\partial_{\theta_i}|\Psi_\beta(\theta_1,\theta_2,\phi)\rangle$ and the Berry curvature $F_{ij}^{\alpha\beta} = \partial_i a_j^{\alpha\beta} - \partial_j a_i^{\alpha\beta} + i[a_i, a_j]^{\alpha\beta}$. Equation (11) can be straightforwardly generalized as

$$C(\phi) = \frac{1}{2\pi}\int_0^{2\pi} d\theta_1 d\theta_2 \mathrm{Tr}F_{12}(\theta_1,\theta_2,\phi). \tag{27}$$

Note that in Sec. II, we considered nondegenerate ground states; therefore, the symbol "Tr" in Eq. (27) is absent in Eq. (11). We can also define the average (first) Chern number for 4D QH as

$$\bar{C}(\phi) = C(\phi)/p. \tag{28}$$

By analogy with Eq. (25), the 4D Hall conductance σ_{4D} for fractional quantum Hall effects is obtained as

$$\sigma_{4D} = \bar{C}(\phi_0) - \bar{C}(0). \tag{29}$$

Equation (29) is among the central results of this paper. In the presence of time-reversal symmetry, the second term vanishes. Equation (29) reduces to Eq. (12) when $p = 1$, namely, the case without ground-state degeneracy.

To conclude this section, we mention that the generalization of Eq. (24) for $d = 2l + 2$-dimensional fractional states reads $\sigma_d = \sum_{\phi_1,\cdots,\phi_l=\phi_0,0} (-1)^{\sum_i \delta(\phi_i,0)} \bar{C}(\phi_1,\cdots,\phi_l)$.

VI. MORE TOPOLOGICAL INVARIANTS FOR 4D FRACTIONAL QH

Having studied the 4D fractional Hall conductance using the $(\theta_1, \theta_2, \phi)$ boundary conditions that we have chosen, let us investigate other choices of boundary conditions. The simplest choice is

$$\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k+L_i\hat{\mathbf{x}}_i,\cdots,\mathbf{r}_N;\theta_1,\theta_2,\theta_3,\theta_4) = \exp(i\theta_i)\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k,\cdots,\mathbf{r}_N;\theta_1,\theta_2,\theta_3,\theta_4) \quad (30)$$

for $i = 1$, 2 3, 4. Suppose that the ground states are p-fold degenerate; then, these ground states form a $U(p)$ fiber bundle on the 4D torus parametrized by $(\theta_1,\theta_2,\theta_3,\theta_4)$, with $0\le\theta_i<2\pi$. We can define a natural topological invariant

$$C_2 = \frac{1}{32\pi^2}\int d^4\theta\epsilon^{ijkl}\mathrm{Tr}F_{ij}F_{kl}, \quad (31)$$

where the matrix elements of non-Abelian Berry curvature F_{ij} are defined as $F_{ij}^{\alpha\beta}(\theta_1,\theta_2,\theta_3,\theta_4) = \partial_i a_j^{\alpha\beta} - \partial_j a_i^{\alpha\beta} + i[a_i,a_j]^{\alpha\beta}$, where $i, j = 1, 2, 3, 4$. Equation (31) is a second Chern number defined for fractional QH states in 4D. It should not be confused with the (lowercase) c_2 in Eq. (2), which is defined in terms of the free Bloch states of noninteracting systems.

For $2n$-dimensional quantum Hall effects, we can straightforwardly generalize C_2 to C_n as

$$C_n = \frac{1}{n!}\int \mathrm{Tr}\left(\frac{F}{2\pi}\right)^n = \frac{1}{2^n n!(2\pi)^n}\int d^{2n}\theta\epsilon^{\alpha_1\cdots\alpha_{2n}}\mathrm{Tr}F_{\alpha_1\alpha_2}\cdots F_{\alpha_{2n-1}\alpha_{2n}}, \quad (32)$$

which are topological invariants for higher-dimensional fractional QH states.

In 2D, the first Chern number C_1 of the $U(p)$ bundle is proportional to the Hall conductance σ_{2D}. In fact, Eq. (25) tells us that $C_1 = p\sigma_{2D}$; thus, C_1 does not give us new topological invariants other than σ_{2D} and p. However, the 4D case is quite different. The key difference between 2D and 4D is as follows. For the 2D QH, both σ_{2D} and C_1 are defined under the same boundary condition parametrized by (θ_1,θ_2). For 4D quantum Hall insulators, the topological invariants C_2 and σ_{4D} are defined using different boundary conditions [Eqs. (5,6), and (7) for σ_{4D}, but Eq. (30) for C_2]; therefore, there is no direct relation between C_2 and σ_{4D}. In principle, C_2 can take different values, given the same value of ground-state degeneracy p and Hall coefficient σ_{4D}. The topological invariant C_2 suggests that there are rich structures in 4D quantum Hall effects. Higher-dimensional QHs are similar: Higher Chern numbers $C_n(n=2,3,\cdots)$ are not directly related to the Hall coefficient σ_d because they are defined under different boundary conditions.

VII. TOPOLOGICAL INSULATORS IN ONE DIMENSION

In this section, we will briefly discuss 1D topological insulators to prepare for the investigation of 3D topological insulators in Sec. VIII. One-dimensional topological insulators can be characterized by a θ term [11]

$$S_{\mathrm{eff}} = \frac{1}{2\pi}\int dtdx\epsilon^{\mu\nu}\theta\partial_\mu A_\nu. \quad (33)$$

Let us study the 1D insulator on a torus T^1, which is just a circle. We take the boundary condition as

$$\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k+L_1\hat{\mathbf{x}}_1,\cdots,\mathbf{r}_N;\theta_1) = \exp(i\theta_1)\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k,\cdots,\mathbf{r}_N;\theta_1); \quad (34)$$

namely, there is a gauge potential $A_1 = \theta_1/L_1$.

Now, there exists a simple topological invariant [89,29]

$$\Gamma = \int_0^{2\pi} d\theta_1 a_1(\theta_1), \quad (35)$$

where the Berry connection is defined as $a_1(\theta_1) = -i\langle\Psi(\theta_1)|\partial_{\theta_1}|\Psi(\theta_1)\rangle$. Equation (35) is an interacting generalization of the Zak phase [90]. It has been applied to 1D models [29,30], though its relation to the θ term was not discussed. Equation (35) is defined modulo 2π because a local gauge transformation of the wave function can change it by 2π.

When the ground state $|\Psi(\theta_1)\rangle$ is not degenerate, the θ value is given by $\theta=\Gamma$. Since we are mainly concerned with higher-dimensional topological insulators, we will not study applications of this 1D formula in detail. It is useful to mention that the quantity $\partial\theta/\partial\lambda$, where λ is a tuning parameter of the many-body Hamiltonian, is usually more useful than θ itself because $\partial\theta/\partial\lambda$ does not have any ambiguity under local gauge transformation of wave functions [89].

When the ground states are p-fold degenerate, the natural generalization of Eq. (35) is

$$\Gamma = \int d\theta_1 \mathrm{Tr}a_1(\theta_1), \quad (36)$$

where the non-Abelian gauge potential is defined as $a_1^{\alpha\beta} = -i\langle\Psi_\alpha(\theta_1)|\partial_{\theta_1}|\Psi_\beta(\theta_1)\rangle$. The θ angle in Eq. (33) is given by

$$\theta = \bar{\Gamma}, \quad (37)$$

where the average $\bar{\Gamma}$ is defined as $\bar{\Gamma} = \frac{1}{p}\Gamma$.

VIII. TOPOLOGICAL INSULATORS IN THREE DIMENSIONS: INTEGER AND FRACTIONAL

The approach we applied to 4D QH states can be naturally generalized to 3D. The 3D boundary conditions are chosen as follows. First,

$$\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k+L_1\hat{\mathbf{x}}_1,\cdots,\mathbf{r}_N;\theta_1,\phi) = \exp(i\theta_1)\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k,\cdots,\mathbf{r}_N;\theta_1,\phi), \quad (38)$$

where $\mathbf{r}_k$ is the coordinate of the kth particle (other variables such as spin are not shown for simplicity of notation), and $\hat{\mathbf{x}}_1$ is the unit vector along the x_1 direction. Second,

$$\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k+L_2\hat{\mathbf{x}}_2,\cdots,\mathbf{r}_N;\theta_1,\phi) = \exp\left(-i\phi\frac{x_3}{L_3}\right)\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k,\cdots,\mathbf{r}_N;\theta_1,\phi) \tag{39}$$

and

$$\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k+L_3\hat{\mathbf{x}}_3,\cdots,\mathbf{r}_N;\theta_1,\phi) = \Psi(\mathbf{r}_1,\cdots,\mathbf{r}_k,\cdots,\mathbf{r}_N;\theta_1,\phi), \tag{40}$$

where ϕ satisfies the same quantization condition as discussed in Sec. II. Now, the θ angle in Eq. (3) is proposed (for the cases without ground-state degeneracy) as

$$\theta=\Gamma(\phi_0)-\Gamma(0), \tag{41}$$

where $\phi_0\equiv 2\pi$, and

$$\Gamma(\phi)=\int_0^{2\pi} d\theta_1 a_1(\theta_1,\phi), \tag{42}$$

with $a_1(\theta_1,\phi)=-i\langle\Psi(\theta_1,\phi)|\partial_{\theta_1}|\Psi(\theta_1,\phi)\rangle$ being the Berry connection defined in terms of the ground-state wave function. One can derive Eq. (41) by calculating the Berry phase gained by the adiabatic evolution $A_1\to A_1+2\pi/L_1$. Because of the topological terms $\frac{\theta}{4\pi^2}\partial_0 A_1(\partial_2 A_3-\partial_3 A_2)$ contained in the θ term, when a flux ϕ exists in T_{23}, as Eqs. (39) and (40) indicate, the adiabatic evolution of $A_1\to A_1+2\pi/L_1$ generates a topological phase $\theta\phi/2\pi$, which should be identified as the Berry phase accumulated by the adiabatic evolution of ground-state wave functions, namely, $\int d\theta_1 a_1(\theta_1,\phi)$. It follows that Eq. (41) is the formula for θ. Note that, potentially, there is another term $\theta'\partial_0 A_1$ that can contribute to the Berry phase in the evolution $A_1\to A_1+2\pi/L_1$, which is the reason why the second term in Eq. (41) appears.

If the Hamiltonian and the ground state depend on a tuning parameter, which we denote as θ_2, then θ is a function of θ_2. The derivative of θ with respect to θ_2 is given by the gauge-invariant formula

$$\frac{\partial\theta}{\partial\theta_2}=\int_0^{2\pi} d\theta_1[F_{21}(\theta_1,\theta_2,\phi_0)-F_{21}(\theta_1,\theta_2,0)], \tag{43}$$

where $F_{21}(\theta_1,\theta_2,\phi)=\partial_{\theta_2}a_1-\partial_{\theta_1}a_2$ and $a_i(\theta_1,\theta_2,\phi)=-i\langle\Psi(\theta_1,\theta_2,\phi)|\frac{\partial}{\partial\theta_i}|\Psi(\theta_1,\theta_2,\phi)\rangle$. Similar to the 1D case discussed in Sec. VII, the quantity $\partial\theta/\partial\theta_2$ is usually more useful than θ itself because $\partial\theta/\partial\theta_2$ is invariant under any local gauge transformation of the wave function.

We will apply Eq. (41) to a noninteracting Dirac model in the Appendix, which gives the same result as obtained [11] from Eq. (4).

In the above calculations, we have assumed that the θ term is isotropic, which is always satisfied if there is time-reversal symmetry (though the Maxwell terms are generally still anisotropic). If the θ term is anisotropic [91,92], namely, if we have $\chi_{ij}E_iB_j=\chi_{ij}E_i\epsilon_{jkl}(\partial_k A_l-\partial_l A_k)$, we should calculate each coefficient χ_{ij} separately, which is also given by Eq. (41) except that the twisted phase θ_1 in Eq. (38) is added in the x_i direction instead of the x_1 direction, and the flux ϕ [see Eqs. (39) and (40)] is added in the (x_k,x_l) plane.

For 3D fractional states with p-fold ground-state degeneracy, we can generalize Eq. (41) as

$$\theta=\bar{\Gamma}(\phi_0)-\bar{\Gamma}(0), \tag{44}$$

where $\bar{\Gamma}(\phi)\equiv\frac{1}{p}\int_0^{2\pi} d\theta_1 \mathrm{Tr} a_1(\theta_1,\phi)$. The logic is similar to Sec. V. An important feature is notable here. We have the transformation rule $a_1\to Ua_1U^\dagger+iU\partial U^\dagger$ under a local gauge transformation of the basis of ground-state wave functions, where $U=U(\theta_1,\phi)$ is a $p\times p$ unitary matrix. This may change $\Gamma(\phi)$ by multiples of $2\pi/p$; therefore, the θ angle of fractional topological insulators is determined modulo $2\pi/p$.

As a digression, let us briefly mention the generalization for a $d=2l+1$-(spatial)-dimensional (isotropic) θ term if the system does not have ground-state degeneracy on a d-dimensional torus. The formula reads

$$\begin{aligned}\theta_d=&\sum_{\phi_1,\cdots,\phi_l=\phi_0,0}(-1)^{\sum_i\delta(\phi_i,0)}\Gamma(\phi_1,\cdots,\phi_l)\\ &=\Gamma(\phi_0,\cdots,\phi_0,\phi_0)-\Gamma(\phi_0,\cdots,\phi_0,0)+\cdots\\ &-\Gamma(0,\cdots,0,0),\end{aligned} \tag{45}$$

which is analogous to Eq. (24). The meanings of the arguments $\phi_1,\cdots,\phi_l$ are similar to that of Eq. (24), and we shall not repeat them here. If the state is fractional, we have $\theta_d=\sum_{\phi_1,\cdots,\phi_l=\phi_0,0}(-1)^{\sum_i\delta(\phi_i,0)}\bar{\Gamma}(\phi_1,\cdots,\phi_l)$, where $\bar{\Gamma}(\phi_1,\cdots,\phi_l)\equiv\Gamma(\phi_1,\cdots,\phi_l)/p$, the integer p being the ground-state degeneracy.

IX. CONCLUSIONS

In this paper, we have defined precise topological invariants in terms of the ground-state wave functions on a torus. This approach provides a conceptual framework in which many topological invariants and topological-field-theoretical coefficients, such as σ_{4D} (in 4D) and θ (in 3D), acquire precise definitions even in the presence of an arbitrary interaction and disorder.

Numerically, we do not expect that the wave function (on a torus) approach followed in the present paper will be as efficient as the topological Hamiltonian approach [68,67] mentioned in Sec. I. However, the present approach has a wider range of validity because it is applicable in the presence of an arbitrary interaction and disorder; therefore, the present approach is highly desirable for certain purposes, especially when both the interaction and disorder are present, or when the interaction is so strong that exotic fractional states are generated. It is also useful to note that the topological invariants in the present paper can also be applied to bosonic topological insulators, for which other topological invariants are hard to define.

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APPENDIX: APPLICATION IN A THREE-DIMENSIONAL NONINTERACTING MODEL

In the noninteracting limit, Eq. (41) should give the same θ as the noninteracting formula [11]. In this Appendix, we will check this result in a simple noninteracting model. This Appendix follows similar calculations as Sec. III.

Let us study a simple 3D noninteracting Dirac model given as

$$h(\mathbf{k}) = v \sin k_1 \tau^1 + [v \sin k_2 \sigma^1 + v \sin k_3 \sigma^2 + M(\mathbf{k})\sigma^3]\tau^3, \tag{A1}$$

where $M(\mathbf{k}) = m + 3 - \sum_{i=1}^{3} \cos k_i$. In the limit that $|m| \ll 1$, the low-energy physics is dominated by the $k \approx 0$ region, and we can linearly expand $h(\mathbf{k})$ as

$$h(\mathbf{k}) \approx vk_1\tau^1 + (vk_2\sigma^1 + vk_3\sigma^2 + m\sigma^3)\tau^3. \tag{A2}$$

The boundary conditions are given in Eqs. (38,39), and (40), which means that there is a flux ϕ inside the 2D torus T_{23}. First, let us take $\phi = \phi_0 \equiv 2\pi$. By a calculation similar to Sec. III, we can first solve $h'(k_2, k_3) = vk_2\sigma^1 + vk_3\sigma^2 + m\sigma^3$ after replacing $k_i \to -i(\partial_i - A_i)$, whose eigenvalues read

$$E_0 = m; \quad E_{n\pm} = \pm\sqrt{m^2 + 2nBv^2}(n = 1, 2, \cdots), \tag{A3}$$

and the corresponding wave functions are $(\psi_0, 0)^T$ and $(\psi_n, \pm\psi_{n-1})^T$. Now, we put these eigenvalues back into the set of parentheses of Eq. (A2); then, we have the 1D Hamiltonians

$$\begin{aligned} h_0 &= vk_1\tau^1 + m\tau^3; \\ h_{n\pm} &= vk_1\tau^1 + E_{n\pm}\tau^3(n = 1, 2, \cdots). \end{aligned} \tag{A4}$$

Now, the $\Gamma(\phi_0)$ in Eq. (41) can be found as $\frac{\pi}{2}[\mathrm{sgn}(E_0) + \sum_n \sum_{\alpha=\pm} \mathrm{sgn}(E_{n\alpha})] = \frac{\pi}{2}\mathrm{sgn}(m)$, which is similar to Sec. III. Again, because of the high-energy regularization, we can only assert that $\Gamma(\phi_0) = \frac{\pi}{2}\mathrm{sgn}(m) + \text{constant}$. Consideration similar to in Sec. III leads to $\Gamma(\phi_0) = \frac{\pi}{2}(\mathrm{sgn}(m) - 1)$. Similarly, we have $\Gamma(0) = 0$; therefore, from Eq. (41) it follows that

$$\theta = \Gamma(\phi_0) - \Gamma(0) = \frac{\pi}{2}(\mathrm{sgn}(m) - 1), \tag{A5}$$

which means that $\theta = -\pi$ when $m < 0$. This is consistent with the result obtained from the noninteracting Chern-Simons term [11].

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[79] This is analogous to the Kaluza-Klein compactification.

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