Many-Body Topological Invariants for Fermionic Symmetry-Protected Topological Phases

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Many-body topological invariants for fermionic symmetry-protected topological phases

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We define and compute many-body topological invariants of interacting fermionic symmetry-protected topological (SPT) phases, protected by an orientation-reversing symmetry, such as time-reversal or reflection symmetry. The topological invariants are given by partition functions obtained by path-integral on unoriented spacetime which, as we show, can be computed for a given ground state wave function by considering a non-local operation, "partial" reflection or transpose. As an application of our scheme, we study the $\mathbb{Z}_8$ and $\mathbb{Z}_{16}$ classification of topological superconductors in one and three dimensions.

The Thouless-Kohmoto-Nightingale-den Nijs (TKNN) formula [1, 2] is the prototype for topological characterization of phases of matter. It relates the quantized Hall conductance to the (first) Chern number defined for Bloch wave functions. At the level of many-body physics, the quantized Hall conductance can also be formulated in terms of ground state wave functions in the presence of twisted boundary conditions ("the many-body Chern number") [3]. In contrast to local order parameters, the TKNN integer distinguishes different quantum phases of matter by focusing on their global topological properties.

More recently, the discovery of topological insulators and superconductors [4, 5] has led to a new research frontier, generally referred to as symmetry protected topological (SPT) phases. These phases are adiabatically connected to topologically trivial states, i.e., atomic insulators which can be represented as simple product states without any entanglement. Nevertheless, they are topologically distinct once a symmetry condition, e.g., time-reversal symmetry, is imposed. A complete classification of the noninteracting fermionic SPT phases protected by non-spatial discrete symmetries [6–8], as well as crystalline SPT phases protected by spatial symmetries [9–12], were achieved.

However, it was later discovered that the non-interacting topological classification is not the full story, and can be dramatically altered once interaction effects are taken into account [13]. Since then, there have been several works which discuss the breakdown of the non-interacting classification in the presence of interactions [14–25].

There are various topological invariants for non-interacting fermionic SPT phases using single-particle states (e.g., Bloch wave functions). For example, the $\mathbb{Z}_2$-valued topological invariants have been introduced for topological insulators both in two and three spatial dimensions [26–29]. For topological superconductors protected by time-reversal symmetry, the integer-valued topological invariants ("the winding number") have been introduced [6]. However, the discovered breakdown of non-interacting classification clearly indicates that the situation at the interacting level is more intricate, and a general framework to distinguish interacting fermionic SPT phases is lacking. This should be contrasted from the quantized Hall conductance, which can be formulated within many-body physics without referring to single-particle wave functions (as it is ultimately related to the response function).

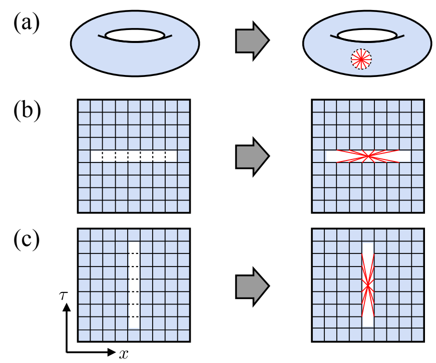

FIG. 1. (a) Introducing a cross-cap in the spacetime. (b) partial reflection, and (c) partial time inversion. First and second columns show the original connectivity after cutting and the twisted bonding after gluing, respectively.

In this letter, we introduce *many-body* topological invariants for topological superconductors protected by an orientation-reversing symmetry, such as time-reversal or reflection symmetry. Our topological invariants do not rely on single-particle descriptions, and have the same status as the many-body Chern number [3].

The basic strategy behind our construction of many-body topological invariants can be best illustrated by drawing an analogy with the many-body Chern-number. The many-body Chern number is formulated as a response of the many-body ground state wave functions to the twisted boundary conditions by $U(1)$ phase. Here, the $U(1)$ phase is associated with the symmetry of the system (i.e., the particle number conservation). Similarly, for phases of matter with more generic symmetry, one can consider twisting the boundary condition *using the symmetry of the system*. For SPT phases protected by orientation reversing symmetry, the symmetry-twisted boundary conditions naturally give rise to unoriented spacetime manifolds [24, 30–34]. From the topological quantum field theory description of topological superconductors [30, 34], one expects that the complex phase of the partition function, when the system is put on an appropriate unoriented manifold, is quantized and serves as a topological invariant [35]. In the following, we design many-body topological invariants, such that they return the quantized phase of the partition function.

One-dimensional topological superconductors in symmetry classes D+R$_-$ and BDI.– We explain our scheme by using the seminal example of 1D topological superconductors discussed by Fidkowski and Kitaev [13] to show the breakdown of non-interacting classification (with a slight variation in terms of symmetry requirements):

$$\hat{H} = -\sum_x \left[t f^\dagger_{x+1} f_x - \Delta f^\dagger_{x+1} f^\dagger_x + \text{H.c.} \right] - \mu \sum_x f^\dagger_x f_x, \tag{1}$$

which describes a superconducting state of spinless fermions. For simplicity, we take Δ as a real parameter and set $\Delta = t$. The SPT phase in this model, realized when $|\mu|/t < 2$, is protected either by time-reversal $\mathcal{T} f_x \mathcal{T}^{-1} = f_x$, $\mathcal{T} i \mathcal{T}^{-1} = -i$, or reflection $\mathcal{R} f_x \mathcal{R}^{-1} = i f_{-x}$. The former case belongs to symmetry class BDI (characterized by time-reversal symmetry where $\mathcal{T}^2 = 1$), while the latter case is referred to as symmetry class "D+R$_-$" (class D with reflection symmetry $\mathcal{R}$ satisfying $\mathcal{R}^2 = (-1)^F$ where F is the fermion number).

In the presence of either one of these symmetries, at the level of non-interacting fermions, one can introduce the integral topological index $\nu \in \mathbb{Z}$ [10–12]. However, the integral classification of the noninteracting fermions collapses into the $\mathbb{Z}_8$ classification in the presence of interactions [13, 36]. Namely, a stack of eight Majorana chains can be adiabatically turned into the trivial phase when symmetry preserving interactions are included.

Spacetime path-integral.– As advocated, we now put the system on an unoriented spacetime and measure the system's response. We first present our many-body invariant using the spacetime path-integral and subsequently present the corresponding formula in the operator formalism, which only involves the many-body ground states.

We start from the ordinary Euclidean path integral representation of the partition function

$$Z = \text{Tr}(e^{-\beta \hat{H}}) = \int \mathcal{D}[\xi]\mathcal{D}[\bar{\xi}]\ e^{-S[\bar{\xi},\xi]}, \tag{2}$$

where $S[\bar{\xi},\xi] = \int_0^\beta d\tau\, [\bar{\xi}\partial_\tau \xi + H(\bar{\xi},\xi)]$, τ is the continuous imaginary time variable, and the Grassmann variables $\xi(\tau,x)$ and $\bar{\xi}(\tau,x)$ are defined at time τ and real-space position x and obey the anti-periodic temporal boundary condition $\xi(\tau+\beta) = -\xi(\tau)$, $\bar{\xi}(\tau+\beta) = -\bar{\xi}(\tau)$. The path integral is defined for the spacetime manifold, which is a torus T^2.

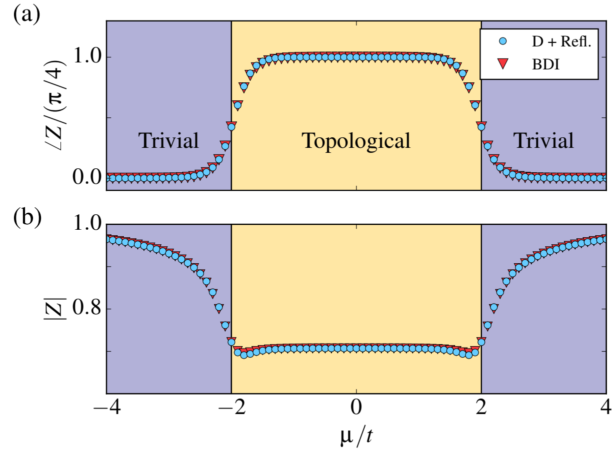

FIG. 2. Phase and amplitude of the partition function in the presence of spatial (Fig. 1(b)) and temporal (Fig. 1(c)) cross-caps (Details in Appendix B [35]. In short, we write the partition function in terms of a Pfaffian and extract the SPT phase by evaluating the ratio of the two Paffafians in the presence and absence of a cross-cap.) Here, we set $\beta = 10$, $N_t = 200$ and $N = 40$. We put $N_{t,\text{part}} = 100$ and $N_{\text{part}} = 20$ for time inversion (BDI) and spatial reflection (D+Refl.), respectively.

In order to create an unoriented spacetime manifold, we "modify" the boundary condition of the path integral, which effectively realizes the real projective plane $\mathbb{R}P^2$. The construction of the real projective plane depends crucially on the type of orientation reversing symmetry (reflection or time-reversal). First, for symmetry class D+R_-, we modify the temporal boundary condition at $\tau = \beta \equiv 0$ as

$$\begin{aligned} \xi(\beta+\epsilon,x) &= -\xi(0,x) \to -i\xi(0,-x), \\ \bar{\xi}(\beta+\epsilon,x) &= -\bar{\xi}(0,x) \to i\bar{\xi}(0,-x), \end{aligned} \tag{3}$$

over the interval $|x| < N_{\text{part}}/2$ where the reflection is done with respect to a vertical line crossing the central bond of the segment (Fig. 1(b)). Here, ϵ is the discretization step along the time axis, $\epsilon = \beta/N_t$. What this procedure does is to first introduce a cut (circle) in the spacetime path-integral and then identify opposite points on the circle by reflection symmetry (Fig. 1(a)). In short, this "cut and glue" process creates a cross-cap in the spacetime manifold, which is now topologically equivalent to $\mathbb{R}P^2$.

As for symmetry class BDI, we begin by noting that in the path-integral formalism, the time-reversal symmetry which is an antiunitary transformation in the operator formalism, should be implemented as an invariance under a change of path-integral variables. For our model, time-reversal transformation is equivalent to the change of Grassmann fields as in $\xi(\tau,x) \to i\bar{\xi}(\beta-\tau,x)$, $\bar{\xi}(\tau,x) \to i\xi(\beta-\tau,x)$. One can check that this transformation leaves

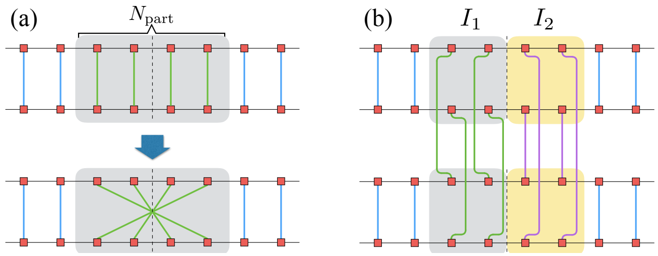

FIG. 3. Schematic representation the ground state overlap (a) partial reflection, $\langle\Psi|\mathcal{R}_{\rm part}|\Psi\rangle$, (b) partial transpose, $\mathrm{tr}\,(\rho_I U_{I_1} \rho_I^{T_1} U_{I_1}^\dagger)$. Solid squares represent physical sites and vertical bonds represent how physical degrees of freedom contracted between $|\Psi\rangle$ and $\langle\Psi|$.

the Hamiltonian (1) or, in fact, generic bilinear forms $H(\bar{\xi},\xi)=\sum_{x,x'}[t_{xx'}\bar{\xi}(x)\xi(x')+\Delta_{xx'}\bar{\xi}(x)\bar{\xi}(x')+\mathrm{H.c.}]$ invariant. It is easy to see that possible two-body interaction terms such as $(\bar{\xi}\xi)^2$ are also invariant. Similar to the cross-cap introduced by twisting the temporal boundary by reflection, one can twist the spatial boundary condition using time-reversal,

$$\xi(\tau,N+1)=-\xi(\tau,0)\to -i\bar{\xi}(\tilde{\tau},0),$$
$$\bar{\xi}(\tau,N+1)=-\bar{\xi}(\tau,0)\to -i\xi(\tilde{\tau},0), \tag{4}$$

over a time interval $t_1<\tau<t_2$ where $0<t_1,t_2<\beta$ and the time inversion $\tau\to\tilde{\tau}$ is performed with respect to the central line $\tau=(t_1+t_2)/2$ of the interval (Fig. 1(c)).

The topological quantum field theory description of topological superconductors implies that the partition function Z of the canonical model (1) on $\mathbb{R}P^2$ is given by $Z\sim e^{i2\pi/8}$ (the eighth root of unity) in the topological regime, corresponding to $\nu=1\in\mathbb{Z}_8$, and $Z\sim 1$ in the trivial regime, corresponding to $\nu=0$. Moreover, the complex phase is additive, i.e., stacking n copies of Majorana chain (1) results in $Z\sim e^{i2\pi n/8}$, and for instance, we have $Z\sim 1$ for $n=8$ that is indicative of the trivial phase. This is how the $\mathbb{Z}_8$ cyclic group is understood in our scheme.

The numerically computed partition function in the presence of a cross-cap is shown in Fig. 2. The results for the symmetry classes BDI and D+R$_-$ match with each other. Well inside the non-trivial SPT phase $|\mu|/t<2$ (i.e., when the size of the cross-cap is much bigger than the correlation length), the phase of the partition function is quantized as $Z\sim e^{i\frac{\pi}{4}}/\sqrt{2}$, whereas in the trivial phase $Z\le 1$ with no complex phase and $Z\to 1$ deep inside the trivial phase (animations and Appendix J [35]). The phase factor $e^{i\frac{\pi}{4}}$ is the $\mathbb{Z}_8$ phase associated with the partition function on $\mathbb{R}P^2$. We shall discuss more about the amplitude $|Z|$ momentarily.

Partial reflection.– The cross-cap in the path-integral can be also implemented in terms of ground state wave functions of the fermionic SPT phases. Let us now discuss this operator formalism. The reflection cross-cap

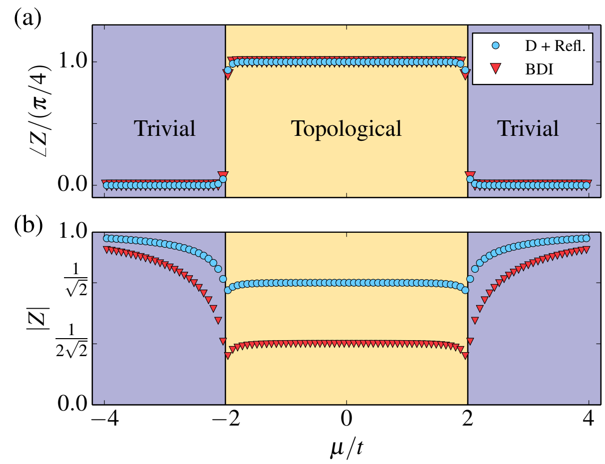

FIG. 4. Partial reflection (5) for class D with reflection and partial transpose (6) for class BDI in the Kitaev Majorana chain. Here, $N=120$ and $N_{\rm part}=60$.

can be expressed as the expectation value of a non-local operator $\mathcal{R}_{\rm part}$ for a given wave function,

$$Z_{\mathcal{R}}=\langle\Psi|\,\mathcal{R}_{\rm part}\,|\Psi\rangle \tag{5}$$

where $\mathcal{R}_{\rm part}$ is the *partial* reflection operator which reflects the sites within a segment of lattice with respect to its central bond (dashed line in Fig. 3 (a)). This quantity has been first proposed as a non-local order parameter to distinguish various topological phases of spin chains [37–42], The overlap $Z_{\mathcal{R}}$ can be also used as an effective method to extract the topological invariant in the reflection symmetric fermionic SPT phases.

Using the definition of reflection symmetry in the Kitaev chain (1), we can construct $\mathcal{R}_{\rm part}$ and compute $Z_{\mathcal{R}}$. The result summarized in Fig. 4 confirms that Eq. (5) shows a similar behavior to its path-integral counterpart. (An analytical derivation of the same result for the fixed point wave function at $\mu=0$ is provided in Appendix D [35]). More examples including the s-wave superconducting nanowire construction [43] of Majorana chain, and the symmetry class A with reflection are provided in Appendix F [35].

Few remarks regarding the amplitude $|Z|$ are in order. First, in the topological phase, the factor $\sqrt{2}$ in the denominator is the quantum dimension of Majorana fermions and physically related to breaking two bonds between the adjacent fermion sites. For instance, in the case of class A, $|Z|=1/2$ in the topological phase corresponding to the quantum dimension of fermionic zero modes (as opposed to Majoranas) at the ends. Second, in the trivial phase $|Z|$ is 1 only in the infinite gap limit and the smooth transition from $1/\sqrt{2}$ to 1 indicates finite size effects. Another important fact is that Z is a bulk quantity and hence independent of the physical boundary conditions at the ends of a long chain.

Partial time-reversal.– Let us now discuss the way to implement the time-reversal cross-cap in terms of a given ground state wave function. To this end, similar to the partial reflection, we need to introduce partial time-reversal transformation. Implementation of partial time-reversal is slightly more complicated than partial reflection, since time-reversal is anti-unitary (i.e., it is not clear how to define a partial complex conjugation). We first explain how to resolve this issue for 1D bosonic SPT phases with time-reversal symmetry $\mathcal{T} = U\mathcal{K}$ where $\mathcal{K}$ is the complex conjugation and U is a unitary acting on local degrees of freedom. Our strategy is to start with the amplitude of full symmetry transformation $|\langle\Psi|\mathcal{T}|\Psi\rangle|$ rather than $\langle\Psi|\mathcal{T}|\Psi\rangle$, since the latter is simply not gauge invariant. Using the definition of time-reversal operator, we write $|\langle\Psi|\mathcal{T}|\Psi\rangle|^2 = \mathrm{tr}\,(\rho U \rho^T U^\dagger)$, where $\rho = |\Psi\rangle\langle\Psi|$ is the density matrix and we use the Hermiticity property $\rho^* = \rho^T$. At this stage, we can conveniently define the topological invariant in terms of a partial symmetry transformation by introducing the *partial transpose* of the density matrix,

$$Z_{\mathcal{T}} = \mathrm{tr}\,\left(\rho_I U_{I_1} \rho_I^{T_1} U_{I_1}^\dagger\right). \tag{6}$$

Here, we consider two adjacent intervals $I_{1,2}$ of the total system S, $\rho_I = \mathrm{tr}_{S\setminus I}(|\Psi\rangle\langle\Psi|)$ is the reduced density matrix for the region $I = I_1 \cup I_2$, and the unitary transformation U_{I_1} acts only in the region I_1. $\rho_I^{T_1}$ is the partial transpose of ρ_I, and for bosonic systems is defined by

$$\rho_I^{T_1} = \sum_{ijkl} |e_i^1, e_j^2\rangle \langle e_k^1, e_j^2|\rho_I|e_i^1, e_l^2\rangle \langle e_k^1, e_l^2|, \tag{7}$$

where $|e_j^1\rangle$ and $|e_k^2\rangle$ denote an orthonormal set of states in the I_1 and I_2 regions. The definition (6) is shown diagrammatically in Fig. 3(b) and is equivalent to the topological invariant discussed previously in Ref. [39] for spin chains. Here, it is important that I_1 and I_2 are adjacent regions; as we show in Appendix G [35], this configuration is topologically equivalent to introducing a cross-cap in the spacetime [41].

The topological invariant (6) may resemble the *concurrence* in the context of quantum information [44–46]; however, Eq. (6) is different from the concurrence where one takes the full transpose of the density matrix. In addition, the eigenvalues of the partially transposed density matrix $\rho_I^{T_1}$ can be used to define another measure of quantum entanglement called the *negativity*, which has been shown as an effective probe of the entanglement in mixed states [47–52].

To generalize the expression (6) for fermionic systems, we need to define a proper partial transpose for fermions. This is more transparent when the density matrix is expanded in the coherent state basis

$$\rho_I = \int d[\bar{\xi},\xi]d[\bar{\chi},\chi]\, |\{\xi_j\}\rangle\, \rho_I\big(\{\bar{\xi}_j\};\{\chi_j\}\big)\, |\{\xi_j\}\rangle \langle\{\bar{\chi}_j\}|,$$

where $d[\bar{\xi},\xi] = \prod_j d\bar{\xi}_j d\xi_j e^{-\sum_j \bar{\xi}_j\xi_j}$ and $\rho_I\big(\{\bar{\xi}_j\};\{\chi_j\}\big) = \big\langle\{\bar{\xi}_j\}\,\big|\,\rho_I\,\big|\,\{\chi_j\}\big\rangle$. Using the transformation rules for constructing a time-reversal cross-cap in the path integral formalism (Eq. (4)), the analog of Eq. (7) for fermions can be defined as

$$\begin{aligned} U_{I_1}\rho_I^{T_1}U_{I_1}^\dagger := \int d[\bar{\xi},\xi]d[\bar{\chi},\chi]\, &|\{-i\bar{\chi}_j\}_{j\in I_1},\{\xi_j\}_{j\in I_2}\rangle \\ &\times \rho_I\big(\{\bar{\xi}_j\};\{\chi_j\}\big)\,\langle\{-i\xi_j\}_{j\in I_1},\{\bar{\chi}_j\}_{j\in I_2}|\,. \end{aligned}$$

The change of variable is effectively equivalent to applying the time-reversal operator only to I_1. An alternative definition of the partial transpose is given in terms of Majorana operators (Appendix G [35]).

Figure 4 shows the numerically computed $Z_{\mathcal{T}}$ of the Majorana chain (1). Well inside the SPT phase, $Z_{\mathcal{T}}$ is given by $Z_{\mathcal{T}} \sim e^{i\frac{\pi}{4}}/2\sqrt{2}$ whereas $Z_{\mathcal{T}} \leq 1$ in the trivial phase. Therefore, partial transpose may serve as a non-local operation to obtain the complex phase of the partition function on $\mathbb{R}P^2$ (See Appendix G [35] for analytical derivation and further examples).

Higher dimensions.– Our scheme, illustrated so far for 1D topological superconductors, can be generalized to other fermionic SPT phases, in particular to higher dimensions. As an example, let us consider the inversion symmetric topological superconductor in class D in 3D (e.g., ^{3}He-B phase). It can be modeled by the BdG Hamiltonian on a cubic lattice, which is given in momentum space as $\hat{H} = (1/2)\sum_{\mathbf{k}} \Psi^\dagger(\mathbf{k})h(\mathbf{k})\Psi(\mathbf{k})$, where $\Psi^\dagger(\mathbf{k}) = (f_\uparrow^\dagger(\mathbf{k}), f_\downarrow^\dagger(\mathbf{k}), f_\downarrow(-\mathbf{k}), -f_\uparrow(-\mathbf{k}))$, and

$$\begin{aligned} h(\mathbf{k}) = &\left[-t(\cos k_x + \cos k_y + \cos k_z) - \mu\right]\tau_z \\ &+ \Delta\left[\sin k_x \tau_x\sigma_x + \sin k_y \tau_x\sigma_y + \sin k_z \tau_x\sigma_z\right]. \end{aligned} \tag{8}$$

This model is invariant under inversion $\mathcal{I}f_\sigma(x,y,z)\mathcal{I}^{-1} = if_\sigma(-x,-y,-z)$ (Appendix H [35]). The topological classification is known to be $\mathbb{Z}_{16}$, and can be captured by the path-integral on the four dimensional real projective space $\mathbb{R}P^4$, which can be realized by introducing a cross-cap in S^4 [30, 34, 53, 54]. To define the corresponding topological invariant in terms of the ground state $|\Psi\rangle$, we consider the expectation value of the partial inversion $Z_{\mathcal{I}} = \langle\Psi|\mathcal{I}_{\mathrm{part}}|\Psi\rangle$, which acts on a closed three ball. The numerically computed SPT invariant is shown in Fig. 5. It is quite remarkable that the partial inversion yields the correct $\mathbb{Z}_{16}$ and $\mathbb{Z}_8$ complex phases in the topological phases characterized by odd and even number of gapless Majorana surface modes, respectively.

Discussion.– In conclusion, we present an approach to detect interacting SPT phases by creating a spacetime cross-cap in the path-integral. We introduce non-local

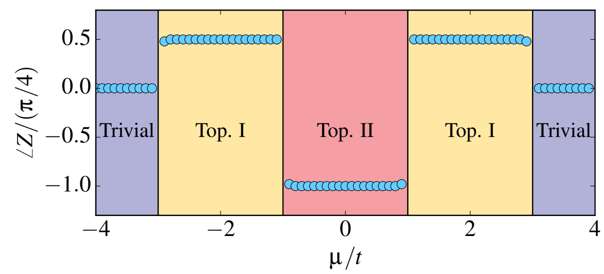

FIG. 5. SPT invariant for the three-dimensional inversion symmetric superconductor (class D), Eq. (8). Top. I (II) corresponds to the phase with odd (even) number of gapless Majorana surface states. Here, $N = 12^3$ and $N_{\rm part} = 6^3$.

order parameters partial reflection/transposition to diagnose many-body SPT phases. While we use a non-interacting fermionic model (the Kitaev chain (1)) to demonstrate our method, we emphasize that our topological invariants are applicable to interacting models and can be used in numerical simulations, such as quantum Monte Carlo. In Appendix F [35], we present the calculation of the topological invariant in an interacting Majorana chain, by making use of the known exact expression of the ground state [55]. In addition, throughout this letter, we consider BCS mean-field wave functions which do not preserve the particle number. One important question is whether the partial transformation works for particle number conserving systems or not [56–60]. As a first step in this direction, we examine the partial reflection for projected-BCS wave functions, obtained by projecting the ground state of the mean-field Hamiltonian (1) to the space of fixed number of particles. Using variational Monte Carlo, we find that the phase of Z remains quantized as in the mean-field wave function (Appendix I [35]). Another important issue is the robustness of SPT invariants in the presence of the random disorder [61].

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