Bulk-boundary correspondence of topological insulators from their respective Green's functions

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Bulk-boundary correspondence of topological insulators from their Green's functions

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Topological insulators are noninteracting, gapped fermionic systems which have gapless boundary excitations. They are characterized by topological invariants, which can be written in many different ways, including in terms of Green's functions. Here we show that the existence of the edge states directly follows from the existence of the topological invariant written in terms of the Green's functions, for all ten classes of topological insulators in all spatial dimensions. We also show that the resulting edge states are characterized by their own topological invariant, whose value is equal to the topological invariant of the bulk insulator. This can be used to test whether a given model Hamiltonian can describe an edge of a topological insulator. Finally, we observe that the results discussed here apply equally well to interacting topological insulators, with certain modifications.

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I. INTRODUCTION

The time-reversal invariant topological insulators of recent interest, and the integer quantum Hall systems of longstanding interest (for recent reviews at a variety of levels, please see Ref. 1), are now known to be just two elements in a classification table of all noninteracting fermionic systems,[2,3] which identifies ten symmetry classes of topological insulators. All of these systems are gapped in the bulk and possess a bulk topological invariant. They are also supposed to have topologically protected gapless excitations at the boundary. These gapless excitations are often taken as the most significant, even the defining, property of topological insulators.

A variety of arguments can be given supporting the existence of gapless edge states based on bulk properties, some more detailed (such as Laughlin's original argument designed for the integer quantum Hall effect[4]) and some more qualitative. For example, consider the case of a model of noninteracting fermions that supports both a topologically trivial phase and a nontrivial phase, with the phase transition driven by varying a parameter in the system's Hamiltonian. At the transition, corresponding to a special value of the parameter, the excitation gap must close. A boundary between two samples in the two phases can then be seen as a domain wall across which the parameter varies spatially through its special value. This "spatial phase transition" should then also result in gapless excitations, which form in the vicinity of the special value. Such arguments, while correct, tell us nothing about what kind of gapless edge excitations might form at the boundary of the topological insulator.

Here we rely on the method of Green's functions to give a general, quantitative argument that proves the existence of the edge states for all topological insulators. Moreover, our argument shows that the edge states are described by their own topological invariant, analogous to the winding number of a vortex in a superfluid or to the charge of a particle as measured by Gauss' law (and similar to the defect invariants of Teo and Kane[5]), whose value must be equal to the invariant of the bulk insulator. This edge invariant vanishes if the edge states are gapped, giving a simple way to see why they must be gapless. The existence of this invariant gives us a tool to test whether a particular Hamiltonian can describe an edge theory, as it is straightforwardly calculable for any Hamiltonian under consideration.

Before we derive this argument later in this article, let us describe the edge topological invariant. A d-dimensional topological insulator that is translationally invariant, so that the d-dimensional momentum $\mathbf{p}^d$ is a good quantum number, possesses a d-dimensional (bulk) topological invariant N_d.[3] If the topological insulator has an edge, translation invariance in the direction perpendicular to the edge is lost, and the good quantum number is the $(d-1)$-dimensional momentum $\mathbf{p}^{d-1}$ parallel to the edge. Let us take one of the components of this momentum, say p_{d-1}, and fix it at some large value Λ. Although we expect the edge to have gapless excitations at some momentum (and so is not an insulator), the Hamiltonian at fixed $p_{d-1} = \Lambda$ is gapped if Λ is sufficiently large (as a function of the remaining $d-2$ momenta), and so describes a $(d-2)$-dimensional insulator. We will show that this insulator is a topological insulator, with the topological invariant $N_{d-2}(\Lambda)$. Finally, we will show that

$$N_d = N_{d-2}(\Lambda) - N_{d-2}(-\Lambda), \tag{1}$$

which constitutes the main result of this article.

As an example, consider the three-dimensional edge of a four-dimensional time-reversal invariant topological insulator with spin-orbit coupling. Suppose the excitations localized at the boundary are described by the Hamiltonian

$$\mathcal{H} = v \sum_{\alpha=x,y,z} p_\alpha \sigma_\alpha - \mu, \tag{2}$$

where σ_α are the Pauli matrices and v is Fermi velocity, which satisfies the appropriate symmetry (time-reversal invariance) $H(p) = \sigma_y H^*(-p)\sigma_y$. Its single-particle excitation spectrum is

$$\epsilon_\pm(\mathbf{p}) = \pm v\sqrt{p_x^2 + p_y^2 + p_z^2} - \mu, \tag{3}$$

and its zero energy excitations occur on a sphere of radius μ/v, as shown in Fig. 1. Let us see that this is indeed the edge of a topological insulator. We fix $p_z = \pm\Lambda$ to obtain the two-dimensional Hamiltonian

$$H_\pm = v\left(p_x\sigma_x + p_y\sigma_y \pm \Lambda\sigma_z\right) - \mu, \tag{4}$$

again as illustrated in Fig. 1. This Hamiltonian, understood as describing a two-dimensional system, is well known. For example, it has been studied as a model of quantum Hall transitions.[6,7] The two-dimensional topological invariant of this Hamiltonian is known to be equal to its Hall conductance in units of e^2/h (note that Eq. (4), unlike Eq. (2), breaks time reversal invariance), and, assuming $\Lambda > \mu/v$, evaluates to

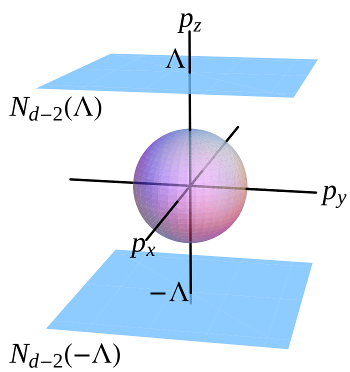

FIG. 1. The Fermi surface of radius μ/v of the topological insulator discussed in the text, and the surfaces $p_z = \pm\Lambda$ on which the edge topological invariant is computed.

$$N_2(\Lambda) - N_2(-\Lambda) = 1. \tag{5}$$

Therefore we conclude that this H is a valid model of the boundary of a four-dimensional topological insulator. This illustrates the usefulness of Eq. (1).

This example assumes an unphysically large bulk dimension, and the reader may doubt that it has any relevance for real-world physics. However, it is known[8] that the experimentally realized time-reversal-invariant topological insulators in 2 and 3 dimensions can be viewed as descending from a four-dimensional parent, simply by setting one or two of the momenta to zero. Similarly, the three-dimensional boundary just discussed can be seen as the parent of the boundary theories of those real systems. In particular, it follows from Eq. (2) that the boundary theory for the two dimensional time-reversal invariant topological insulator is $H = v\,\sigma_x p_x - \mu$, while that of the three dimensional time-reversal invariant insulator is $H = v\left(\sigma_x p_x + \sigma_y p_y\right) - \mu$. We will return to this "dimensional reduction" later in this article.

The Green's function formalism we use is quite powerful: it remains applicable even when interactions are added to the system, since Green's functions exist for interacting as well as for noninteracting systems. Here one must comment that the power of topological invariants often lies in the fact that they represent the response of noninteracting systems to external electromagnetic field. Once the interactions are turned on, the topological invariant written in terms of interacting Green's functions may or may not represent the response, and this could be considered an impediment to using the Green's function formalism to describe interacting topological insulators. However, the main result, Eq. (1), is correct regardless of the presence of interactions as will be clear from its derivation. If one takes as the most physically relevant property of topological insulators is the existence of edge states, then since the relation Eq. (1) relates the topological invariant to the property of the edge, this relation, and not the response, can in principle be taken as a starting point of the application of this formalism to the interacting topological insulators.

Yet the interpretation of Eq. (1) may change once the interactions are turned on. As discussed in a recent paper by one of us,[9] in the presence of interactions the (eigenvalues of the) Green's functions may have zeroes localized at the edge, in addition to the poles that indicate the usual edge states. From the point of view of the topological invariants, zeroes are similar to poles, and can result in a nonzero edge invariant even in the absence of zero-energy edge states.[10] In fact, it can be shown that the recent result of Ref. 11, where a model topological insulator loses its edge states in the presence of interactions, is due to the replacement of the edge states by the zeros of the Green's function.[12] The study of the effects of interactions using the formalism developed here appears to be a useful direction of further research, but goes beyond the scope of this article. In what follows we mostly assume that the fermions do not interact, although throughout this article we point out what exactly changes if interactions are taken into account.

To connect this article to previous publications, we remark that the relation Eq. (1) was discussed for $d = 2$ in Ref. 13. Subsequently, it was extended for $d = 1$ and discussed in the presence of interactions in Ref. 9. Here we extend it for all topological insulators, in any number of dimensions.

We proceed as follows: in section II we derive Eq. (1) for systems with no symmetry other than translational (class A in the Altand-Zirnbauer classification[14,15]), which only have integer-valued topological invariants in even spacial dimensions. Then in section III we describe the effects of discrete symmetries on the invariants; and then describe how these results imply the relation between bulk and surface physics for $\mathbb{Z}_2$ topological systems. Finally in section IV we discuss systems with chiral symmetry. Appendix A contains the derivation of a key step in our derivation of Eq. (1), and Appendix B presents a more complete discussion of 1D topological insulators.

II. TOPOLOGICAL INSULATORS WITHOUT ANY SYMMETRIES

We start with a translationally invariant topological insulator with a single particle Green's function $G_{\alpha\beta}(\omega, \mathbf{p})$. If interactions are absent, the insulator can be described by the Hamiltonian

$$H = \sum_{\mathbf{p}} \mathcal{H}_{\alpha\beta}(\mathbf{p})\, \hat{a}^{\dagger}_{\alpha\mathbf{p}} \hat{a}_{\beta\mathbf{p}}. \tag{6}$$

Here $\hat{a}^{\dagger}_{\alpha\mathbf{p}}$ creates a fermion with momentum $\mathbf{p}$ in d dimensions, and the species label α runs over the spin, bands, as well as particle/hole space for a superconductor (summation on indices should be always understood). In that case, the Green's function is simply given by

$$G(\omega, \mathbf{p}) = [i\omega - \mathcal{H}(\mathbf{p})]^{-1}. \tag{7}$$

Once interactions are switched on, simple expressions of this kind are no longer available, but Green's function can still be defined in a standard way (see, for example, 16).

The bulk topological invariant is

$$N_d = C_d\, \epsilon_{a_0 \ldots a_d} \int d\omega d^d p \,\mathrm{tr}\, G^{-1}\partial_{a_0} G \ldots G^{-1}\partial_{a_d} G, \tag{8}$$

where a runs over $(\omega, \mathbf{p})$, and ϵ is fully antisymmetric tensor, with $\epsilon_{\omega p_1 \ldots p_d} = +1$ (the other nonvanishing components are obtained by permutation). The constant C_d is given by[3]

$$C_d = -(2\pi i)^{-(d/2)-1}(d/2)!/(d+1)! \tag{9}$$

The spatial dimension d is even, as N_d vanishes when d is odd (by antisymmetry of ϵ and cyclicity of the trace tr); we will later introduce a different expression, valid for chiral systems in odd dimensions, that we denote by the same symbol.

This topological invariant always evaluates to an integer, and gives the Hall conductance in two-dimensional space,[17] at least in the absence of interactions — it remains a topological quantity (an integer) even with interactions. This is true simply because it measures the winding of the map from a $(d+1)$-dimensional space $(\omega, \mathbf{p}^d)$ to a space of matrices G; it is known that such a map can be topologically nontrivial if d is even. Moreover, it is clear that in the absence of interactions, to change the value topological invariant one needs to deform the Green's function in such a way that either G or G^{-1} becomes singular. For noninteracting systems, this is only possible if $\omega = 0$ and $\mathcal{H}$ has zero energy states as follows from Eq. (7); this results in infinite G at $\omega = 0$ and the closing of the gap in the spectrum. For interacting systems G itself can acquire zero eigenvalues at $\omega = 0$,[9] so that G^{-1} is singular; thus interacting systems can change the value of their invariant Eq. (8) without ever closing the gap. All of this matches known results.

Now we introduce some technology, inspired by Volovik.[13] Consider a d-dimensional system with a domain wall of dimension $d-1$; the Hamiltonian varies in the direction perpendicular to the domain wall in such a way that far from the domain wall the Hamiltonian describes a topological insulator with the invariant N_d^R or N_d^L, on the right or left side of the domain wall (what this means precisely will be defined below). Since there are only $d-1$ good momenta, it is described by the mixed Green's function $\tilde{G}(\omega, \mathbf{p}^{d-1}; s, s')$, where s is the coordinate normal to the boundary and is effectively another matrix index. A Fourier transform with respect to $s - s'$ produces the Wigner (-Weyl) transform $G(\omega, \mathbf{p}^d, \bar{s})$,[18,19] with $\bar{s} = (s + s')/2$ and p_d the momentum conjugate to $s - s'$. Far from the domain wall, this will become $\bar{s}$-independent and coincide with the bulk Green's function (that is, with translation invariance the Wigner and Fourier transforms are the same).

Importantly, two objects exist which can be interpreted as the inverse of G. The "true" inverse satisfies

$$\sum_{\beta} \int ds' \tilde{K}_{\alpha\beta}(s, s')\, \tilde{G}_{\beta\gamma}(s', s'') = \delta_{\alpha\gamma}\delta(s - s'') \tag{10}$$

(in this expression the ω and $\mathbf{p}^{d-1}$ dependence of $\tilde{K}$ and $\tilde{G}$ was suppressed for brevity). For noninteracting systems

$$\tilde{K}(\omega, \mathbf{p}^{d-1}; s, s') = i\omega - \mathcal{H}(\omega, \mathbf{p}^{d-1}; s, s'), \tag{11}$$

but for interacting systems one should rely solely on Eq. (10) to calculate $\tilde{K}$. At the same time, matrix (or local) inverse G^{-1} satisfies

$$G^{-1}_{\alpha\beta}(\omega, \mathbf{p}^d, \bar{s})\, G_{\beta\gamma}(\omega, \mathbf{p}^d, \bar{s}) = \delta_{\alpha\gamma}. \tag{12}$$

With translation invariance along s, $K = G^{-1}$, but in the presence of a domain wall $K \neq G^{-1}$ [here $K(\omega, \mathbf{p}^d, \bar{s})$ is the Wigner transform of $\tilde{K}(\omega, \mathbf{p}^{d-1}; s, s')$].

With these tools, we define the $(d+2)$-dimensional vector

$$n_{a_0} = C_d\, \epsilon_{a_0 a_1 \ldots a_{d+1}} \mathrm{tr}\, G^{-1}\partial_{a_1} G \ldots G^{-1}\partial_{a_d} G \tag{13}$$

in the space $(\omega, \mathbf{p}^d, \bar{s})$. Remarkably, the divergence of this vector is zero except where G (or G^{-1} if interactions are present) is singular, as can be checked by direct differentiation. This is completely analogous to the electric field in electrostatics with point charges or charged surfaces. Here, the sources of $\mathbf{n}$ are singularities (or zeros) of G. The analogy to electrostatics is productive; we will essentially measure the charge of a singularity with Gauss' law, integrating the flux of $\mathbf{n}$ over a surface that surrounds the charge.

For the rest of this section, for simplicity we will always refer to these as "singularities" having in mind that in the absence of interactions G cannot have zeros. We will also keep in mind that if interactions are present, singularities will imply either infinite or zero G.

The singularities of G may occur at multiple points of the $d+2$ dimensional space or on surfaces in the space spanned by $(\omega, \mathbf{p}^d, \bar{s})$. We denote these f_i.

Because $G(\omega, \mathbf{p}^d, \bar{s})$ reduces to the bulk Green's function far from the boundary (domain wall), the definitions Eqs. (8) and (13) mean that we can compute N_d as the flux of $\mathbf{n}$ through the surface $\bar{s} = L$ for large L. That is, the difference between topological invariants on either side (right N_d^R and left N_d^L, say) of the boundary,

$$N_d^R - N_d^L = \int d\omega d^d p \, [n_{\bar{s}}(\bar{s} = L) - n_{\bar{s}}(\bar{s} = -L)], \quad (14)$$

is just the flux of $\mathbf{n}$ through the combined surface $(\omega, \mathbf{p}^d, \pm L)$, shown in Fig. 2. On the other hand, and this is the crucial point, because $\partial_a n_a = 0$ we can use *any surface we like* to compute $N_d^R - N_d^L$ so long as it encloses the singular surfaces of G. Denoting by S_{f_i} any $(d+1)$-dimensional "Gaussian" surface (for example, a sphere) surrounding f_i we find

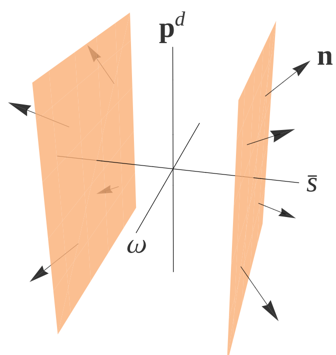

FIG. 2. The surfaces $\bar{s} = \pm L$ on which N_d is computed as the flux of $\mathbf{n}$.

$$N_d^R - N_d^L = \sum_i \int \mathbf{dS}_{f_i} \cdot \mathbf{n}. \quad (15)$$

Eq. (15) constitutes the first half of our argument.[20]

To relate the flux of $\mathbf{n}$ to the edge properties of the system, we construct a d-dimensional vector $\mathbf{r}$ out of the mixed Green's function $\tilde{G}(\omega, \mathbf{p}^{d-1}; s, s')$, which allows us to define a topological invariant that directly captures the behavior of the edge states. We define

$$r_{a_0} = C_{d-2} \, \epsilon_{a_0 \ldots a_{d-1}} \mathrm{Tr} \, \tilde{K} \circ \partial_{a_0} \tilde{G} \circ \cdots \circ \tilde{K} \circ \partial_{a_{d-1}} \tilde{G}. \quad (16)$$

The convolution $(\tilde{A} \circ \tilde{B})(s, s'') = \int ds' \tilde{A}(s, s') \tilde{B}(s', s'')$ that appears here is really a generalization of matrix multiplication to functions of two coordinates s, s'. That is, the coordinates s, s' are treated as matrix indices of the functions $\tilde{A}$ and $\tilde{B}$, and $\tilde{G}$; of course, these functions also carry the ordinary matrix indices α, β that label fermion species, *etc*, and which are being summed over in the usual way. Then $\mathrm{Tr} \, \tilde{A} \equiv \int ds \, \mathrm{tr} \tilde{A}(s, s)$ is just the trace for these generalized matrices. The index a here runs over $(\omega, \mathbf{p}^{d-1})$, the space of the vector $\mathbf{r}$.

The vector $\mathbf{r}$, just like the vector $\mathbf{n}$ above, is divergence-free, except at singularities of the mixed Green's function $\tilde{G}$. These singularities can also be interpreted as "electrostatic" sources for the vector $\mathbf{r}$ emanating from them.

It is clear that the singular surfaces f_i — the sources of $\mathbf{n}$ — become the sources of $\mathbf{r}$ as well when projected from the $(d+2)$-dimensional space $(\omega, \mathbf{p}^d, \bar{s})$ onto the d-dimensional edge space $(\omega, \mathbf{p}^{d-1})$. Since the Green's function $\tilde{G} = [i\omega - \mathcal{H}]^{-1}$ can only be singular where $\omega = 0$ and $\mathcal{H}$ has zero energy eigenstates, these sources are confined to $\omega = 0$ and form surfaces (or points) in the $(d-1)$-dimensional space spanned by $\mathbf{p}^{d-1}$, which we identify with the edge Fermi surfaces and Dirac points and denote F_i (having in mind that in the presence of interactions surfaces and points of zero $\tilde{G}$ play an equivalent role).

Remarkably, we can prove the following statement:

$$\sum_i \int \mathbf{dS}_{f_i} \cdot \mathbf{n} = \sum_i \int \mathbf{dS}_{F_i} \cdot \mathbf{r}. \quad (17)$$

Here S_{F_i} is the $(d-2)$-dimensional surface surrounding the Fermi surface (or Dirac point) F_i. The proof of this statement is given in Appendix A and is quite involved (although for $d = 2$ the proof is significantly simpler; it is given in Ref. 13). It relies on the approximation of the domain wall being smooth. However, the corrections to this equation form a series expansion in powers of the gradient $\partial_{\bar{s}} G$. Since both sides of this equation are integers due to Eq. (15), small corrections to it must vanish.

It follows from Eqs. (15) and (17) that

$$N_d^R - N_d^L = \sum_i \int \mathbf{dS}_{F_i} \cdot \mathbf{r}. \quad (18)$$

In words, this says that the Fermi surfaces (and Dirac points) on the edge are characterized by "topological charges," or fluxes of $\mathbf{r}$ emanating from these surfaces and points. This charge is equal to the difference in the bulk topological invariants on either side of the boundary. Eq. (18) is the quantitative statement of the fact that gapless excitations are required at a boundary between bulk insulators with different values of the topological invariant N_d (in the presence of interactions, there can be zeroes instead[9]). Indeed, in the absence of such excitations, $\mathbf{r}$ is divergence-free everywhere and its flux is always zero.

What remains is to interpret this charge as a difference of topological invariants, as discussed in the beginning of this article. So long as the Fermi surface does not traverse the Brillouin zone in the p_{d-1} direction, we can choose S_F to be the surfaces $(\omega, \mathbf{p}^{d-2}, \pm\Lambda)$ for suitable Λ, instead of the spheres closely surrounding the Fermi surface(s) that we assumed until this point [see Fig. 3].

The flux through S_F is then the difference of the fluxes of $\mathbf{r}$ through these two surfaces. In turn, those fluxes can be reinterpreted as the difference $N_{d-2}(\Lambda) - N_{d-2}(-\Lambda)$,

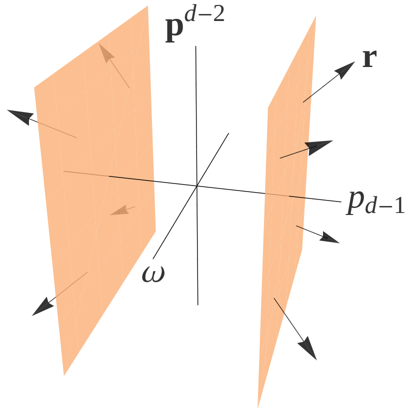

FIG. 3. The surfaces $p^{d-1} = \pm\Lambda$ on which N_{d-2} is computed as the flux of $\mathbf{r}$.

where

$$N_{d-2}(p_{d-1}) = \int d\omega\, d^{d-2}p\, r_{p_{d-1}} \qquad (19)$$

is a $(d-2)$-dimensional topological invariant calculated in the space $(\omega, \mathbf{p}^{d-2})$ with p_{d-1} fixed, as can be verified with Eq. (16). The main result of this article Eq. (1) (where N^L_d is assumed to be 0 for simplicity) immediately follows.

In the simplest case $d = 2$ this result was derived in Ref. 13, where $N_0(\Lambda) - N_0(-\Lambda)$ was interpreted as a number of energy levels crossing zero as the momentum along the one-dimensional edge changes from $-\Lambda$ to Λ, corresponding to the standard picture of edge states in the integer quantum Hall effect. In higher number of even dimensions d, this result's interpretation is more complicated, but the result is nonetheless useful, as in the example given in the Introduction.

This concludes the discussion of topological insulators without symmetries (systems of class A).

III. TOPOLOGICAL INSULATORS WITH TIME-REVERSAL OR PARTICLE-HOLE SYMMETRY

Now let us apply this formalism to systems in the nine remaining classes of topological insulators with symmetry, beginning from non-chiral insulators. Nonchiral insulators, termed classes AI, AII, C and D, are those which possess either time-reversal or particle-hole symmetry (it can be helpful to refer to the "periodic table" of topological insulators in Refs. 2 and 3 for the discussion of this section and the next). We have seen that with no symmetry (class A), bulk insulators are classified by an integer in even dimensions. The same invariants describe the other nonchiral classes in even dimensions. However the presence of discrete symmetries can force them to vanish in some dimensions, as follows. Classes AI and AII represent time-reversal (T) invariant systems with integer and half-integer spin respectively, and the Green's function satisfies the constraint

$$G(\omega, \mathbf{p}, \bar{s}) = U_T^\dagger\, G^T(\omega, -\mathbf{p}, \bar{s})\, U_T, \qquad (20)$$

where U_T is a unitary matrix such that $U_T^* U_T = \epsilon_T = +1$ for AI and $\epsilon_T = -1$ for AII (G^T is the transposed Green's function). The same constraint holds for $\tilde{G}$. Putting this into N_d, relabeling $\mathbf{p} \to -\mathbf{p}$, taking the transpose, using cyclicity, and relabeling indices, we see that this forces $N_d = 0$ when $d = 4n + 2$ (an anticyclic permutation is odd in $d = 4n + 2$). Similarly, classes C and D have particle-hole (C) symmetry

$$G(\omega, \mathbf{p}, \bar{s}) = -U_C^\dagger\, G^T(-\omega, -\mathbf{p}, \bar{s})\, U_C, \qquad (21)$$

where $U_C^* U_C = \epsilon_C = +1$ for class D and $\epsilon_C = -1$ for class C. An additional minus sign in the integrals is generated by $\omega \to -\omega$, so that N_d is nonzero only in spaces of dimension $d = 4n + 2$. All of this matches what was established elsewhere using a different language.[3]

The conclusion here is that if we are in a spatial dimension where the topological invariant can be nonzero, the bulk-boundary correspondence Eq. (1) applies just as it does for systems without any symmetry. One might worry that the relation Eq. (1) involves not only N_d but also N_{d-2}; as we just saw, in systems with symmetries if N_d is nonzero, N_{d-2} appears to be zero. However, in Eq. (1) N_{d-2} is calculated with p^{d-1} fixed at some value Λ, so the Green's function no longer satisfies Eq. (20) or (21). Thus both sides of Eq. (1) can be nonzero, as they should.

Let us now account for the appearance of $\mathbb{Z}_2$ invariants, which in time-reversal-invariant insulators which belong to class AII appear for example in $d = 2$ and $d = 3$. To explain these, we appeal to the dimensional reduction picture of Qi, Hughes, and Zhang,[8] in which the physical system is considered as embedded within a space of higher dimension, with one or two of the momenta being fictitious additional parameters in the Green's function. The real physical system corresponds to the fictitious momenta set to zero. Under T (or C) almost every point in the momentum space has an image at the opposite momentum, the exceptions being the time-reversal-invariant (TRI) points. As a result, if a Green's function has a point singularity at a non-TRI point, this contributes 2 to Eq. (18), since each point and its image contribute. So, if $N^R_d - N^L_d$ is odd and all singularities are points, some of the singular points must be located at the TRI points in the momentum space. Finally, it is possible to make sure, by choosing the appropriate extension of G to the unphysical momenta, that all singular TRI points are in the physical space. This leads to the conclusion that if the topological invariant in the extended space is an odd integer, there must be singular points, or as we saw edge states, in the physical (reduced-dimension) theory.

The same arguments apply if, instead of a Fermi point, there is a Fermi surface surrounding a TRI point. The case of a surface is also crucial for showing that generally the dimensionality cannot be reduced by more than 2. Indeed, generalizing a result due to Hořava,[21] generic topological insulators characterized by integer invariants have two-dimensional Fermi surfaces at the boundary. A Fermi surface (spherical, for simplicity) centered on zero is defined by the equation $p_x^2 + p_y^2 + p_z^2 = p_F^2$, with the remaining momenta, if any, being arbitrary. This can be dimensionally reduced by one or two by setting $p_z = 0$ or $p_y = p_z = 0$. However, to reduce the dimensionality by more than 2 requires setting $p_x = p_y = p_z = 0$, which eliminates gapless excitations.

An example of two-dimensional Fermi surfaces located at the three-dimensional edge of a four-dimensional topological insulator with time-reversal invariance is shown in Fig. 4. Three Fermi surfaces are depicted, giving

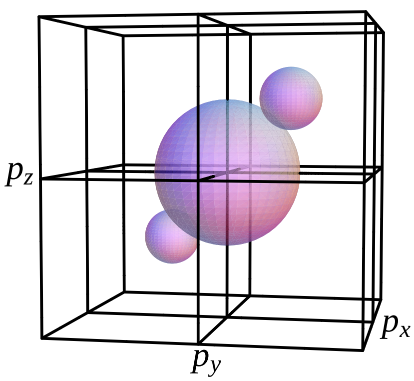

FIG. 4. Example of an edge Brillouin zone containing a time-reversal-invariant, multicomponent Fermi surface. The two smaller spheres each contribute to the three-dimensional edge topological invariant, but they do not intersect the time-reversal invariant planes of the Brillouin zone and so do not contribute to dimensionally reduced edges.

$N_4 = N_2(\Lambda) - N_2(-\Lambda) = 3$. At the same time, two of those Fermi surfaces located at opposite momenta play no role if dimensions are reduced by setting, for example, $p_z = 0$. The remaining Fermi surface centered on the origin still yields zero energy excitations even if $p_z = 0$, thus in this example the edge state survives in lower dimensions. On the other hand, if N_4 were even, then the central Fermi surface would necessarily be absent (or there would be a pair that could be deformed off the $p_z = 0$ plane), and there would be no edge excitations in lower dimensions. Here, as everywhere else, in the presence of interactions, the Fermi surfaces could be the surfaces of zero energy excitations as well as surfaces of zeroes of Green's functions.

Note that if one breaks time reversal invariance by adding appropriate terms in the Hamiltonian, the excitations no longer have to be symmetric under reflection of momenta. Then the central Fermi surface can move off the center of the Brillouin zone and no longer contribute to the lower dimensional edge excitations. This is the mechanism by which breaking time reversal invariance removes edge states in lower dimensions (but not in the original 3-dimensional edge where edge excitations survive even if time reversal invariance is broken).

Finally, the dimensional reduction gives a trivial result in some dimensions because the bulk invariant N_d takes only even values for the dimensionally extended system, which washes out the $\mathbb{Z}_2$ structure.

These arguments conclude our discussions of topological insulators in classes AI, AII, C and D.

IV. TOPOLOGICAL INSULATORS WITH CHIRAL SYMMETRY

We also want to show that analogous results hold for the classes with chiral, or sublattice (S), symmetry (AIII, BDI, CII, CI and DIII). In these systems there is a matrix Σ such that

$$G(\omega, \mathbf{p}, \bar{s}) = -\Sigma\, G(-\omega, \mathbf{p}, \bar{s})\, \Sigma, \quad \Sigma^2 = 1. \tag{22}$$

The bulk invariant for chiral systems, analogous to Eq. (8), can be written as

$$N_d = \frac{C_{d-1}}{2} \epsilon_{a_1 \ldots a_d} \int d^d p \, \mathrm{tr}\, \Sigma\, G^{-1} \partial_{a_1} G \ldots G^{-1} \partial_{a_d} G, \tag{23}$$

where G is evaluated at $\omega = 0$, a runs over the components of $\mathbf{p}$, and the bulk dimension d is now odd.[22] Unlike the even-dimensional topological invariant Eq. (8), this expression does not treat momenta and frequency in a symmetric fashion and in fact is derived directly from the topological invariant written in terms of the Hamiltonian in Ref. 3 by replacing $\mathcal{H} \to G^{-1}\big|_{\omega=0}$. An expression for N_d with d odd which involves integration over frequency and momenta is also possible,[9] however for the purpose of this article it is not needed.

Expressions strictly analogous to Eqs. (13), (15), and (16) can be formulated for the chiral case, leading to a relation just like the bulk-boundary correspondence Eq. (18). In particular,

$$n_{a_0} = \frac{C_{d-1}}{2} \epsilon_{a_0 \ldots a_d} \mathrm{tr}\, \Sigma\, G^{-1} \partial_{a_1} G \ldots G^{-1} \partial_{a_d} G, \tag{24}$$

where a runs over $(\mathbf{p}^d, s)$, is a $(d+1)$-dimensional divergence-free vector, while

$$r_{a_0} = \frac{C_{d-3}}{2} \epsilon_{a_0 \ldots a_{d-2}} \mathrm{Tr}\, \Sigma\, \tilde{K} \circ \partial_{a_1} \tilde{G} \circ \cdots \circ \tilde{K} \partial_{a_{d-2}} \tilde{G} \tag{25}$$

(a runs over $\mathbf{p}^{d-1}$) is a $(d-1)$-dimensional divergence-free vector. Here everything is evaluated at $\omega = 0$.

Class AIII, without T or C symmetry, is potentially nontrivial in any odd dimension. Classes BDI, CII, CI, and DIII are characterized by the presence of both T and C symmetries, with $\epsilon_T \epsilon_C = \eta$ equal to $+1$ in the first two classes and -1 in the other two. The invariant Eq. (23) vanishes if $\eta = 1$ and $d = 3 + 4n$, or if $\eta =$

-1 and $d = 1 + 4n$, because Σ and G anticommute at $\omega = 0$ as a consequence of S-symmetry and $U_T \Sigma U_T^\dagger = \eta \Sigma^T$. Arguments similar to the ones employed above in nonchiral classes can now be used to see the emergence of the chiral $\mathbb{Z}_2$ invariant in appropriate dimensions.

For example if $d = 1$, the vector $\mathbf{r}$ reduces to a scalar $r = -\mathrm{Tr}\,\Sigma$. As is well known, zero-energy states are eigenstates of Σ, with the eigenvalue $+1$ (right zero modes) or -1 (left). $\mathrm{Tr}\,\Sigma$, the difference of the number of right and left eigenstates, is then equal to the difference of the bulk invariants on both sides of this zero-dimensional boundary. A reader may worry that the formalism reported earlier in this article becomes somewhat degenerate at $d = 1$, therefore we present a slightly more detailed derivation of this result in Appendix B.

This concludes the derivation of Eq. (1) for all classes of topological insulators in all spacial dimensions.

V. CONCLUSIONS

In this article we presented a derivation of the relationship Eq. (1) between the bulk and the boundary of topological insulators. Even when there are no interactions and no disorder, this relation is quite useful and allows to test whether a particular proposed boundary theory can indeed be at the edge of a topological insulator. When interactions are present, the relationship Eq. (1) remains true and still allows to relate the the bulk to the edge, although the edge states may get replaced by zeroes.[9] In addition to the extension to interacting systems already described, the method described here can also be extended to disordered topological insulators, by periodically repeating the finite size system. The results obtained in this way will be reported elsewhere.

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Appendix A: Derivation of Eq. (17).

Given a matrix $\tilde{A}(s, s')$ which is also a function of two variables s and s', one can introduce its Wigner (or Weyl) transform

$$A\left(p_d, \bar{s}\right) = \int dr\, e^{ip_d r} \tilde{A}\left(\bar{s} + \frac{r}{2}, \bar{s} - \frac{r}{2}\right). \qquad \text{(A1)}$$

The technical tool we need in the following calculation is the Moyal product expansion, which allows us to write the Wigner transform of $\tilde{C} = \tilde{A} \circ \tilde{B}$ (this stands for $\tilde{C}(s, s'') = \int ds'\, A(s, s') B(s', s'')$) as

$$C = AB + \frac{1}{2i} \epsilon_{\mu\nu}\, \partial_\mu A\, \partial_\nu B + \ldots, \qquad \text{(A2)}$$

where μ, ν stand for $\bar{s}$, p_d. In particular, this means that

$$K = G^{-1} + \frac{1}{2i} \epsilon_{\mu\nu} \chi_\mu \chi_\nu G^{-1} + \ldots, \quad \chi_\mu \equiv G^{-1} \partial_\mu G. \qquad \text{(A3)}$$

This can be checked by demanding that $\tilde{K} \circ \tilde{G} = 1$, applying Wigner transform and using Eq. (A2).

The Moyal product expansion is a formal expansion in powers of the gradient of G, and the omitted terms involve higher gradients of G. As mentioned in the text, this does not limit the applicability of our results to slow domain walls; since we are deriving a relation between integer-valued quantities, any corrections from higher powers of the gradient must vanish (unless they also evaluate to integers, in which case they would indicate extra topological structure).

We would like to relate the vector $\mathbf{r}$ to the vector $\mathbf{n}$. The former involves Green's functions in real space, while the latter involves Wigner-transformed Green's functions. Therefore, we need to apply the gradient expansion to

$$r_{a_0} = C_{d-2} \epsilon_{a_0 \ldots a_{d-1}} \mathrm{Tr}\, X_{a_1} \circ \cdots \circ X_{a_{d-1}}, \quad X_a \equiv \tilde{G}^{-1} \circ \partial_\mu \tilde{G}. \qquad \text{(A4)}$$

First, consider the trace of a product:

$$\begin{aligned} \mathrm{Tr}\, \tilde{A} \circ \tilde{B} &= \int ds ds'\, \mathrm{tr}\, \tilde{A}(s, s') \tilde{B}(s', s) \\ &= \int \frac{ds ds' dp_d dp'_d}{(2\pi)^2}\, e^{-ip_d(s-s') - ip'_d(s'-s)} \\ &\qquad \mathrm{tr}\, A\left(p_d, \frac{s+s'}{2}\right) B\left(p'_d, \frac{s+s'}{2}\right) \\ &= \int \frac{d\bar{s} dp_d}{2\pi}\, \mathrm{tr}\, A(p_d, \bar{s}) B(p_d, \bar{s}). \end{aligned} \qquad \text{(A5)}$$

This states that the trace is invariant upon changing to the Wigner-Weyl basis. The expansion we need is therefore

$$\mathrm{Tr}\, \tilde{K} \circ \partial_{a_1} \tilde{G} \circ \cdots \circ \tilde{K} \circ \partial_{a_{d-1}} \tilde{G} = \int \frac{d\bar{s} dp_d}{2\pi}\, \mathrm{tr}\, KM, \qquad \text{(A6)}$$

where M is the Wigner transform of $\partial_{a_1} \tilde{G} \circ \tilde{K} \cdots \circ \partial_{a_{d-2}} \tilde{G} \circ \tilde{K} \circ \partial_{a_{d-1}} \tilde{G}$:

$$M = \left[\left(\partial_{a_1} G + \frac{\epsilon_{\mu_1\nu_1}}{2i}\partial_{\mu_1,a_1} G\partial_{\nu_1}\right)\left(K + \frac{\epsilon_{\mu'_1\nu'_1}}{2i}\partial_{\mu'_1} K\partial_{\nu'_1}\right)\right]$$
$$\dots\left[\left(\partial_{a_{d-2}} G + \frac{\epsilon_{\mu_{d-2}\nu_{d-2}}}{2i}\partial_{\mu_{d-2},a_{d-2}} G\partial_{\nu_{d-2}}\right)\left(K + \frac{\epsilon_{\mu'_{d-2}\nu'_{d-2}}}{2i}\partial_{\mu'_{d-2}} K\partial_{\nu'_{d-2}}\right)\right]\partial_{a_{d-1}} G + \dots$$
$$= \left[\partial_{a_1} GK + \frac{\epsilon_{\mu_1\nu_1}}{2i}\partial_{\mu_1,a_1} G\partial_{\nu_1}(K\,\cdot) + \frac{\epsilon_{\mu_1\nu_1}}{2i}\partial_{\mu_1} K\partial_{\nu_1}\right]$$
$$\dots\left[\partial_{a_{d-2}} GK + \frac{\epsilon_{\mu_{d-2}\nu_{d-2}}}{2i}\partial_{\mu_{d-2},a_{d-2}} G\partial_{\nu_{d-2}}(K\,\cdot) + \frac{\epsilon_{\mu_{d-2}\nu_{d-2}}}{2i}\partial_{a_{d-2}} G\partial_{\mu_{d-2}} K\partial_{\nu_{d-2}}\right]\partial_{a_{d-1}} G + \dots. \quad \text{(A7)}$$

Eq. (A7) comes from applying the Moyal product expansion, Eq. (A2), to every $\circ$-product.

The notation is quite unwieldy, so we make the following notational simplifications. First, we suppress all $\epsilon_{\mu\nu}$; since we will only be keeping terms of first order in the gradient, there should be no confusion about how indices are contracted. Second, the factor $\epsilon_{a_0\dots a_{d-1}}$ is suppressed as well, and every other symbol that carries an index a_i is written in bold face, with the index suppressed: $\chi_{a_i} \to \boldsymbol{\chi}$ and $\partial_{a_i} \to \mathbf{d}$. It must be remembered that these symbols form a completely antisymmetric tensor. In more formal language, these are one-forms. We can also rewrite products (and $\circ$ products)

$$A_{a_1}\dots A_{a_j} \to \mathbf{A}^j. \quad \text{(A8)}$$

Finally, we will write $d-1 = n$ (which is odd by assumption).

Then the quantity to be computed, up to the overall constant, is

$$\mathrm{Tr}\,\mathbf{X}^n = \int \frac{d\bar{s}dp_d}{2\pi}\,\mathrm{tr}\;K\left[\mathbf{d}GK + \frac{1}{2i}\partial_\mu \mathbf{d}G\partial_\nu(K\,\cdot) + \frac{1}{2i}\mathbf{d}G\partial_\mu K\partial_\nu\right]^{n-1}\mathbf{d}G + \dots. \quad \text{(A9)}$$

The bracket expands to

$$(\mathbf{d}GK)^{n-1} + \frac{1}{2i}\sum_{j=0}^{n-2}(\mathbf{d}GG^{-1})^{n-2-j}\left[\partial_\mu\mathbf{d}G\partial_\nu(G^{-1}\,\cdot) + \mathbf{d}G\partial_\mu G^{-1}\partial_\nu\right](\mathbf{d}GG^{-1})^j + \dots, \quad \text{(A10)}$$

where $K \to G^{-1}$ in the sum because we keep only first order in the gradient. Then

$$\mathrm{Tr}\,\mathbf{X}^n = \int\frac{d\bar{s}dp_d}{2\pi}\,\mathrm{tr}\left\{(K\mathbf{d}G)^n\right.$$
$$\left. + \frac{1}{2i}\sum_{j=0}^{n-2}(G^{-1}\mathbf{d}G)^{n-2-j}G^{-1}\left[\partial_\mu\mathbf{d}G\partial_\nu(G^{-1}\,\cdot) + \mathbf{d}G\partial_\mu G^{-1}\partial_\nu\right]\mathbf{d}G(G^{-1}\mathbf{d}G)^j\right\} + \dots$$
$$= \int\frac{d\bar{s}dp_d}{2\pi}\left\{\mathrm{tr}\;\boldsymbol{\chi}^n + \frac{1}{2i}\sum_{j=1}^{n}\mathrm{tr}\;\boldsymbol{\chi}^{n-j}\chi_\mu\chi_\nu\boldsymbol{\chi}^j\right.$$
$$\left. + \frac{1}{2i}\sum_{j=0}^{n-2}\mathrm{tr}\;\boldsymbol{\chi}^{n-2-j}\left[G^{-1}\partial_\mu\mathbf{d}G\partial_\nu(\boldsymbol{\chi}^{j+1}) - \boldsymbol{\chi}\chi_\mu G^{-1}\partial_\nu(G\boldsymbol{\chi}^{j+1})\right]\right\} + \dots, \quad \text{(A11)}$$

where we have expanded K in the first term according to Eq. (A3) and replaced $\boldsymbol{\chi} = G^{-1}\mathbf{d}G$ and $\partial_\mu G^{-1} = -\chi_\mu G^{-1}$.

Note that the the zeroth-order term in the expansion,

$$\int\frac{d\bar{s}dp_d}{2\pi}\,\mathrm{tr}\;\boldsymbol{\chi}^n, \quad \text{(A12)}$$

produces what is often termed a "weak" topological invariant, that is, a topological invariant of lower dimension than the bulk system; we will ignore this term from now on. AE

Because n is odd, no sign is picked up under cyclic relabeling of the indices hidden in the bold-face notation, so we can use cyclicity of the trace. Therefore, we can combine terms to obtain the first order quantity

$$\mathbf{T} \equiv \sum_{j=1}^{n} \mathrm{tr}\ \boldsymbol{\chi}^{n-j}\chi_\mu\chi_\nu\boldsymbol{\chi}^j + \sum_{j=0}^{n-2} \mathrm{tr}\ \boldsymbol{\chi}^{n-2-j} \times \left[G^{-1}\partial_\mu \mathbf{d} G \partial_\nu(\boldsymbol{\chi}^{j+1}) - \boldsymbol{\chi}\chi_\mu G^{-1}\partial_\nu(G\boldsymbol{\chi}^{j+1})\right]$$
$$= \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \sum_{j=0}^{n-2} \mathrm{tr}\ \boldsymbol{\chi}^{n-2-j}\left[G^{-1}\partial_\mu \mathbf{d}G - \boldsymbol{\chi}\chi_\mu\right]\partial_\nu(\boldsymbol{\chi}^{j+1}).$$

The combination in square brackets is simply $\mathbf{d}\chi_\mu$ so, shifting the summation index,

$$= \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \sum_{j=1}^{n-1} \mathrm{tr}\ \boldsymbol{\chi}^{n-1-j}(\mathbf{d}\chi_\mu)\partial_\nu(\boldsymbol{\chi}^j). \quad \text{(A13)}$$

The factor $\mathbf{d}\chi_\mu$ contains double derivatives of G, which do not appear in our desired result. Therefore, we will separate out total derivatives in $\mathbf{d}$, which produce no flux on the (closed) Gaussian surfaces S_F on which the topological invariant is built [see Eq. (17)]. To do this, note that $\mathbf{d}^2 = 0$ and that, when using the product rule to expand these derivatives, a sign appears every time $\mathbf{d}$ moves past a $\boldsymbol{\chi}$. This gives

$$\mathbf{d}(\boldsymbol{\chi}^j) = \sum_{j'=0}^{j-1}(-1)^{j'}\boldsymbol{\chi}^{j'}(\mathbf{d}\boldsymbol{\chi})\boldsymbol{\chi}^{j-1-j'}$$
$$= \sum_{j'=0}^{j-1}(-1)^{j'+1}\boldsymbol{\chi}^{j+1} = \begin{cases} 0 & j\ \text{even} \\ -\boldsymbol{\chi}^{j+1} & j\ \text{odd} \end{cases}, \quad \text{(A14)}$$

which implies

$$\mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}(\mathbf{d}\chi_\mu)\partial_\nu(\boldsymbol{\chi}^j) = \begin{cases} \mathbf{d}\,\mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j) & j\ \text{even} \\ -\mathbf{d}\,\mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j) - \mathrm{tr}\ \boldsymbol{\chi}^{n-j}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j) + \mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}\chi_\mu\partial_\nu(\boldsymbol{\chi}^{j+1}) & j\ \text{odd} \end{cases} \quad \text{(A15)}$$

since n is odd. Then

$$\mathbf{T} = \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \mathbf{d}\sum_{j=1}^{n-1}(-1)^j\mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j) + \sum_{\substack{j=1 \\ j\ \text{odd}}}^{n-1}\left[\mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}\chi_\mu\partial_\nu(\boldsymbol{\chi}^{j+1}) - \mathrm{tr}\ \boldsymbol{\chi}^{n-j}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j)\right]$$
$$= \mathbf{d}\sum_{j=1}^{n-1}(-1)^j\mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j) + \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \sum_{j=1}^{n-1}(-1)^j\mathrm{tr}\ \boldsymbol{\chi}^{n-j}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j), \quad \text{(A16)}$$

where we have shifted the summation index in the last term. The total derivative is of no further interest, so we set $\mathbf{D}_1 = \mathbf{d}\sum_{j=1}^{n-1}(-1)^j\mathrm{tr}\ \boldsymbol{\chi}^{n-j-1}\chi_\mu\partial_\nu(\boldsymbol{\chi}^j)$. In the last term, expanding the derivative ∂_ν and using cyclicity gives

$$\mathbf{T} = \mathbf{D}_1 + \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \sum_{j=1}^{n-1}\sum_{m=1}^{j}(-1)^j\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\partial_\nu\boldsymbol{\chi}$$
$$= \mathbf{D}_1 + \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \sum_{m=1}^{n-1}\left[\sum_{j=m}^{n-1}(-1)^j\right]\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\partial_\nu\boldsymbol{\chi}$$
$$= \mathbf{D}_1 + \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \sum_{\substack{m=2 \\ m\ \text{even}}}^{n-1}\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\partial_\nu\boldsymbol{\chi}.$$

With $\partial_\nu\boldsymbol{\chi} = \mathbf{d}\chi_\nu + \boldsymbol{\chi}\chi_\nu - \chi_\nu\boldsymbol{\chi}$,

$$= \mathbf{D}_1 + \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu + \sum_{\substack{m=2 \\ m\ \text{even}}}^{n-1}\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\mathbf{d}\chi_\nu + \sum_{\substack{m=2 \\ m\ \text{even}}}^{n-1}\left[\mathrm{tr}\,\boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^m\chi_\nu - \mathrm{tr}\,\boldsymbol{\chi}^{n-m+1}\chi_\mu\boldsymbol{\chi}^{m-1}\chi_\nu\right]. \quad \text{(A17)}$$

Now, because n is odd and m is even,

$$\sum_{\substack{m=2\\ m\,\mathrm{even}}}^{n-1} \mathbf{d}\,\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\chi_\nu$$
$$= \sum_{\substack{m=2\\ m\,\mathrm{even}}}^{n-1} \big[-\mathrm{tr}\ \boldsymbol{\chi}^{n-m+1}\chi_\mu\boldsymbol{\chi}^{m-1}\chi_\nu$$
$$-\mathrm{tr}\ \boldsymbol{\chi}^{n-m}(\mathbf{d}\chi_\mu)\boldsymbol{\chi}^{m-1}\chi_\nu$$
$$+\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m}\chi_\nu + \mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\mathbf{d}\chi_\nu\big]$$
$$= \sum_{\substack{m=2\\ m\,\mathrm{even}}}^{n-1} \big[2\,\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\mathbf{d}\chi_\nu + \mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m}\chi_\nu$$
$$-\mathrm{tr}\ \boldsymbol{\chi}^{n-m+1}\chi_\mu\boldsymbol{\chi}^{m-1}\chi_\nu\big]\,, \quad \text{(A18)}$$

where the second equality follows from antisymmetry in μ and ν after a relabeling of the summation index in the second term of the first equality. This means

$$\mathbf{T} = \mathbf{D}_1 + \mathrm{tr}\ \boldsymbol{\chi}^{n}\chi_\mu\chi_\nu$$
$$+\frac{1}{2}\sum_{\substack{m=2\\ m\,\mathrm{even}}}^{n-1}\{\mathbf{d}\,\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m-1}\chi_\nu$$
$$+\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m}\chi_\nu$$
$$-\mathrm{tr}\ \boldsymbol{\chi}^{n-m+1}\chi_\mu\boldsymbol{\chi}^{m-1}\chi_\nu\}. \quad \text{(A19)}$$

We can collect the total derivatives as $\mathbf{D}_2$, shift the summation index in the last term, and rewrite $2\,\mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu = \mathrm{tr}\ \boldsymbol{\chi}^n\chi_\mu\chi_\nu - \mathrm{tr}\ \chi_\mu\boldsymbol{\chi}^n\chi_\nu$ to obtain

$$\mathbf{T} = \mathbf{D}_2 + \frac{1}{2}\sum_{m=0}^{n}(-1)^m\,\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m}\chi_\nu. \quad \text{(A20)}$$

Including $\mathbf{D}_2$ with the suppressed terms and restoring $\epsilon_{\mu\nu}$, this means that

$$\mathrm{Tr}\,\mathbf{X}^n = \int\frac{d\bar{s}dp_d}{8\pi i}\sum_{m=0}^{n}(-1)^m\epsilon_{\mu\nu}\mathrm{tr}\ \boldsymbol{\chi}^{n-m}\chi_\mu\boldsymbol{\chi}^{m}\chi_\nu + \ldots. \quad \text{(A21)}$$

This expression is sufficiently simple that we can return to the original, more explict notation:

$$\epsilon_{a_0a_1\ldots a_n}\mathrm{Tr}\,X_{a_1}\circ\cdots\circ X_{a_n}$$
$$= \int\frac{d\bar{s}dp_d}{8\pi i}\sum_{m=0}^{n}(-1)^m\epsilon_{\mu\nu}\epsilon_{a_0a_1\ldots a_n}$$
$$\times\,\mathrm{tr}\ \chi_{a_1}\ldots\chi_{a_{n-m}}\chi_\mu\chi_{a_{n-m+1}}\ldots\chi_{a_n}\chi_\nu + \ldots. \quad \text{(A22)}$$

The right-hand side has $2n!(n+1) = 2(n+1)!$ terms and is totally antisymmetric, while using the Levi-Civita symbol gives $(n+2)!$ terms. Therefore,

$$\epsilon_{a_0a_1\ldots a_n}\mathrm{Tr}\,X_{a_1}\circ\cdots\circ X_{a_n}$$
$$= \frac{1}{4\pi i(n+2)}\int d\bar{s}dp_d\,\epsilon_{a_0a_1\ldots a_{n+2}}\mathrm{tr}\ \chi_{a_1}\ldots\chi_{a_{n+2}} + \ldots, \quad \text{(A23)}$$

assuming that we choose to order the new indices appropriately.

Finally, it is important that the constant be correct:

$$C_d = -(2\pi i)^{-\frac{d}{2}-1}\frac{(d/2)!}{(d+1)!}$$
$$= (2\pi i)^{-1}\frac{d/2}{d(d+1)}\left[-(2\pi i)^{-\frac{d}{2}}\frac{(d/2-1)!}{(d-1)!}\right]$$
$$= \frac{1}{4\pi i(d+1)}C_{d-2}, \quad \text{(A24)}$$

so (substituting back $d = n+1$)

$$C_{d-2}\epsilon_{a_0a_1\ldots a_{d-1}}\mathrm{Tr}\,X_{a_1}\circ\cdots\circ X_{a_{d-1}}$$
$$= \frac{1}{4\pi i(d+1)}C_{d-2}\int d\bar{s}dp_d\,\epsilon_{a_0a_1\ldots a_{d+1}}\mathrm{tr}\,\chi_{a_1}\ldots\chi_{a_{d+1}}$$
$$+\ldots$$
$$= C_d\int d\bar{s}dp_d\,\epsilon_{a_0a_1\ldots a_{d+1}}\mathrm{tr}\ \chi_{a_1}\ldots\chi_{a_{d+1}} + \ldots, \quad \text{(A25)}$$

or

$$r_a = \int d\bar{s}dp_d\,n_a + \ldots. \quad \text{(A26)}$$

This is valid for values of a in $(\omega, \mathbf{p}^{d-1})$, but does not make sense for $a = \bar{s}$ or $a = p_d$ since $\mathbf{r}$ does not have such components.

We would like to calculate

$$\int d\mathbf{S}_f^{d+1}\cdot\mathbf{n}. \quad \text{(A27)}$$

We deform the sphere S_f to the space $S_F\times M$ where S_F is the sphere in the space $(\omega, \mathbf{p}^{d-1})$ and M is the entire space $(\mathbb{R}^2)$ spanned by p_d and $\bar{s}$. This can be termed a "hypercylinder," since a cylinder is the product of a circle (analogous to our sphere S_F) and a straight line (analogous to the flat space $M = \mathbb{R}^2$).

The flux of $\mathbf{n}$ through such a surface can be computed with only the components of $\mathbf{n}$ for which the relation Eq. (A26) holds. Part of that flux involves integration over $dsdp_d$, which then naturally leads to

$$\int d\mathbf{S}_f^{d+1}\cdot\mathbf{n} = \int d\mathbf{S}_F^{d-1}\cdot\int d\bar{s}dp_d\,\mathbf{n} = \int d\mathbf{S}_f^{d-1}\cdot\mathbf{r}, \quad \text{(A28)}$$

where Eq. (A26) was used. This is the result asserted in the text as Eq. (17).

Appendix B: Chiral systems in one dimensional space

We start by writing $\mathrm{Tr}\,\Sigma$ as

$$\mathrm{Tr}\,\Sigma = \mathrm{Tr}\,\Sigma\,\tilde{K}\circ\tilde{G}. \quad \text{(B1)}$$

Notice that this is true at arbitrary ω. We then take advantage of Eqs. (A3) and (A5) to rewrite this as

$$\frac{1}{4\pi i}\mathrm{tr}\,\Sigma\int d\bar{s}dp\left(G^{-1}\partial_{\bar{s}}GG^{-1}\partial_p G - G^{-1}\partial_p GG^{-1}\partial_{\bar{s}}G\right). \tag{B2}$$

The expression to be integrated is a total derivative and results, upon integrating, in

$$\mathrm{Tr}\,\Sigma = N_1(s=-L) - N_1(s=L), \tag{B3}$$

where N_1, defined in Eq. (23), is evaluated at $\bar{s}=-L$ and $\bar{s}=L$. This is indeed what is claimed in section IV. What remains is to remark that while these expressions are written at arbitrary ω, the limit $\omega\to 0$ is convenient as only in this limit $\mathrm{Tr}\,\Sigma$ counts zero energy states (and zeroes of Green's functions if there are interactions) localized at the boundary. This derivation can be used instead of the much more involved procedure reported in Ref. 9.

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