Chiral-Symmetric Higher-Order Topological Phases of Matter: Supplemental Material

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This Supplemental Material is divided into 4 sections. In Section I, we describe the structure of chiral-symmetric Hamiltonians and how to calculate the *winding number* in discrete periodic extended systems (i.e., lattice systems) in terms of a sublattice dipole moment operator, which will allow us to derive the general class of multipole chiral numbers in any dimension. In Section II, we enunciate the generalizations of these invariants for 2D and 3D, which label topological phases with higher-order topology. We also show that these invariants are strictly quantized under chiral symmetry, and provide expressions for them in the form of Bott index. Finally, we differentiate these invariants from other first-order topological indices that protect zero-dimensional states in 2D crystals. In Section III, we detail properties of the model proposed in the Main Text, and show the correspondence between the index N_{xy} and its corner states. Finally, in Section IV, we comment on the existence of bulk and boundary obstructions separating these phases.

I. Chiral-symmetric systems: general characteristics

Chiral-symmetric systems are described by Hamiltonians \mathcal{H} that obey

$$\Pi \mathcal{H} \Pi = -\mathcal{H},\tag{S1}$$

where Π is the *chiral operator*. The degrees of freedom in chiral-symmetric systems can be divided into two sublattices, A and B. The chiral operator is equal to

$$\Pi = \sum_{\mathbf{R},\alpha \in A} c^{\dagger}_{\mathbf{R},\alpha} \left| 0 \right\rangle \left\langle 0 \right| c_{\mathbf{R},\alpha} - \sum_{\mathbf{R},\beta \in B} c^{\dagger}_{\mathbf{R},\beta} \left| 0 \right\rangle \left\langle 0 \right| c_{\mathbf{R},\beta}.$$
(S2)

From now on, we will constrain our problem to the case in which the two sublattices have equal number of degrees of freedom, $N_A = N_B$. For an eigenstate of the Hamiltonian $|\psi_n\rangle$ with energy ϵ_n , there is a partner eigenstate $\Pi |\psi_n\rangle$ with opposite energy,

$$\mathcal{H}\Pi \left| \psi_n \right\rangle = -\Pi \mathcal{H} \left| \psi_n \right\rangle = -\epsilon_n \Pi \left| \psi_n \right\rangle. \tag{S3}$$

Thus, the energy spectrum of a chiral-symmetric system is symmetric with respect to zero energy.

In the basis in which the degrees of freedom are ordered so that those of sublattice A come first and then those of sublattice B, the chiral operator takes the form $\Pi = \sigma_z \otimes I_{N_A \times N_A}$, where σ_z the third Pauli matrix and $I_{n \times n}$ is the identity matrix of size n. In that same basis, the Hamiltonian takes the form

$$\mathcal{H} = \begin{pmatrix} 0 & h \\ h^{\dagger} & 0 \end{pmatrix}. \tag{S4}$$

The eigenstates of \mathcal{H} can be written as $|\psi\rangle = \frac{1}{\sqrt{2}}(\psi_n^A, \psi_n^B)^T$, where ψ_A and ψ_B are normalized vectors that exist only in the A, B subspaces, respectively. The chiral partner state with opposite energy is $\Pi |\psi_n\rangle = \frac{1}{\sqrt{2}}(\psi_n^A, -\psi_n^B)^T$. Evaluating $\mathcal{H}^2 |\psi_n\rangle = \epsilon_n^2 |\psi_n\rangle$ leads to the eigenvalue problems

$$(hh^{\dagger})\psi_n^A = \epsilon_n^2 \psi_n^A (h^{\dagger}h)\psi_n^B = \epsilon_n^2 \psi_n^B,$$
(S5)

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so that ψ_n^A and ψ_n^B can be easily obtained by diagonalizing hh^{\dagger} or $h^{\dagger}h$, respectively. Equation (S5) has a structure compatible with a singular value decomposition. Indeed, it is possible to write h as

$$h = U_A \Sigma U_B^{\dagger} \tag{S6}$$

where U_A is a unitary matrix representing the space spanned by $\{\psi_n^A\}$, i.e., $U_A = (\psi_1^A, \psi_2^A, \dots, \psi_{N_A}^A)$ and similarly for U_B , and Σ is a diagonal matrix containing the singular values. Notice, for example, that

$$hh^{\dagger} = U_A \Sigma^2 U_A^{\dagger}$$

$$h^{\dagger}h = U_B \Sigma^2 U_B^{\dagger}$$
(S7)

which are compatible with Eq. (S5) if we identify the squared energies $\{\epsilon_n^2\}$ with the square of the singular values in Σ .

In what follows, it will be convenient to have a 'flattened' version of Hamiltonian (S4), given by

$$\mathcal{H} = \begin{pmatrix} 0 & q \\ q^{\dagger} & 0 \end{pmatrix}, \quad q = U_A U_B^{\dagger}, \tag{S8}$$

whose energies are $\epsilon_n = \pm 1$. The flattening was achieved by dropping the singular value matrix Σ in the definition of q in Eq. (S8). Contrast this with the equivalent expression in Eq. (S6) for Hamiltonian (S4). Although the Hamiltonians (S4) and (S8) represent different systems, those two systems will belong to the same topological phase. We will see, however, that Hamiltonian (S8) facilitates the calculation of the topological invariants associated with its topological phase.

A. The winding number as a sublattice polarization

We now turn our attention to chiral-symmetric Hamiltonians that are extended and periodic (i.e., lattice systems). These systems have topological phases labelled by an integer invariant, known as the *winding number*. Since topological properties of a topological phase are preserved under adiabatic deformations, i.e., those deformations that preserve the energy gap and symmetry, let us consider, without loss of generality, a flattened version of Hamiltonian (S4) at each crystal momentum k,

$$\mathcal{H}(k) = \begin{pmatrix} 0 & q(k) \\ q(k)^{\dagger} & 0 \end{pmatrix}, \quad q(k) = U_A(k)U_B^{\dagger}(k), \tag{S9}$$

where $\mathcal{H}(k)$ is a Bloch Hamiltonian with a *flat* energy spectrum $\epsilon = \pm 1$ at all k. The winding number, which classifies different homotopy classes $\pi_1[U(n)] \cong \mathbb{Z}$ in 1D, is given by

$$N_x = \frac{\mathrm{i}}{2\pi} \int_{-\pi}^{\pi} \operatorname{Tr}\left[q(k)^{\dagger} \partial_k q(k)\right] dk \in \mathbb{Z}.$$
(S10)

By replacing $q(k) = U_A(k)U_B^{\dagger}(k)$ in Eq. (S10), we have

$$N_x = \frac{\mathrm{i}}{2\pi} \int_{-\pi}^{\pi} \mathrm{Tr} \left[U_A^{\dagger}(k) \partial_k U_A(k) \right] dk + \frac{\mathrm{i}}{2\pi} \int_{-\pi}^{\pi} \mathrm{Tr} \left[U_B(k) \partial_k U_B^{\dagger}(k) \right] dk.$$
$$= -\frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{Tr} \left[\mathcal{A}_A(k) \right] dk + \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{Tr} \left[\mathcal{A}_B(k) \right] dk.$$
(S11)

Here $\mathcal{A}_A(k) = -iU_A^{\dagger}(k)\partial_k U_A(k)$ is the Berry connection in the A sublattice, as is \mathcal{A}_B for the B sublattice. In the second step we have used $\operatorname{Tr}[U^{\dagger}(k)\partial_k U(k)] = -\operatorname{Tr}[U(k)\partial_k U^{\dagger}(k)]$. Notice that Eq. (S11) is not defined mod 1.

B. Winding number in discrete space

We now seek to derive an expression equivalent to the winding number but in real space instead of momentum space. Such an expression would enable the characterization of disordered lattices. A first step is to discretize Eq. (S11). For that purpose, consider the following expression,

$$U^{\dagger}(k)\partial_k U(k) \approx U^{\dagger}(k)(U(k+\delta k) - U(k))/\delta k$$

valid as $\delta k \to 0$. Rearranging this expression,

$$I + \delta k U^{\dagger}(k) \partial_k U(k) \approx U^{\dagger}(k) U(k + \delta k).$$

Taking the logarithm on both sides, and using the approximation $Log(1 + x) \approx x$ on the LHS, we have

$$\delta k U^{\dagger}(k) \partial_k U(k) \approx \log(U^{\dagger}(k)U(k+\delta k)).$$
 (S12)

Let us now use this expression on Eq. (S11) to have a discretized version of it,

$$N_{x} = \frac{\mathrm{i}}{2\pi} \sum_{k} \operatorname{Tr} \left[\operatorname{Log}(U_{A,k}^{\dagger} U_{A,k+\delta k}) - \operatorname{Log}(U_{B,k}^{\dagger} U_{B,k+\delta k}) \right]$$
$$= \frac{1}{2\pi \mathrm{i}} \sum_{k} \operatorname{Tr} \operatorname{Log} \left[F_{A,k} F_{B,k}^{\dagger} \right],$$
(S13)

where in the last step we used the fact that, for a unitary matrix M, $Log(M) = -Log(M^{\dagger})$. The unitary matrices $F_{S,k}$ are determined by first considering the matrices

$$G_{\mathcal{S},k} = U_{\mathcal{S},k+\delta k}^{\dagger} U_{\mathcal{S},k},\tag{S14}$$

which are not unitary due to the discretization of k [1]. To restore unitativy, consider the singular value decomposition

$$G_{\mathcal{S},k} = V_{\mathcal{S},k} D_{\mathcal{S},k} W^{\dagger}_{\mathcal{S},k}, \tag{S15}$$

where $D_{S,k}$ is the diagonal matrix containing the singular values. In the thermodynamic limit, $D_{S,k}$ is the identity matrix. For finite L, on the other hand, the magnitud of the diagonal elements of $D_{S,k}$ are less than 1. We define

$$F_{\mathcal{S},k} = V_{\mathcal{S},k} W_{\mathcal{S},k}^{\dagger} \tag{S16}$$

which is unitary.

C. Winding number in position space

Having discretized the expression for the winding number for the case in which the momenta is discrete, we now derive the position space version of the winding number [2]. For that purpose, consider the second-quantization operators for the anihilation of electrons in real space and crystal momentum space, which are related by the Fourier transform

$$c_{R,\alpha} = \frac{1}{\sqrt{L}} \sum_{k} e^{-ikR} c_{k,\alpha},$$

$$c_{k,\alpha} = \frac{1}{\sqrt{L}} \sum_{R} e^{ikR} c_{R,\alpha}.$$
(S17)

To enforce periodic boundary conditions, we impose the constraint

$$c_{R+L,\alpha} = c_{R,\alpha} \to k = \frac{2\pi}{L}m, \ m \in \mathbb{Z},$$
(S18)

which means that in Eq. (S17), $k \in \delta_k(0, 1, \dots L - 1)$, where $\delta_k = 2\pi/L$.

To determine the winding number, we will need to make use of the operator associated with polarization [3] defined

over each sublattice $\mathcal{S} = A, B$ [2],

$$\hat{P}_{x}^{\mathcal{S}} = \sum_{R,\alpha\in\mathcal{S}} c_{R,\alpha}^{\dagger} \left|0\right\rangle \exp\left[-\mathrm{i}\frac{2\pi}{L}R\right] \left\langle 0\right| c_{R,\alpha}.$$
(S19)

This operator can be written in momentum space as

$$\hat{P}_{x}^{\mathcal{S}} = \sum_{k,\alpha\in\mathcal{S}} c_{k+\delta_{k},\alpha}^{\dagger} \left|0\right\rangle \left\langle 0\right| c_{k,\alpha}.$$
(S20)

The action of $\hat{P}_x^{\mathcal{S}}$ on a state $|k, \alpha\rangle = c_{k,\alpha}^{\dagger} |0\rangle$ is to shift the momentum of the state on sublattice \mathcal{S} , i.e., $\hat{P}_x^{\mathcal{S}} |k, \alpha\rangle = |k + \delta_k, \alpha\rangle$.

In what follows, we show that the most general expression for the winding number is

$$N_x = \frac{1}{2\pi i} \operatorname{TrLog}\left(\bar{P}_x^A \bar{P}_x^{B\dagger}\right)$$
(S21)

where $\bar{P}_x^{\mathcal{S}} = U_{\mathcal{S}}^{\dagger} P_x^{\mathcal{S}} U_{\mathcal{S}}.$

For that purpose, we will transform Eq. (S21) into crystal momentum space and show that it reduces to Eq. (S13). For that purpose, let us consider the projectors into sublattice S

$$\mathcal{P}_{\mathcal{S}} = \sum_{n,k,\alpha,\beta} [u_{n,k}^{\mathcal{S}}]_{\alpha} c_{k,\alpha}^{\dagger} |0\rangle \langle 0| c_{k,\beta} [u_{n,k}^{\mathcal{S}}]_{\beta}^{*},$$
(S22)

where $[u_{n,k}^{\mathcal{S}}]_{\alpha}$ denotes the α th component of the *n*th singular state in the SVD decomposition of Eq. (S6), corresponding to the *n*th column of $U_{\mathcal{S}}$, for $\mathcal{S} = A$ or B, and * denotes complex conjugation. Written compactly, $\mathcal{P}_{\mathcal{S}} = U_{\mathcal{S}}U_{\mathcal{S}}^{\dagger}$. Similarly, we can spell out $q = U_A U_B^{\dagger}$ [Eq. (S8)] as

$$q = \sum_{n,k,\alpha,\beta} [u_{n,k}^A]_{\alpha} c_{k,\alpha}^{\dagger} |0\rangle \langle 0| c_{k,\beta} \cdot [u_{n,k}^B]_{\beta}^*$$
(S23)

We need to calculate $\mathcal{P}_A P_x^A q P_x^{B\dagger} \mathcal{P}_B = U_A U_A^{\dagger} P_x^A U_A U_B^{\dagger} P_x^{B\dagger} U_B U_B^{\dagger}$. First, let us calculate

$$\mathcal{P}_{A}P_{x}^{A} = \sum_{n,k,\alpha} \left| u_{n,k+\delta k}^{A} \right\rangle \left[u_{n,k+\delta k}^{A} \right]_{\alpha}^{*} \left\langle 0 \right| c_{k,\alpha}$$

$$P_{x}^{B\dagger} \mathcal{P}_{B} = \sum_{n,k,\alpha} c_{k,\alpha}^{\dagger} \left| 0 \right\rangle \left[u_{n,k+\delta k}^{B} \right]_{\alpha}^{*} \left\langle u_{n,k+\delta k}^{B} \right|, \qquad (S24)$$

where $\left|u_{n,k}^{S}\right\rangle = \sum_{\alpha} [u_{n,k}^{S}]_{\alpha} c_{k,\alpha}^{\dagger} \left|0\right\rangle$. Using Eqs. S23 and S24, we have

$$\mathcal{P}_{A}P_{x}^{A}qP_{x}^{B\dagger}\mathcal{P}_{B} = \sum_{k,n,m,l} \sum_{\alpha,\beta} \left| u_{n,k+\delta k}^{A} \right\rangle [u_{n,k+\delta k}^{A}]_{\alpha}^{*} [u_{m,k}^{A}]_{\alpha} [u_{m,k}^{B}]_{\beta}^{*} [u_{l,k+\delta k}^{B}]_{\beta} \left\langle u_{l,k+\delta k}^{B} \right|$$

$$= \sum_{k,n,m,l} \left| u_{n,k+\delta k}^{A} \right\rangle [F_{A,k}]_{n,m} [F_{B,k}^{\dagger}]_{m,l} \left\langle u_{l,k+\delta k}^{B} \right|$$

$$= \sum_{k,n,l} \left| u_{n,k+\delta k}^{A} \right\rangle [F_{A,k}F_{B,k}^{\dagger}]_{n,l} \left\langle u_{l,k+\delta k}^{B} \right|$$

$$= \sum_{k,n,l} \left| u_{n,k}^{A} \right\rangle [F_{A,k-\delta k}F_{B,k-\delta k}^{\dagger}]_{n,l} \left\langle u_{l,k}^{B} \right|. \tag{S25}$$

The expression (S25) implies that $\bar{P}_x^A \bar{P}_x^{B\dagger} = U_A^{\dagger} P_x^A U_A U_B^{\dagger} P_x^{B\dagger} U_B$ takes the form

$$\bar{P}_{x}^{A}\bar{P}_{x}^{B\dagger} = \begin{pmatrix} F_{A,k_{0}}F_{B,k_{0}}^{\dagger} & 0 & \dots & 0\\ 0 & F_{A,k_{1}}F_{B,k_{1}}^{\dagger} & \dots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \dots & F_{A,k_{L-1}}F_{B,k_{L-1}}^{\dagger} \end{pmatrix}.$$
(S26)

Notice that the matrix is diagonal in k. Therefore, we have

$$N_{x} = \frac{1}{2\pi i} \operatorname{TrLog} \left(\bar{P}_{x}^{A} \bar{P}_{x}^{B\dagger} \right)$$
$$= \frac{1}{2\pi i} \sum_{k} \operatorname{TrLog} \left[F_{A,k} F_{B,k}^{\dagger} \right]$$
(S27)

which is identical to the expression for the winding number (S13).

In contrast, the invariant that protects the quantization of the dipole moment in chiral-symmetric insulators at half-filling is

$$p_x = -\frac{1}{2\pi} \operatorname{ImLog}[\operatorname{Det}(U_{\operatorname{occ}}^{\dagger} P_x U_{\operatorname{occ}}) \operatorname{Det}(P_x^{\dagger 1/2})],$$
(S28)

where U_{occ} is the subspace of occupied bands at half filling and $P_x = \sum_{R,\alpha} |R, \alpha\rangle \mathcal{U}_D(R) \langle R, \alpha|$ is the position operator defined over the entire lattice [3]. The dipole moment invariant is quantized to $p_x = 0$ or 1/2 under chiral symmetry, and is related to the winding number by the expression $p_x = N_x/2 \mod 1$.

II. Generalizations of the winding number to higher-order topological systems with chiral symmetry

As stated in the Main Text, we generalize the invariant (S21) to 2D and 3D. In 2D, the invariant is

$$N_{xy} = \frac{1}{2\pi i} \operatorname{TrLog}\left(\bar{Q}_{xy}^{A} \bar{Q}_{xy}^{B\dagger}\right) \in \mathbb{Z}$$
(S29)

where $\bar{Q}_{xy}^{S} = U_{S}^{\dagger} Q_{xy}^{S} U_{S}$ for S = A, B, and Q_{xy}^{S} is the sublattice quadrupole moment operator

$$Q_{xy}^{\mathcal{S}} = \sum_{\mathbf{R},\alpha\in\mathcal{S}} |\mathbf{R},\alpha\rangle \operatorname{Exp}\left(-\mathrm{i}\frac{2\pi xy}{L_x L_y}\right) \langle \mathbf{R},\alpha| \,.$$
(S30)

Similarly, in 3D the invariant is

$$N_{xyz} = \frac{1}{2\pi i} \operatorname{TrLog}\left(\bar{O}_{xyz}^{A} \bar{O}_{xyz}^{B\dagger}\right) \in \mathbb{Z}$$
(S31)

where $\bar{O}_{xyz}^{S} = U_{S}^{\dagger}O_{xyz}^{S}U_{S}$, for S = A, B, and O_{xyz}^{S} is the sublattice octupole moment operator

$$O_{xyz}^{\mathcal{S}} = \sum_{\mathbf{R}, \alpha \in \mathcal{S}} |\mathbf{R}, \alpha\rangle \operatorname{Exp}\left(-\mathrm{i}\frac{2\pi xyz}{L_x L_y L_z}\right) \langle \mathbf{R}, \alpha|, \qquad (S32)$$

A. Quantization of the real space invariants

The invariants (S21), (S29), and (S31) take the form

$$N = \frac{1}{2\pi i} \operatorname{TrLog} \left(U_A^{\dagger} M_A U_A U_B^{\dagger} M_B^{\dagger} U_B \right)$$
(S33)

where $M_{\mathcal{S}}$ (for $\mathcal{S} = A, B$) is $P_x^{\mathcal{S}}, Q_{xy}^{\mathcal{S}}$, or $O_{xyz}^{\mathcal{S}}$ in 1D, 2D, or 3D, respectively. Notice that since the matrices $M_{\mathcal{S}}$ and $U_{\mathcal{S}}$ are unitary, we have

$$\operatorname{Det}(U_A^{\dagger} M_A U_A U_B^{\dagger} M_B^{\dagger} U_B) = \operatorname{Det}(M_A M_B^{\dagger}) = 1,$$
(S34)

where in the last step we use the fact that $M_x^A = M_x^B$, which is true because the two sublattices have (i) equal number of degrees of freedom in each unit cell and (ii) the same number of unit cells, from which it follows that M_A and M_B are identical. From (S34) it follows that tracing the logarithm of $U_A^{\dagger}M_A U_A U_B^{\dagger}M_B^{\dagger}U_B$ in (S33) will necessarily have to give a phase that is a multiple of $2\pi i$, i.e., it will be of the form $2\pi iN$, with $N \in \mathbb{Z}$. This integer N is indeed the topological invariant.

B. Real space invariants written as a Bott index

Starting again with Eq. S33, and performing a unitary transformation using U_B of the matrix product on the interior of the matrix logarithm, we can rewrite (S33) as

$$N = \frac{1}{2\pi i} \text{TrLog} \left(U_B U_A^{\dagger} M_A U_A U_B^{\dagger} M_B^{\dagger} U_B U_B^{\dagger} \right).$$
(S35)

Noting the definition of $q = U_A U_B^{\dagger}$ and again that $M_A = M_B = M$ are unitary (see discussion in previous section),

$$N = \frac{1}{2\pi i} \operatorname{TrLog} \left(q^{-1} M_A q M_B^{\dagger} \right)$$

= $\frac{1}{2\pi i} \operatorname{TrLog} \left(q^{-1} M q M^{-1} \right)$
= $\operatorname{Bott}(q^{-1}, M).$ (S36)

C. Topological protection of zero-dimensional states of first-order topolgy

Chiral-symmetric systems can also protect zero-dimensional states at topological defects. For a point defect in d dimensions, $q(\mathbf{k}, \mathbf{r})$ in Eq. (S4) is parametrized by d momentum variables \mathbf{k} and d-1 position variables \mathbf{r} , and the number of protected states is given by the homotopy class $\pi_{2d-1}[U(N)] = \mathbb{Z}$ into which $q(\mathbf{k}, \mathbf{r})$ falls [4], such as in the 2D Jackiw and Rossi lattice model for the protection of 0D topological states bound to vortices. Nontrivial homotopies exist only in odd dimensional manifolds, and thus rule out, for example, the protection of 0D states at the corners of 2D crystals. In contrast, our invariants, Eqs. (5) and (6) of the Main Text (Eq. (S29) and (S31) here), allow for such protection, and thus are of different nature than first-order topological indices based on homotopy classes.

III. The extended QTI model

In this section we describe in detail certain characteristics of the QTI model with long-range hopping terms (Eq. (7), (8), and (9) in the Main Text). We show (A) how these phases are in general outside the framework of topological quantum chemistry [5, 6], (B) how the phase diagram is modified when the horizontal hopping terms are different from the vertical ones, (C) the support of the corner states, (D) the correspondence between the topological index N_{xy} [Eq. (5) in the Main Text, or Eq. (S29) here] and the number and chiral charge of the corner states, (E) some subtleties regarding how the phase diagrams in the Main Text were determined, and (F) the convergence of our results with disorder with system size.

A. Symmetry representations of the topological phases

The extended QTI model has the Hamiltonian of Eq. (S4) with off-diagonal term

$$h(\mathbf{k}) = h_{QTI}(\mathbf{k}) + C_s h_{SLR}(\mathbf{k}) + C_d h_{DLR}(\mathbf{k})$$
(S37)

where $h_{\text{QTI}}(\mathbf{k})$, $h_{\text{SLR}}(\mathbf{k})$, and $h_{\text{DLR}}(\mathbf{k})$ are defined in Eqs. (7), (8), and (9) of the Main Text.

Consider the case $C_s = 1$, $C_d = 0$. In that case, the Hamiltonian is C_{4v} symmetric and supports bulk-obstructed topological phases. At high-symmetry points (HSPs) and lines of the BZ, the representations of the elements of C_{4v} are given in Table S1. To capture more directly the topological protection due to crystalline symmetries, Table S1 also shows the symmetry indicator invariants, defined as

$$[M_j] = \#M_j - \#\Gamma_j \tag{S38}$$

where $\#M_j$ is the number of bands below the gap with C_4 symmetry representations $M_j = e^{i\pi(2j-1)/4}$, for j = 1, 2, 3, 4, at the **M** point of the BZ, and similarly for the Γ point.

phase	irreps at Γ	irreps at ${\bf M}$	$([M_1], [M_2], [M_3], [M_4])$
$N_{xy} = 0$	$\{e^{i3\pi/4}, e^{-i3\pi/4}\}$	$\{e^{i3\pi/4}, e^{-i3\pi/4}\}$	(0,0,0,0)
$N_{xy} = 1$	$\{e^{i3\pi/4}, e^{-i3\pi/4}\}$	$\{e^{i\pi/4}, e^{-i\pi/4}\}$	(1, -1, -1, 1)
$N_{xy} = 4$	$\{e^{i3\pi/4}, e^{-i3\pi/4}\}$	$\{e^{i3\pi/4}, e^{-i3\pi/4}\}$	$(0,\!0,\!0,\!0)$

TABLE S1. C_4 symmetry representations and symmetry indicator invariants (S38) for the lowest two bands of Hamiltonian (S37) at the C_4 invariant points of the BZ Γ and **M** for all topological phases. At all C_2 -invariant points, the representations are $\pm i$. Similarly, at all M_x and M_y invariant lines, the representations are ± 1 . In both cases, those representations lead to trivial symmetry indicator invariants for C_2 and reflection symmetries.

A result worth noting from Table S1 is that, while the $N_{xy} = 1$ phase (i.e., the QTI nontrivial phase with $q_{xy} = e/2$) has nontrivial symmetry indicator invariants, the $N_{xy} = 4$ does not. Consequently, the topology of this last phase cannot be captured by the theory of induction of representations and symmetry indicator invariants [5, 6]. Nevertheless, its nontrivial nature is evident in both the existence of a nonvanishing bulk invariant $N_{xy} = 4$ and the existence of an equal number of topological zero-energy states at each corner [Fig. 1(d) of the Main Text and Fig. S2 here].

The representations due to C_2 symmetry and reflection symmetries are equal at all HSPs of the BZ in all phases, and thus have trivial symmetry indicator invariants.

B. Phase diagram for the ordered C_{2v} symmetric system

In the interest of completeness, in Fig. S1 we show the phase diagram for a system which is C_{2v} symmetric, with $w_{m,x} = 3w_{m,y}$, $w_D = 0$, and $w_{m\geq 0} = 0$.



FIG. S1. Phase diagram of the chiral-symmetric second-order topological phase, N_{xy} (left), and the quadrupole phase q_{xy} (right), for a C_{2v} symmetric system with open boundaries as a function of the hopping ratios, $w_{1,y}/v$ and $w_{2,y}/v$, with $w_{m,x} = 3w_{m,y}$ and $w_D = 0$. Phase transitions where the boundary band gap closes along the x edge are shown in green, while those which close along the y edge are shown in cyan.

C. Corner states and their support

In this section, we show the form and localization of two sets of corner states for phases indicated in the Main Text. First, in Fig. S2, we show one possible choice of the four corner-localized states of the lattice considered in Fig. 1 in the Main Text with $N_{xy} = 4$. As can be seen, the summation of the probability density functions of the four orthogonal states equals that of the total set of four states in a single corner, as shown in the Main Text. Second, in Fig. S3 we show the probability density function of the corner states of a $N_{xy} = -1$ phase from the system considered in Fig. 2 in the Main Text. Notice that the corner states have support on the opposite sublattice as those in the $N_{xy} = 4$ phase (Fig. S2) due to the reversal in the sign of the bulk index N_{xy} .



FIG. S2. Probability density functions of the four corner states at one of the corners of a $N_{xy} = 4$ phase (four left plots) and cumulative PDF for all the four states (rightmost plot). Support at each sublattice is indicated by blue and red colors, respectively. All corner states in the same corner have the same chiral charge and thus have support on only one sublattice. In this simulation, v = 1, $w_1 = 2$, $w_2 = 2$, $w_D = 0$.



FIG. S3. Probability density functions of all the corner states of a $N_{xy} = -1$ phase (4 states in total, one per corner). Support at each sublattice is indicated by blue and red colors, respectively. In this simulation, v = 1, $w_1 = 1$, $w_2 = 0.8$, $w_D = 0.5$.

D. Correspondence between N_{xy} , band gap closings, and corner states

To claim that the multipole chiral numbers introduced here are the topological invariant connected with the appearance of corner-localized modes across a band gap closing, one must show that all three phenomena are causally connected. In other words, changes in either N_{xy} or the number (or type) of corner-localized modes necessarily imply a change in other quantity, and moreover that these changes can only occur at a band gap closing.

To support this claim, Fig. S4(a-d) presents numerical simulations of all three of these quantities, N_{xy} , the distribution of states in energy, and the bulk band gap, for the long-range quadrupole topological insulator model considered in Fig. 1(b) of the Main Text with fixed $w_1/v = 0.4$. As can be seen, the closing of the bulk band gap at $w_2/v = 1$ coincides with 8 states departing from each of the upper and lower bulk bands and becoming pinned at $\epsilon = 0$. These 16 states in total are those corner-localized states shown in Fig. 1(d) of the Main Text, which are predicted to exist as $N_{xy} = 4$ for $w_2/v > 1$. The slight discrepancy between the change in N_{xy} and the closing of the bulk band gap is due to finite system effects, where the topological invariant does not change until the bulk band gap is larger that the approximate coupling strength between the corner states in adjacent corners.

In Fig. S4(e-i), we show this same correspondence for the quadrupole topological insulator with both long-range straight and long-range diagonal hoppings considered in Fig. 2(b) of the Main Text with fixed $w_1/v = 0.8$. As w_2/v is increased from 0 to 2, this system undergoes three separate phase transitions. The first transition, $N_{xy} = 1 \rightarrow -1$ near $w_2/v = 0.4$, occurs at a closing of the edge band gap, not the bulk band gap. This particular phase transition also does not change the number of corner-localized states, as there is only one state localized to each corner in both phases. Rather, across the phase transition, the corner states swap the sublattices on which they are supported. The



FIG. S4. Correspondence between the appearance of zero energy states, change in the topological invariant N_{xy} , and the closing of the bulk and edge band gaps for two of the systems considered in the Main Text in Figs. 1(b) and 2(a). (a) Copy of Fig. 1(b) from the Main Text, red line indicates the choice of w_1/v and w_2/v in (b-d). (b) Number of states relative to their energy and w_2/v calculated with open boundary conditions. (c) N_{xy} as a function of w_2/v calculated using open boundary conditions. (d) Bulk band gap, $\Delta \epsilon$ as a function of w_2/v calculated using periodic boundary conditions. (e-h) Similar to (a-d), except for the system in Fig. 2(a) of the Main Text. (i) Edge band gap calculated using a semi-open boundary, i.e. periodic in x, but open in y. In all simulations of both systems, the system size was 80×80 unit cells.

other two phase transitions, $N_{xy} = -1 \rightarrow 0$ and $N_{xy} = 0 \rightarrow 4$, both occur when the bulk band gap closes, and result in changes in the number of corner-localized states. Again, discrepancies between the change in N_{xy} from the band gap closings are due to finite system size effects. There are some subtleties in how the phase diagrams shown in Figs. 1(b) and 2(a) of the Main Text are constructed due to finite system size effects. As was shown in Fig. S4, computing the topological invariants N_{xy} in finite systems causes the topological invariant not to change at exactly the same location where the band gap closes. Moreover, it is not numerically feasible to calculate an entire 2D phase diagram at a reasonable sampling density even at the system sizes shown in Fig. S4 (80 × 80 unit cells), due to the memory requirements necessary to calculate the full singular value decomposition of H. In the definition of N_{xy} , every single singular value is necessary to achieve accurate results.

As such, the phase diagrams shown in Figs. 1b, 2a, and 2b are constructed by first finding closings in the bulk and edge band structures, assuming the system is infinite in any non-open direction. Numerically, artifacts can appear in the calculation of the band gap closings due to finite system sizes, as shown in Fig. S5, but simulations strongly suggest that the phase diagrams converge to those shown in the Main Text in the thermodynamic limit. Then, we calculate N_{xy} within each region at an ensemble of points using open boundaries in all directions and using large system sizes. We also verify these calculations through direct calculation of N_{xy} across the entire 2D parameter space but using smaller system sizes.



FIG. S5. Bulk band gaps of the C_{4v} symmetric system considered in Fig. 1(b) of the Main Text calculated using periodic boundary conditions with the spacing between adjacent points in the Brillouin zone being $\delta k = 0.1$ (left) and $\delta k = 0.025$ (right).

F. Finite system size effects in disordered systems

Another manifestation of the difficulties associated with finite system sizes is in calculating the topological invariant and band gaps for disordered systems. In Fig. S6 we show the variation and (slow) convergence of both the topological invariant, N_{xy} , as well as the bulk and edge band gaps as a function of system size. Here, the system contains some disorder with a fixed strength, W/v = 4.8, with W defined in the Main Text. The underlying system possess C_{4v} symmetry, with $W_1/v = 1$ and $w_2/v = 4$, while the added disorder breaks all of the system's symmetries (including C_4) except for chiral symmetry. Only a single realization of the disorder is shown here at each system size.

IV. Bulk and boundary energy gap closing at phase transitions

As shown in the Main Text, the phase transitions between phases of different multipole chiral numbers close the gap at either the boundary or the bulk. This has to be the case since changing the winding number across the phase transition goes hand in hand with the delocalization of the topological corner states, which necesitates extended gapless channels. The existence of these gapless extended channels is necessary because the hybridization of topological states away from zero energy can only occur by fusing pairs of topological states having opposite chiral charge, and such pairs do not exist within any single corner.

This is illustrated in Fig. S7. At the phase transition critical points, the bulk (a) or edges (b,c) close the energy gap, allowing the topological corner states to delocalize and hybridize away from zero energy. In (a), a C_4 symmetric lattice within a bulk-obstructed phase transition hybridizes corner states via bulk low energy channels, reducing the bulk invariant by 1. In (b), a C_4 symmetric boundary-obstructed phase transition hybridize the corner states via the boundary, reducing the bulk invariant by 2. In (c), a C_2 symmetric boundary obstructed transition reduces the bulk invariant by 1.



FIG. S6. Dependence of the topological invariant N_{xy} , the bulk band gap, and the two edge band gaps on the number of unit cells per side in a square lattice. The underlying system has C_{4v} symmetry, while the added disorder breaks all of the symmetries (including C_4) except for chiral symmetry.



FIG. S7. Schematics that illustrates the hybridization of topological corner states during phase transitions. Red and blue dots represent topological corner states of opposite chiral charge. Topological corner states hybridize only if they have opposite chiral charge and bulk (a) or edge (b,c) low energy channels are available for their delocalization.

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