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Chiral-symmetric higher-order topological phases protected by multipole winding number invariants

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Abstract: We introduce novel higher-order topological phases in chiral-symmetric systems protected by multipole winding numbers, bulk integer topological invariants that can yield multiple topological states per corner. © 2021 The Author(s)

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Higher-order topological band theory [1, 2] has expanded the classification of topological phases of matter across insulators, semimetals, and superconductors. This theory generalizes the bulk-boundary correspondence of topological phases, so that an nth-order topological phase in d dimensions has protected features, such as gapless states or fractional charges, only at its $(d-n)$-dimensional boundaries. Currently, two complementary mechanisms explain the existence of higher-order topological phases (HOTPs); (1) corner-induced filling anomalies [3] which arise due to certain Wannier center configurations, and (2) boundary mass domain arguments [2]. While the first mechanism is responsible for the fractional quantization of corner charge, the second one predicts the existence of single in-gap states at corners. However, neither of these mechanisms allows for HOTPs that protect multiple states at each corner. Yet, in principle, such phases should exist. In first-order topology, for example, phases with multiple degenerate mid-gap states exist in 1D chiral symmetric systems (class AIII in the tenfold classification [4]), whose topological phases are identified by a *winding number*, an integer topological invariant that – unlike the Wannier center and mass domain mechanisms – can protect several zero-energy states at each boundary.

In this presentation, we show the existence of a $\mathbb{Z}$ classification for HOTPs in chiral-symmetric systems (class AIII) and identify the topological invariants in 2D and 3D that protect them [5]. We refer to these invariants as *multipole winding numbers* (MWNs) because they are built from sublattice multipole moment operators and are a generalization of the 1D winding number to higher dimensional systems. These invariants are calculated in the bulk of the crystal, i.e., with periodic boundary conditions, and their integer values coincide with the number of degenerate zero-energy states at each corner of a crystal with open boundaries. Thus, MWNs provide a novel higher-order bulk-boundary correspondence for topological phases of matter. We show that phases with nonzero MWNs are in general boundary-obstructed, and probe their remarkable robustness in the presence of chiral symmetry-preserving disorder. The existence of phases with MWNs reveals a richer classification of HOTPs and provides a broader understanding of boundary-obstructed topological phases beyond the Wannier center and mass domain perspectives.

We thus focus our attention on chiral symmetric Hamiltonians $\mathscr{H}$, which satisfy $\Pi\mathscr{H}\Pi = -\mathscr{H}$, where Π is the chiral operator, which allows a partition of the lattice into two sublattices, A and B, with opposite chiral charge. The eigenstates of $\mathscr{H}$ can be written as $|\psi_n\rangle = (1/\sqrt{2})(\psi_n^A, \psi_n^B)^T$, where ψ_n^A and ψ_n^B are normalized vectors that exist only in the A, B subspaces, respectively. In the basis in which the chiral operator is $\Pi = \tau_z$, $\mathscr{H} = [0, h; h^\dagger, 0]$, and the energies, ε_n, can be solved for using singular value decomposition (SVD), $h = U_A \Sigma U_B^\dagger$. Here, where $U_{\mathscr{S}}$, for $\mathscr{S} = A, B$, is a unitary matrix representing the space spanned by $\{\psi_n^{\mathscr{S}}\}$, and Σ is a diagonal matrix containing the singular values. Using this decomposition, it follows that $hh^\dagger = U_A \Sigma^2 U_A^\dagger$ and $h^\dagger h = U_B \Sigma^2 U_B^\dagger$, so that the squared energies $\{\varepsilon_n^2\}$ correspond to the squared singular values in Σ^2.

To derive the MWNs for higher-order topological phases, consider a lattice in 2D (3D) with L_i unit cells along direction $i = x, y$ ($i = x, y, z$). Each unit cell is labelled by $\mathbf{R} = (x, y)$ [$\mathbf{R} = (x, y, z)$] and has N_T orbitals (or, more generally, N_T internal degrees or freedom). To build the topological indices for chiral symmetric higher-order topological phases in the basis $\{|\mathbf{R}, \alpha\rangle\}$, we define the following sublattice multipole moment operators

$$Q_{xy}^{\mathscr{S}} = \sum_{\mathbf{R}, \alpha \in \mathscr{S}} |\mathbf{R}, \alpha\rangle \,\mathrm{Exp}\left(-\mathrm{i}\frac{2\pi xy}{L_x L_y}\right) \langle \mathbf{R}, \alpha|, \qquad O_{xyz}^{\mathscr{S}} = \sum_{\mathbf{R}, \alpha \in \mathscr{S}} |\mathbf{R}, \alpha\rangle \,\mathrm{Exp}\left(-\mathrm{i}\frac{2\pi xyz}{L_x L_y L_z}\right) \langle \mathbf{R}, \alpha|, \tag{1}$$

for 2D and 3D lattices, respectively. We claim that the integer invariants for chiral symmetric second-order topological phases in 2D and third-order topological phases in 3D are, respectively,

$$N_{xy} = \frac{1}{2\pi\mathrm{i}} \mathrm{TrLog}\left(\bar{Q}_{xy}^{A} \bar{Q}_{xy}^{B\dagger}\right) \in \mathbb{Z}, \qquad N_{xyz} = \frac{1}{2\pi\mathrm{i}} \mathrm{TrLog}\left(\bar{O}_{xyz}^{A} \bar{O}_{xyz}^{B\dagger}\right) \in \mathbb{Z}, \tag{2}$$

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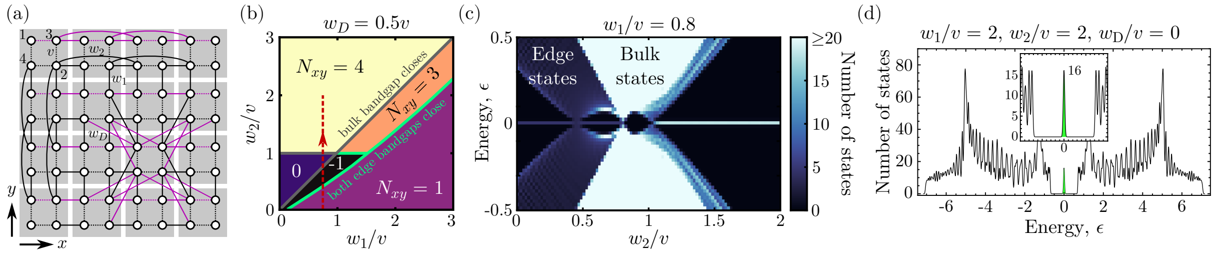

Fig. 1. (a) Schematic depicting the tight-binding model used. Not all non-nearest neighbor hoppings are shown for clarity. All purple hoppings are multiplied by -1 such that each plaquette has a uniform flux of π. (b) Phase diagram of N_{xy} for a C_{4v} symmetric, separability-broken system with $w_D/v = 0.5$ and $w_{m>2} = 0$. Bulk-obstructed phase transitions are shown in gray, while boundary-obstructed phase transitions are shown in lime. (c) Density of states for this system for fixed $w_1/v = 0.8$, indicated as the red line in (b). (d) Density of states the $N_{xy} = 4$ phase with $w_D/v = 0$.

where $\bar{Q}^{\mathscr{S}}_{xy} = U^\dagger_{\mathscr{S}} Q^{\mathscr{S}}_{xy} U_{\mathscr{S}}$ and $\bar{O}^{\mathscr{S}}_{xyz} = U^\dagger_{\mathscr{S}} O^{\mathscr{S}}_{xyz} U_{\mathscr{S}}$, for $\mathscr{S} = A, B$, are the sublattice multipole moment operators projected into the spaces $U_{\mathscr{S}}$.

To prove that the invariants (2) are strictly quantized, notice that they take the form $N = (1/2\pi\mathrm{i})\mathrm{TrLog}(U^\dagger_A M_A U_A U^\dagger_B M^\dagger_B U_B)$, where $M_{\mathscr{S}}$ (for $\mathscr{S} = A, B$) is $Q^{\mathscr{S}}_{xy}$ in 2D, or $O^{\mathscr{S}}_{xyz}$ in 3D. Since the matrices $M_{\mathscr{S}}$ and $U_{\mathscr{S}}$ are unitary, we have $\det(U^\dagger_A M_A U_A U^\dagger_B M^\dagger_B U_B) = \det(M_A M^\dagger_B) = 1$, where the last step follows if the two sublattices have (i) equal number of degrees of freedom in each unit cell and (ii) the same number of unit cells. Under these conditions, tracing the logarithm of $U^\dagger_A M_A U_A U^\dagger_B M^\dagger_B U_B$ will necessarily give a phase that is a multiple of $2\pi\mathrm{i}$, i.e., it will be of the form $2\pi\mathrm{i}N$, with $N \in \mathbb{Z}$. This integer N is the topological invariant.

We now illustrate some of the topological phases with nonzero values of N_{xy} and demonstrate that this invariant corresponds to the number of corner-localized states in each corner. Consider the quadrupole topological insulator (QTI) [1] with additional long-range hopping terms that preserve chiral symmetry, see Fig. 1a.

First, consider a chiral and C_4 symmetric, long-range QTI model with $w_D/v = 0.5$. For $w_2/v < 1$ and $w_1 < w_2$, this system possesses a bulk bandgap around zero energy and both the quadrupole moment, q_{xy} [1], and the quadrupole winding number, N_{xy} (Eq. 2), identify it as trivial ($q_{xy} = 0$, $N_{xy} = 0$), Fig. 1b. Starting from this phase and increasing w_2/v, a bulk bandgap-closing phase transition occurs, after which the system possesses a non-trivial MWN, $N_{xy} = 4$, but a trivial quadrupole moment, $q_{xy} = 0$. Simulations of the open system reveal that each corner of the lattice in this new phase possesses four degenerate modes with $\varepsilon = 0$ and that all such states within a corner exist only on a single sublattice of the system. Not only is the $N_{xy} = 4$ phase not captured by the quadrupole index, but more generally, it lies beyond the framework of induced band representations. Consequently, topological indices based on calculating the representations of the bulk bands at high-symmetry points of the Brillouin zone will fail to find this phase, as the representations of the lowest two bands at all of the high-symmetry points are identical in the $N_{xy} = 4$ phase, leading to trivial symmetry indicator invariants.

Phase transitions between phases with different MWNs need not close the bulk bandgap but, at a minimum, must close some lower-dimensional edge or surface bandgap. As can be seen in Fig. 1b, the $N_{xy} = -1$ and $N_{xy} = 3$ phases each have a phase boundary in which the bulk bandgap closes, and boundaries with other phases where only the edge bandgap closes. Both of these types of boundaries can be explicitly seen in the density of states across these phase transitions, Fig. 1c. For all of the different phases identified in Fig. 1b, the number of states localized in each corner of the system is equal to $|N_{xy}|$ and the sublattice over which the corner states are supported is given by $\mathrm{sgn}(N_{xy})$. Thus, for example, the $N_{xy} = -1$ phase in Fig. 1b indicates that the system possesses one state localized in each corner with support only on the *opposite* sublattice when compared with those in phases with $N_{xy} > 0$.

Finally, one can show that the topological phases protected by MWNs are robust in the presence of disorder that breaks all spatial symmetries and time-reversal symmetry. As such, these phases do *not* require crystalline symmetries to exist, but will generally be boundary obstructed.

In conclusion, we have demonstrated a novel higher-order topological phases protected by MWNs in chiral-symmetric systems, many of which would be misidentified as trivial by current theories.

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