Topological Insulators beyond Energy Band Characterization

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Topological phases of matter are generally characterized by topological properties of energy bands of a system. Their transitions under preserved symmetries occur through closing a gap of energy bands, leading to topologically protected edge states in energy spectra in topological phases. Here we predict a new topological phase that emerges through closing a gap of bands constructed by energy bands, instead of through closing an energy gap with preserved symmetries. From this perspective, topological phases may arise from topological properties of the "bands of bands" associated with their gap closure and corresponding edge states. We demonstrate this idea by studying a tight-binding model. We find that the Wannier bands constructed by energy bands exhibit a gap closure associated with a change of a winding number, while the energy bands remain gapped and trivial without any zero energy modes. In addition, the topological Wannier bands give rise to quantized edge polarizations. Since the emergence of this topological phase does not involve any energy gap closure, we expect its appearance under unitary time evolution. Indeed, this phase appears as we perform a quench dynamics. Our study opens a new direction for exploring topological phases beyond conventional energy band characterization.

In recent years, topological phases of matter have witnessed a rapid advance in quantum physics [1, 2]. They are generally characterized by topological invariants of energy bands of a system. Their change usually involves closure of an energy band gap of a Hamiltonian with preserved symmetries. Examples include quantum Hall insulators [3], topological insulators with time-reversal symmetry [4–7] and topological crystalline insulators [8, 9]. Recently, a quadrupole topological insulator has been theoretically proposed [10, 11] and experimentally observed [12–15]. Besides zero energy corner-localized modes and quantized quadrupole moments, this insulator supports quantized edge polarizations along all boundaries. It has been further shown that a type-II quadrupole topological insulator can exist [16]. Distinct from the original one, the type-II has only a pair of quantized edge polarizations violating a basic relation required by the classical electromagnetic theory. Such exotic phenomena arise because the Wannier bands close their gap while the energy band gap is maintained. There, the energy bands are also topological with quantized quadrupole moment and zero energy corner states. Here, we generalize this concept and propose that topological phases can change due to a gap closure of bands constructed by energy bands, i.e., the "bands of bands", even though the energy bands do not involve any gap closure, remaining topologically trivial from the conventional perspective. We demonstrate this idea by constructing a Hamiltonian which exhibits a gap closure of the Wannier bands while preserving the gap in the energy spectrum. Although the zero energy corner modes are lacking in the energy spectrum, the quantized edge polarization arises from the gap closure of the Wannier bands. Such a topological phase can also be characterized by a winding number of the Wannier bands.

Since the appearance of this new topological phenomenon does not require closure of an energy band gap, it is natural to expect their emergence under unitary time evolution. Nonequilibrium dynamics under unitary time evolution between distinct topological phases have been studied in cold atoms from various aspects [17–33]. Given that the unitary evolution does not change the determinant of a parent Hamiltonian, the topology of the evolved states remains unchanged if symmetries of the parent Hamiltonian are preserved during unitary time evolution [17, 18, 29]. On the other hand, a physical quantity, such as the Berry phase, can change continuously if symmetries of the parent Hamiltonian are allowed to change during unitary time evolution [30, 31]. However, in our case, while symmetries are maintained throughout, we show that the topology of evolved states can change. We find that the Wannier band gap can vanish as time evolves, leading to topological phases without zero energy modes in nested entanglement spectra. Such a gap closure also results in a sudden change of a winding number and edge polarizations. We also find type-II quadrupole topological insulators as time evolves.

Model Hamiltonian.— We start by considering a tight-binding Hamiltonian in a square lattice with reflection symmetries [as schematically shown in Fig. 1(a)] described by [34]

$$H = \sum_{\mathbf{R}} \sum_{2 \leq d_x, d_y \leq 2} \hat{c}_{\mathbf{R}, \alpha}^{\dagger} c_{\mathbf{R} + d_x, e_x + d_y, e_y} h(d_x, d_y) \hat{c}_{\mathbf{R}},$$

where \(\hat{c}_{\mathbf{R}, \alpha}^{\dagger}\) and \(\hat{c}_{\mathbf{R}, \alpha}\) create (annihilates) a particle at a site denoted by a lattice vector \(\mathbf{R} = R_x e_x + R_y e_y\) with \(R_x\) and \(R_y\) being integers and orbital index \(\alpha = 1, 2, 3, 4\) within a unit cell. When \(d_x = d_y = 0\), the sum over \(d_x\) and \(d_y\) describes the particle hopping between distinct orbitals within a unit cell; otherwise, the sum describes the hopping between nearby unit cells. Here, we choose the lattice constant \(a_{x,y} = 1\) throughout for simplicity. To generate the new topological phase, we include the long-range tunnelling.
To be specific, we take $h_{(00)} = -t_2 \tau_x \sigma_2 + \beta \tau_1 \sigma_0 + \gamma \tau_2 \sigma_2$, $h_{(10)} = t_3 (-i \tau_2 \sigma_3 + \tau_3 \sigma_0 - \tau_1 \sigma_2) + t_1 (\tau_1 \sigma_0 - i \tau_2 \sigma_3)/2$, $h_{(01)} = -t_3 \tau_3 \sigma_3 - it_3 \tau_2 \sigma_1$, $h_{(11)} = t_3 (\tau_1 \sigma_0 - i \tau_2 \sigma_1)$, $h_{(20)} = -t_3 (i \tau_1 \sigma_3 + i \tau_2 \sigma_1) + t_1 \tau_1 \sigma_0 - t_2 \tau_2 \sigma_2$, $h_{(21)} = 0$, $h_{(12)} = t_2 (-i \tau_3 \sigma_3 + \tau_3 \sigma_0 + i \tau_2 \sigma_1 + \tau_2 \sigma_3)/2$, $h_{(22)} = t_2 \tau_3 \sigma_3 + t_3 (-\tau_1 \sigma_0 + i \tau_2 \sigma_3 - \tau_3 \sigma_0 - i \tau_2 \sigma_1)/2$, where $\sigma, \tau$ represent Pauli matrices for the degrees of freedom within a unit cell. We can obtain the other hopping matrices for $d_x \neq 0$ and $d_y \neq 0$ by $h_{(d_x,d_y)} = (h_{(d_x,d_y)})^\dagger$, $\tilde{m}_x h_{(d_x,d_y)} \tilde{m}_x^\dagger = h_{(-d_x,d_y)}$ and $\tilde{m}_y h_{(d_x,d_y)} \tilde{m}_y^\dagger = h_{(d_x,-d_y)}$ because of the Hermiticity and reflection symmetries of the system with $\tilde{m}_x = \tau_1 \sigma_3$ and $\tilde{m}_y = \tau_1 \sigma_1$. The presence of reflection symmetries: $x \rightarrow -x$ and $y \rightarrow -y$, maintains the vanishing of bulk dipole moments [10, 11]. Specifically, we set $\beta = 0.4$, $t_1 = 0.3$, $t_2 = 0.2$, and $t_3 = 0.1$.

In Fig. 1(b), we plot the energy spectrum of the Hamiltonian under open boundary conditions in our considered region of a system parameter $\gamma$. The figure shows the absence of an energy gap closure and the absence of zero energy corner states, implying that the energy bands are topologically trivial. We further calculate the quadrupole moment [35] and find that it remains zero as $\gamma$ varies, further suggesting the absence of topological properties directly dictated by the energy bands. In the following, we will show that the Wannier bands constructed by energy bands experience a gap closure as $\gamma$ changes, leading to the appearance of edges states in the Wannier spectrum, which give rise to the quantized edge polarizations. We will also demonstrate that these edge states are topologically protected by a winding number [16].

To define the Wannier band, we introduce the Wilson loop $W_y = F_{y,k_y} F_{y,k_y-\delta y} \cdots F_{y,k_y}$ (similarly for $W_x$), where $[F_{y,k_y}]_{mn} = \langle u_k^m | + \delta k_y u_k^n \rangle$ [10, 11, 36]. Here, $|u_k^n\rangle$ is the $n$th occupied eigenstate of our Hamiltonian, $k_y$ is the quasimomentum along $y$ and $\delta k_y = 2\pi/N_y$ with $N_y$ being the number of unit cells along $y$. We define the Wannier Hamiltonian $H_{W_y}$ by [10, 11]

$$W_y \equiv e^{iH_{W_y}}. \tag{2}$$

We refer to its eigenvalues $2\nu_y$ as the Wannier band, where $\nu_y$ is the Wannier center determining the polarization contributed by each state. Since our system has reflection symmetries, the eigenvalues appear in pairs as $\{\nu_y, -\nu_y\}$, leading to zero total polarization in the bulk [10, 11]. In a torus geometry, we can write the Wannier Hamiltonian in momentum space as $H_{W_y}(k_x)$ with eigenvalues of $2\nu_y(k_x)$. Because $e^{i2\pi \nu_y(k_x)}$ is 1-periodic with respect to $\nu_y(k_x)$, we restrict $\nu_y(k_x)$ to $(0,1)$. Similar to an energy band, the Wannier bands can be gapped with one band $\nu_y^+(k_x) \in (0,0.5)$ and the other $\nu_y^-(k_x) \in (0.5,1)$. However, in contrast to energy bands, the Wannier bands have two gaps: one is around $\nu_y = 0$ and the other around $\nu_y = 0.5$ [37]. Because of the reflection symmetries, the Wannier gap can vanish at either $\nu_y = 0$ or $\nu_y = 0.5$. Yet, only the gap closure for the latter results in the quantized edge polarizations.

Figure 1(c) explicitly illustrates that the gap of the Wannier bands of $\nu_y$ vanishes at $\gamma = -0.62$, leading to the edge states at $\nu_y = 0.5$ of the Wannier Hamiltonian localized at two opposite $x$-normal boundaries (see the red line). These edge states give rise to edge polarizations [see the inset of Fig. 1(d)], which are quantized to $p_y^{\text{edge}} = \pm e/2$ for a half along $x$.

The topological phase can also be characterized by the winding number [16].

$$W_{\nu_y}^{\gamma=\pi} = \frac{1}{2\pi i} \int_0^{2\pi} dk_y \log U_{\nu_y}^{\gamma=\pi}(k_x), \tag{3}$$

where $U_{\nu_y}^{\gamma=\pi}(k_x)$ is a submatrix of $W_{\nu_y}^{\gamma=\pi}(k_x) = [U_{\nu_y}^{\gamma=\pi}(k_x), 0, 0, U_{\nu_y}^{\gamma=\pi}(k_x)]$, a Wilson line with respect to $\epsilon$ defined as $W_{\nu_y}^{\gamma=\pi}(k_x) \equiv W_{k_y \leftarrow 0}(k_x) e^{-iH_{W_y}(k_x)\epsilon/(2\pi)}$, where $W_{k_y \leftarrow 0}(k_x) = F_{y,k_y} F_{y,k_y-k_x} \cdots F_{y,k_y}$ and $H_{W_y}(k_x) \equiv -i\log W_{\nu_y}^{\gamma=\pi}(k_x)$ is the Wannier
Hamiltonian with respect to $\epsilon$ with $\log_\epsilon(e^{i\phi}) = i\phi$ with $\epsilon \leq \phi < \epsilon + 2\pi$. We associate the change of the polarization with the winding number as

$$p_y^{\text{edge}}(\gamma_1) - p_y^{\text{edge}}(\gamma_0) = \left(\frac{[W^{\epsilon=\pi}_{\nu_y}(\gamma_1) - W^{\epsilon=\pi}_{\nu_y}(\gamma_0)}{-\Delta N_{q,x}}\right)/2 \text{mod}(1),$$

where $\Delta N_{q,x}$ denotes the number of times that the quadrupole moment changes arising from the gap closure of the edge energy spectrum at the $x$-normal boundaries, when $\gamma$ varies from $\gamma_0$ to $\gamma_1$. In our case, since the quadrupole moment remains zero, the change of the polarization is only dictated by the winding number.

Figure 1(d) shows that the winding number $W^{\epsilon=\pi}_{\nu_y}$ suddenly changes from zero to one at $\gamma = -0.62$, where the gap of the Wannier bands $\nu_y$ vanishes at $\nu_y = 0.5$, accounting for the sudden emergence of quantized edge polarizations $p_y^{\text{edge}}$ afterwards. In contrast, the winding number $W^{\epsilon=\pi}_{\nu_x}$ remains zero, consistent with lacking a gap closure for the Wannier bands $\nu_x$ at $\nu_x = 0.5$, explaining the absence of the edge polarizations $p_x^{\text{edge}}$. We emphasize that the energy bands remain gapped as we deform the Hamiltonian continuously in the entire considered parameter region, suggesting that they remain topologically trivial from conventional perspective.

Quench dynamics.— Since the change of topological phases does not involve any energy gap closure, we expect the appearance of these phases under time evolution. Let us start with a many-body ground state $|\psi_k\rangle$ of an initial Hamiltonian $H_i(k)$ and then suddenly change the Hamiltonian to $H_f(k)$ by tuning system parameters.

The state then evolves under the final Hamiltonian, i.e., $|\psi_k(t)\rangle = e^{-iH_f(k)t}|\psi_k\rangle$. Since the evolved state is an eigenstate of a parent Hamiltonian $H_p(k) = e^{-iH_f(k)t}H_i(k)e^{iH_f(k)t}$, the topological properties of the evolved states are dictated by the parent Hamiltonian. Given $\det(H_p(k)) = \det(H_i(k))$, the parent Hamiltonian cannot close its energy gaps during time evolution.

Specifically, we consider the type-I quadrupole Hamiltonian \[ H_f(k) = (\gamma_x + \lambda \cos k_x)\Gamma_4 + \lambda \sin k_x \Gamma_3 + (\gamma_y + \lambda \cos k_y)\Gamma_2 + \lambda \sin k_y \Gamma_1, \] where $\Gamma_j = -\tau_2 \sigma_j$ ($j = 1, 2, 3$) and $\Gamma_4 = \tau_1 \sigma_0$. The phase diagram is shown in Fig. 2 with respect to $\gamma_x/\lambda$ and $\gamma_y/\lambda$ (see also Ref. [11]). We choose the ground state of $H_i/\gamma_x = \tau_1 \sigma_0 - \tau_2 \sigma_2$ (i.e., $\gamma_x = \gamma_y$ and $\lambda = 0$) as the initial state and then suddenly tune $\gamma_x$, $\gamma_y$ and $\lambda$ to the values as shown in Fig. 2(a). During time evolution, the parent Hamiltonian maintains reflection symmetries, i.e., $\hat{m}_\mu H_f \hat{m}_\mu^{-1} = H_f(k_\mu \to k_\mu)$ with $\mu = x, y$. Without loss of generality, we study two scenarios: one corresponds to the final Hamiltonian in the topologically trivial region and the other in the quadrupole insulating region.
Figure 2(b1-d1) illustrate the entanglement spectrum [35], Wannier spectrum and edge polarizations as a function of time, after the Hamiltonian is quenched into a topologically trivial phase. At $t = 1.1$, the gap of the entanglement spectrum $\text{ES}_x$ vanishes, revealing the vanishing of the energy gap for the parent Hamiltonian under open boundary conditions along $x$ [39]. This gap closure leads to the appearance of the quantized quadrupole moment ($q_{xy} = e/2$) and edge polarizations along $y$ ($p_{y}^{\text{edge}} = \pm e/2$). Here, the edge polarizations are calculated by the formula (5), where $\Delta N_{\mu \nu} (\mu = x, y)$ are evaluated by the number of times that the gap of $\text{ES}_x$ closes. Since there is neither gap closure for $\text{ES}_y$ nor Wannier gap closure for $\nu_x$, $p_{x}^{\text{edge}}$ remains zero. In addition, the nested entanglement spectra $\text{ES}_{xy}$ exhibit zero energy modes (see the blue region) (the nested entanglement spectrum $\text{ES}_{xy} = 0.5$ corresponds to the entanglement zero mode [35, 40]), reflecting the existence of fractional corner charges ($Q^{\text{corner}} = \pm e/2$) for the parent Hamiltonian in a geometry with open boundary conditions. This shows that the system enters into a type-II quadrupole topological insulating region with the basic relation $Q^{\text{corner}} = (p_{y}^{\text{edge}} + p_{x}^{\text{edge}} - q_{xy})\text{mod}(1)$ being violated. At $t = 2.5$, $\text{ES}_x$ experiences a gap closure, leading to a topologically trivial phase with zero quadrupole moment ($q_{xy} = 0$) and edge polarizations ($p_{x}^{\text{edge}} = p_{y}^{\text{edge}} = 0$).

Remarkably, shortly afterwards, the gap of the Wannier bands $\nu_x$ vanishes at $t = 2.55$ and $\nu_x = 0.5$, resulting in nonzero quantized edge polarizations $p_{x}^{\text{edge}} = e/2$. However, in this phase, the entanglement spectra do not exhibit any gap closure, reflecting the absence of the edge energy gap closure for the parent Hamiltonian under open boundary conditions. This accounts for the absence of the quadrupole moment and zero modes in the nested entanglement spectrum. When the gap of these Wannier bands $\nu_x$ closes again at $t = 3.54$, the edge polarization $p_{x}^{\text{edge}}$ vanishes so that the topological phase becomes trivial. The appearance and disappearance of this new topological phase are caused only by the gap closure of the Wannier bands at $\nu = 0.5$ (in other words, topological properties of the Wannier bands change due to the Wannier gap closure). This shows that the quench dynamics can produce new topological phases, although the coherent dynamics do not involve any energy gap closure.

Figure 2(b2-d2) present the results for the final Hamiltonian in the type-I quadrupole insulating phase. We find that the states evolve into the type-II QTI phase at $t = 1.04$ with quantized quadrupole moments ($q_{xy} = e/2$) and quantized edge polarizations $p_{x}^{\text{edge}} = \pm e/2$ but $p_{y}^{\text{edge}} = 0$ due to closure of the gap of $\text{ES}_y$. The nested entanglement spectrum has zero energy modes in the region, reflecting the existence of fractional corner charges ($Q^{\text{corner}} = \pm e/2$) for the parent Hamiltonian under open boundary conditions. At $t = 1.14$, the gap of the Wannier bands $\nu_x$ vanishes, yielding quantized edge polarizations $p_{y}^{\text{edge}} = \pm e/2$, which signals the transition into the type-I QTI where the basic relation $Q^{\text{corner}} = (p_{y}^{\text{edge}} + p_{x}^{\text{edge}} - q_{xy})\text{mod}(1)$ is satisfied. This phase remains until the Wannier bands $\nu_y$ close the gap at $t = 1.66$, followed by the emergence of the type-II QTI. We also observe that the type-II QTI reappears at $t = 3.94$ as a result of the vanishing of the gap of $\text{ES}_y$.

This new topological phase may be experimentally observed in cold atoms, photonic crystals, solid-state materials and electric circuits. For the electric circuits, one can design connections with electric devices to simulate the Hamiltonian (1), similar to the electric network for realizing the type-II QTI [16]. These new phases can also be observed through quench dynamics in cold atom experiments. In fact, Ref. [10] has introduced an experimental scheme to realize the type-I quadrupole model (6). In the scheme, laser beams are used to engineer a superlattice with four sites in each unit cell [see Fig. 1(a)]. Tunnelling along $y$ is suppressed by a linear potential. Then, Raman laser beams are applied to restore the hopping with a phase of $\pi$ per plaquette [41, 42]. Initially, we can tune the superlattice to realize large barriers between unit cells, which suppress the tunnelling between unit cells despite the presence of Raman lasers, realizing our initial Hamiltonian with almost zero $\lambda$. The cold atoms are prepared in the ground state of this Hamiltonian. After that, we suddenly change the model to our final Hamiltonian by tuning the superlattice and Raman lasers and perform the tomography of the evolved states. We can achieve the tomography by first removing atoms at two sites in each unit cell and then performing the tomography of the remaining sites by time-of-flight measurements [43, 44]. We can kick the atoms out of the trap by shining resonant laser beams to these sites to excite them to the $P$ state, which rapidly decays through spontaneous emission and escapes the trap. This is feasible given that current experiments can realize laser beams with the diameter as small as 600 nm [45, 46], comparable to the lattice constant. With measured states, the quadrupole moments, entanglement spectrum, and edge polarization can be obtained.

In summary, we have discovered a new class of topological phases solely characterized by topological properties of the Wannier bands. The topological phase transition occurs as a result of the Wannier band gap closing rather than the energy band gap closing. Such a transition is associated with a sudden change of the winding number of the Wannier bands. In fact, we find that the new topological phase appears without involving any energy band gap closure, suggesting that the phase is topologically trivial from traditional perspective. We further demonstrate that the new topological phase emerges in the quench dynamics of cold atoms. Our study opens a new direction for searching for topological phases characterized by topological properties of the "bands of bands" beyond conventional energy band characterization.
We thank T. Tian and H.-X. Yang for helpful discussions. This work is supported by the start-up fund from Tsinghua University, the National Thousand-Young-Talents Program and the National Natural Science Foundation of China (11974201).

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SUPPLEMENTAL MATERIAL

In the supplementary material, we will give the Hamiltonian in momentum space in Section 1, show the method to calculate the quadrupole moment in Section 2, and discuss the entanglement spectrum in detail in Section 3.
The reduced density matrix for the subsystem from atomic positive charges.

respectively, and the sum is performed over

\[ \text{tracing out the subsystem} \]

\[ \text{subsystems} \]

\[ \text{FIG. S1. (Color online) The entanglement spectrum (a) ES}_x \text{ and (b) ES}_y \text{ are evaluated by partitioning a system into two subsystems A and B and tracing out the subsystem B. (c) The nested entanglement spectrum ES}_{xy} \text{ is obtained by further tracing out the subsystem A}_2.} \]

S-1. HAMILTONIAN IN MOMENTUM SPACE

The Hamiltonian in Eq. (1) in the main text can be expressed in momentum space as

\[ H(k) = \sum_{i,j=0}^{3} g_{ij}(k) \tau_i \otimes \sigma_j, \quad (S1) \]

where all nonzero \( g_{ij} \)'s are given by

\[ g_{01} = -t_3(\sin(2k_x) + 2 \sin(2k_x) \cos(2k_y)), \quad (S2) \]
\[ g_{03} = -2t_3 \sin(2k_y), \quad (S3) \]
\[ g_{10} = \beta + t_1(\cos(k_x) + 2 \cos(2k_y)) + t_3(\cos(2k_x) - 2 \cos(2k_x) \cos(2k_y)), \quad (S4) \]
\[ g_{21} = -2t_2 \sin(k_y) + 4t_3(\cos(k_x) \sin(2k_y) - \cos(k_x) \sin(k_y)), \quad (S5) \]
\[ g_{22} = \gamma - 2t_3 \cos(k_x) - 2t_2 \cos(2k_y), \quad (S6) \]
\[ g_{23} = -t_1 \sin(k_x) + t_3(-\sin(2k_x) + 4 \sin(k_x) \cos(2k_y) + 2 \sin(2k_x) \cos(2k_y)), \quad (S7) \]
\[ g_{31} = -2t_3 \sin(k_y), \quad (S8) \]
\[ g_{32} = -t_2 + t_3(2 \cos(k_x) - \cos(2k_x) - 2 \cos(k_y) + 4 \cos(k_x) \cos(2k_y) + 4 \cos(k_x) \cos(2k_y) - 2 \cos(2k_x) \cos(2k_y)), \quad (S9) \]
\[ g_{33} = t_3(-2 \sin(k_x) + 2 \sin(2k_x) - 4 \sin(k_x) \cos(2k_y) + 4 \sin(2k_x) \cos(2k_y)). \quad (S10) \]

This Hamiltonian respects the reflection symmetry: \( \hat{m}_x H(k_x, k_y) \hat{m}^{-1}_x = H(-k_x, k_y) \) with \( \hat{m}_x = \tau_1 \otimes \sigma_3 \), and \( \hat{m}_y H(k_x, k_y) \hat{m}^{-1}_y = H(k_x, -k_y) \) with \( \hat{m}_y = \tau_1 \otimes \sigma_1 \).

S-2. THE QUADRUPOLE MOMENT

The quadrupole moment is calculated based on the formula \([S1, S2]\)

\[ q_{xy} = \frac{1}{2\pi} \Im \log \langle \Psi_G | \hat{U}_2 | \Psi_G \rangle, \quad (S11) \]

where \( |\Psi_G\rangle \) is the many-body ground state of a system under periodic boundary conditions and \( \hat{U}_2 = e^{2\pi i \sum_r \hat{q}_{xy}(r)} \) with \( \hat{q}_{xy}(r) = xy \hat{n}(r)/(L_xL_y) \) characterizing the quadrupole moment per unit cell measured with respect to \( x = y = 0 \) at site \( r \). \( \hat{n}(r) \) is the number of particles at site \( r \), \( L_x \) and \( L_y \) are the sizes of the system along \( x \) and \( y \) directions, respectively, and the sum is performed over \( (x, y) \in (0, L_x] \times (0, L_y] \). Note that we have eliminated the contribution from atomic positive charges.

S-3. ENTANGLEMENT SPECTRA

To define the entanglement spectrum, let us partition a system into two subsystems labelled by \( A \) and \( B \), respectively. The reduced density matrix for the subsystem \( A \) can be obtained by performing partial trace over the subsystem \( B \),
that is,
\[
\rho_A = \text{Tr}_B |\Psi\rangle \langle \Psi| = \frac{e^{-H_A}}{Z_A},
\]  
(S12)
where $|\Psi\rangle$ is a many-body ground state, $H_A$ is defined as a Hamiltonian corresponding to the reduced density matrix $\rho_A$ and $Z_A = \text{Tr} e^{-H_A}$. The entanglement spectrum refers to the eigenvalues of $\rho_A$ [S3–S5].

In the single-particle case, the entanglement spectrum can be determined by diagonalizing the correlation matrix [S6]

\[
[C_A]_{ij} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle,
\]  
(S13)
where $i, j \in A$. If we diagonalize $H_A$ as $H_A = \sum_n \varepsilon_n \hat{a}_n^\dagger \hat{a}_n$, the single-particle entanglement spectrum $\xi_n$ and $\varepsilon_n$ are related by

\[
\xi_n = \frac{1}{\varepsilon_n + 1}.
\]  
(S14)

Clearly, the entanglement spectrum $\xi_n = 0.5$ corresponds to an entanglement zero mode $\varepsilon_n = 0$. In the main text, we show the entanglement spectrum $\text{ES}_x$ and $\text{ES}_y$ obtained by tracing out the right part and top part of a system as shown in Fig. S1(a) and (b), respectively.

To characterize the edge modes of quadrupole topological insulators, which are localized at the corners, nested entanglement spectra are introduced [S7], as detailed in the following.

For a 2D quadrupole insulator, the Hamiltonian can be diagonalized as

\[
H = \sum_{k_x, k_y, n} E_{k_x, k_y}^n \hat{f}_{k_x, k_y, n}^\dagger \hat{f}_{k_x, k_y, n},
\]  
(S15)
where $\hat{f}_{k_x, k_y, n}^\dagger = \sum_\alpha [u_{k_x, k_y}^n]_\alpha \hat{c}_{k_x, k_y, \alpha}$ and $|u_{k_x, k_y}^n\rangle$ is the $n$th eigenstate of $H(k)$ corresponding to the eigenenergy $E_{k_x, k_y}^n$. Suppose that the system has $L_x \times L_y$ unit cells with $L_x = 2N_x$ and $L_y = 2N_y$. We first partition the system into two subsystems $A$ and $B$ along the $x$ direction: $A = \{(x, y)|1 \leq x \leq N_x, 1 \leq y \leq L_y\}$ and $B = \{(x, y)|N_x < x \leq L_x, 1 \leq y \leq L_y\}$. The correlation matrix in the subsystem $A$ is given by

\[
[C_{A,k_y}]_{x\alpha,x'\alpha'} = \langle \Psi_G | \hat{c}_{x\alpha,k_y}^\dagger \hat{c}_{x'\alpha',k_y} | \Psi_G \rangle = \frac{1}{L_x} \sum_{k_x} e^{i k_x (x-x')} \sum_{n \in \text{occ}} |U_{k_x,k_y}|_{\alpha n} |U_{k_x,k_y}^\dagger|_{\alpha' n},
\]  
(S16)
where $|\Psi_G\rangle$ is the many-body ground state of $H$ and $U_{k_x,k_y}$ consists of all occupied eigenstates $|u_{k_x,k_y}^n\rangle$ as column vectors. Diagonalizing $C_{A,k_y}$ yields the eigenvalues $\xi_{k_y}^n$ and eigenvectors $|v_{k_y}^n\rangle$ of $C_{A,k_y}$. The Hamiltonian $H_A$ of the reduced density matrix $\rho_A$ can be diagonalized as

\[
H_A = \sum_{k_y,m} \log(\frac{1}{\xi_{k_y}^m} - 1) g_{k_y,m}^\dagger g_{k_y,m},
\]  
(S17)
where $g_{k_y,m}^\dagger = \sum_{\alpha} [v_{k_y}^m]_{\alpha x} \hat{c}_{x\alpha,k_y}^\dagger$. The subsystem $A$ is further partitioned into two parts along the $y$ direction [as shown in Fig. S1(c)]: $A_1 = \{(x,y)|1 \leq x \leq N_x, 1 \leq y \leq N_y\}$ and $A_2 = \{(x,y)|1 \leq x \leq N_x, N_y < y \leq L_y\}$. The correlation matrix in the region $A_1$ is given by

\[
[C_{A_1}]_{x\alpha,y\alpha'} = \langle \Psi_A | \hat{c}_{x\alpha,k_y}^\dagger \hat{c}_{y\alpha',k_y} | \Psi_A \rangle = \frac{1}{L_y} \sum_{k_y} e^{i k_y (y-y')} \sum_{m \in \text{occ}} |V_{k_y}|_{\alpha m} |V_{k_y}^\dagger|_{m,x\alpha'},
\]  
(S18)
where $|\Psi_A\rangle$ is the many-body ground state of $H_A$ and the average is over all occupied states of $H_A$. $V_{k_y}$ is made up of all occupied eigenvectors $|v_{k_y}^n\rangle$ as column vectors. We can determine the nested entanglement spectrum by calculating the eigenvalues of $C_{A_1}$. 

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