Are atomic insulators distinguishable?

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Topological classification of quantum solids often (if not always) groups all trivial atomic or normal insulators (NIs) into the same featureless family. As we argue here, this is not necessarily the case always. In particular, when the global phase diagram of electronic crystals harbors topological insulators with the band inversion at various time reversal invariant momenta $K_{\text{inv}}^{\text{TI}}$ in the Brillouin zone, their proximal NIs display noninverted band gap minima at $K_{\text{min}}^{\text{NI}} = K_{\text{inv}}^{\text{TI}}$. In such systems, once topological superconductors nucleate from NIs, the inversion of the Bogoliubov de Gennes bands takes place at $K_{\text{inv}}^{\text{BdG}} = K_{\text{min}}^{\text{NI}}$, inheriting from the parent state. We showcase this (possibly general) proposal for two-dimensional time reversal symmetry breaking insulators. Then distinct quantized thermal Hall conductivity and responses to dislocation lattice defects inside the paired states (tied with $K_{\text{inv}}^{\text{BdG}}$ or $K_{\text{min}}^{\text{NI}}$), in turn unambiguously identify different parent atomic NIs.

**Introduction.** The world of insulators fragments into two sectors according to the topology and geometry of the bulk electronic wavefunction in quantum crystals: topological insulators (TIs) and normal insulators (NIs) [1, 2]. TIs manifest bulk-boundary correspondence, featuring robust gapless modes at crystal interfaces, such as edge, surface, corner and hinge, for example. When combined with the crystal symmetry, the family of TIs hosts a rich fair showcasing strong, weak, crystalline, higher-order and atomically obstructed TIs [3–21]. By contrast, atomic or normal insulators, although abundant in nature, do not accommodate any gapless topological boundary modes. Naturally, within the topological classification scheme of quantum materials, NIs are grouped into a single featureless family. A question therefore can be raised. *Can we topologically distinguish such NIs?*

Here we provide an indirect affirmative answer to this question by considering a paradigmatic toy square lattice model for two-dimensional (2D) time-reversal symmetry ($T$) breaking insulators [22]. We show if the global phase diagram of quantum materials supports TIs featuring the hallmark band inversion at different time reversal invariant momenta $K_{\text{inv}}^{\text{TI}}$ in the Brillouin zone (BZ), then their respective proximal NIs display a band gap minima at $K_{\text{min}}^{\text{NI}} = K_{\text{inv}}^{\text{TI}}$ [Fig. 1]. In such systems, when topological superconductors (TSCs) nucleate from NIs [Fig. 2(a)], the inversion of the Bogoliubov de Gennes (BdG) bands takes place at $K_{\text{inv}}^{\text{BdG}} = K_{\text{min}}^{\text{NI}}$ [Fig. 3]. While half-quantized thermal Hall conductivity ($\kappa_{xy}$) reveals the topological nature of the paired states [Fig. 2(b)], dislocation lattice defects, sensitive to $K_{\text{inv}}^{\text{BdG}}$, in turn underpins $K_{\text{min}}^{\text{NI}}$ [Fig. 4]. Therefore, responses of TSCs allow us to identify and distinguish their parent NIs. Specifically, when a TSC, characterized by a half-quantized $\kappa_{xy}$, stems from a NI with the band gap minima at a finite momentum, only then robust zero energy localized Majorana modes appear near the dislocation core. We present a simple mathematical proof to generalize this proposal to arbitrary dimensions (larger than one) and symmetry class to classify NIs from the responses of their proximal TSCs, operative under the only assumption that a half-filled system always describes an insulator.

**Normal state.** The Hamiltonian for 2D $T$-breaking insulators on a square lattice reads $H = \sum_k \hat{\Psi}_k^\dagger \hat{H}(k) \hat{\Psi}_k$, where $\hat{\Psi}_k = [c_k^\dagger, c_k]$, and $c_k^\dagger$ is the fermionic annihilation operator. 

![Diagram](https://example.com/figure1.png) **Fig. 1.** (a) Phase diagram of the normal state Hamiltonian [Eq. (1)] in terms of the Chern number $C$ [Eq. (2)] for $t = t_0 = 1$. In each insulating phase, the band structure displays parity polarization of the eigenvectors in red (+) and blue (−) for (i) $m_0 = 2.25$, (ii) $m_0 = −0.75$, (iii) $m_0 = 0.75$ and (iv) $m_0 = −2.25$. Hence, bands are noninverted (inverted) in NIs (TIs). Here we follow the path $\Gamma \to X \to M \to \Gamma$ in the BZ. (b) The Six-terminal electrical ($\sigma_{xy}$) and thermal ($\kappa_{xy}$) Hall conductivities as a function of $m_0$, computed in a rectangular system (see insets) of length $L = 200$ and width $W = 100$. In TIs, both $\sigma_{xy} = C$ (in units of $e^2/h$) and $\kappa_{xy} = C$ (in units of $\pi^2 k_B^2/(3h)$). Dotted lines are guide to the eye.
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supports one chiral edge mode, encoding the first Chern

Vector Pauli matrix \( \tau \)

operator with momentum \( k \) and parity \( \tau = \pm \) \[22\]. The \( k \)-dependent operator is given by \( \mathcal{H}(k) = \tau \cdot \mathbf{d}(k) \) with

\[
\mathbf{d}(k) = \left( t \sin(k_x a), t \sin(k_y a), m_0 - t_0 \sum_{j=x,y} \cos(k_j a) \right).
\]

Vector Pauli matrix \( \tau = (\tau_x, \tau_y, \tau_z) \) operates on the parity indices (±). Throughout, we set \( t = t_0 = 1 \), and the lattice constant \( a = 1 \). Then this model hosts TIs in the regime \( -2 < m_0 < 2 \), and NIs otherwise. Each TI supports one chiral edge mode, encoding the first Chern number \( C = \pm 1 \), defined within the first BZ as \[23\]

\[
C = \int_{\text{BZ}} \frac{d^2k}{4\pi} \left[ \partial_{k_x} \mathbf{d}(k) \times \partial_{k_y} \mathbf{d}(k) \right] \cdot \mathbf{d}(k),
\]

manifesting the bulk-boundary correspondence, where \( \mathbf{d}(k) = \mathbf{d}(k) / |\mathbf{d}(k)| \). In NIs \( C = 0 \). The nontrivial Chern number gives rise to quantized electrical and thermal Hall conductivities, which we discuss shortly.

Various phases of this model Hamiltonian in terms of the Chern number and the associated band structures are shown in Fig. 1(a). The topological regime fragments

into two sectors depending on the band inversion moment in the BZ (\( \mathbf{K}_{\text{inv}}^{\text{Tl}} \)). Specifically, \( \mathbf{K}_{\text{inv}}^{\text{Tl}} = (0,0) \) (\( \Gamma \) point) for \( 0 < m_0 < 2 \) and \( (\pi,\pi) \) (M point) for \( -2 < m_0 < 0 \). In these two phases, \( C = +1 \) and \( -1 \), respectively. The transition between them takes place through a band gap closing at the \( X = (\pi,0) \) or \( Y = (0,\pi) \) point when \( m_0 = 0 \). Two NIs are born from these TIs via bulk gap closings at the M and \( \Gamma \) points when \( m_0 = -2 \) and \( +2 \), respectively. Even though the bands are noninverted in NIs, the parity-polarized conduction (valence) band displays band minima (maxima) near the \( \Gamma \) and \( M \) points, respectively for \( m_0 > 2 \) and \( m_0 < -2 \). In this respect, the band gap minima in NIs occurs at \( \mathbf{K}_{\text{min}}^{\text{NI}} = \mathbf{K}_{\text{inv}}^{\text{Tl}} \) of their proximal parent TIs.

Before addressing the proposal to distinguish NIs with different \( \mathbf{K}_{\text{min}}^{\text{NI}} \), we characterize the normal state in terms of the electrical (\( \sigma_{xy} \)) and thermal (\( \kappa_{xy} \)) Hall responses to facilitate the forthcoming discussion.

**Electrical Hall conductivity.** We compute \( \sigma_{xy} \) in a six-terminal geometry at zero temperature \[24\]. Since mesoscopic details of the device or scattering region and
leads play a pivotal role in obtaining meaningful transport responses, here we briefly discuss their geometry used for the calculations [Fig. 1(b)]. A rectangular scattering region containing the system is maintained at a voltage $V$. It is connected to six terminals. All of them are kept at different voltages with the help of reservoirs. To generate transverse electrical response, we apply a voltage gradient between lead 1 ($V_1 = -\Delta V/2$) and lead 4 ($V_4 = \Delta V/2$), resulting in a longitudinal electrical current ($I_{xy}$) between them. No current is flowing between the transverse leads. They serve as the voltage probes. This setup allows us to calculate $\sigma_{xy}$, generated between the transverse leads by extracting the scattering matrix using Kwant [25]. The current-voltage relation is given by $I_{el} = G_{el}V$, with $G_{el} = (I_{el}, 0, 0, -I_{el}, 0, 0)$ and $V = (-\Delta V/2, V_2, V_3, \Delta V/2, V_5, V_6)$. The conductance matrix $G_{el}$ contains only the transmission blocks of the scattering matrix. Upon finding $G_{el}$, we extract different voltages from the above current-voltage relation. Subsequently, we compute the transverse electrical resistance $R_{xy}^e = (V_2 + V_3 - V_5 - V_6)/(2I_{el})$ [26–28], yielding $\sigma_{xy} = (e^2/h)(R_{xy}^e)^{-1}$. Setting $e = h = 1$, we find $\sigma_{xy} = C$, as shown in Fig. 1(b).

**Thermal Hall conductivity.** The same six-terminal geometry can be used to compute $\kappa_{xy}$. The scattering region is now maintained at a temperature $T$. All six terminals are kept at different temperatures. We apply a temperature gradient between lead 1 ($T_1 = -\Delta T/2$) and lead 4 ($T_4 = \Delta T/2$). It results in a longitudinal thermal current ($I_{th}$) from lead 1 to lead 4. The current-temperature relation is captured by the matrix equation $I_{th} = A_{th}T$, where $I_{th} = (I_{th}, 0, 0, -I_{th}, 0, 0)$ and $T = (-\Delta T/2, T_2, T_3, \Delta T/2, T_5, T_6)$. The matrix elements of $A_{th}$ are given by [29, 30]

$$A_{th,ij} = \int_0^\infty \frac{E^2}{T} \left( -\frac{\partial f(E,T)}{\partial E} \right) \left[ \delta_{ij} \mu_j - \text{Tr}(t^\dagger_{ij} t_{ij}) \right] dE,$$

where $\mu_j$ denotes the number of propagating modes in the $j$th lead, $f(E,T) = 1/(1 + \exp[E/(k_BT)])$ is the Fermi-Dirac distribution function, $t_{ij}$ is the transmission part of the scattering matrix between the leads $i$ and $j$, and the trace ($\text{Tr}$) is taken over the conducting channels. Upon obtaining $A_{th}$, we calculate temperature at various leads from the current-temperature relation. The transverse thermal resistance is $R_{xy}^{th} = (T_2 + T_3 - T_5 - T_6)/(2I_{th})$. For both electrical and thermal Hall resistances, average over different terminals is taken to avoid contact resistance effects, giving rise to robust quantized values. Inverting $R_{xy}^{th}$, we obtain $\kappa_{xy} = \pi^2 k_B^2 T/(3h) (R_{xy}^{th})^{-1}$, where we further set $k_B = 1$ [29–32]. Notice that the integrand in Eq. (3) depends on the derivative of the Fermi-Dirac function, which is valid in the limit $T \rightarrow 0$ [24]. We compute $\kappa_{xy}$ for $T = 0.01$ (in the energy unit). Then in units of $\pi^2/3$, we find $\kappa_{xy}/T = C$, as shown in Fig. 1(b).

**Superconductivity.** Therefore, NIs with distinct $K_{\text{Ni}}^{\text{min}}$ cannot be distinguished from any response of charged fermions. Such a goal can nevertheless be accomplished when the system is conducive to Cooper pairing. The charge conjugation symmetry allows this system to support only one local pairing [33]. The effective single-particle BdG Hamiltonian then reads

$$H_{\text{BdG}} = \frac{1}{2} \sum_k (\Psi_k^{\text{Nam}})^\dagger H_{\text{BdG}}(k) \Psi_k^{\text{Nam}},$$

where $\Psi_k^{\text{Nam}} = [\Psi_k, \tau_1 \Psi_k^\dagger]$, is the Nambu-doubled spinor and

$$H_{\text{BdG}}(k) = d_1^\dagger(k) \Gamma_0 d_1(k) + d_2^\dagger(k) \Gamma_0 d_2(k) + d_3^\dagger(k) \Gamma_0 d_3(k) + \Delta \Gamma_3.$$  (4)

The $4 \times 4$ Dirac matrices are $\Gamma_{ab} = \eta_a \otimes \tau_b$. The new set of Pauli matrices $\{\eta_a\}$ act on the Nambu space. The factor of $1/2$ in $H_{\text{BdG}}$ stems from the Nambu doubling.

Computation of the phase diagram of $H_{\text{BdG}}(k)$ is greatly simplified by noting that a unitary rotation by $U = \exp[-i\pi \Gamma_{20}/4]$ brings it to a block diagonal form $U^\dagger H_{\text{BdG}}(k) U = \mathcal{H}_{\text{BdG}}^+(k) \oplus \mathcal{H}_{\text{BdG}}^-(k)$, where $\mathcal{H}_{\text{BdG}}^\pm(k) = \tau \cdot d^\dagger(k)$ with $d^\dagger(k) = (d_1^\dagger, d_2^\dagger, d_3^\dagger)$ and

$$d_0^\dagger(k) = m_0 + \Delta - t_0(\cos(k_x a) + \cos(k_y a)).$$

(5)

The global phase diagram of $H_{\text{BdG}}(k)$ can now be constructed in terms of the total Chern number $C_{\text{tot}} = C_+ + C_-$, as shown in Fig. 2(a), where $C_{\pm}$ are the Chern numbers for $\mathcal{H}_{\text{BdG}}^\pm(k)$, computed from Eq. (2). It features TSCs with $C_{\text{tot}} = \pm 1$ and $\pm 2$, besides the ones

![FIG. 4. Energy spectra of $H_{\text{BdG}}(k)$ [Eq. (4)] in the presence of an edge dislocation-antidislocation pair with $b = \pm a\hat{e}_x$, placed symmetrically in a periodic system with linear dimensions $L = 24$ in the $x$ and $y$ directions, for $\Delta = 0.5$, and (a) $m_0 = -1.0$, (b) $m_0 = -2.0$, and (c) $m_0 = 0.0$, yielding $C_{\text{tot}} = +2, +1$ and 0 (with nontrivial Zak phase) [Fig. 2(a)], respectively. Insets show near zero energy states, whose local density of states is always highly localized around the defect cores.](image-url)
with $C_{\text{tot}} = 0$. The $C_{\text{tot}} = 0$ sector fragments into two classes, which can be distinguished in terms of a weak topological invariant, namely the Zak phase [34–37]. The one with a nontrivial Zak phase is named weak TSC [24].

**Thermal Hall effect.** We now compute responses of the paired states from Fig. 2(a), capturing the signatures of their nontrivial topological invariants. At this point, we should note that once superconductivity develops in the system, electrical charge responses become ill-defined as Cooper pairs do not obey the charge conservation. However, as the energy of the system is conserved, $\kappa_{xy}$ serves as a bonafide topological response to characterize the paired states. Details of the computation of $\kappa_{xy}$ in a six terminal geometry has already been discussed. So, here we only quote the final results. We find that $\kappa_{xy}$ is nonvanishing only when $C_{\text{tot}}$ is nonzero and half-integer quantized, namely $\kappa_{xy} = -2C_{\text{tot}}/2$ in units of $\pi^2/3$, once we set $k_y = h = 1$ [29–31]. Therefore, TSCs with $C_{\text{tot}} = \pm 1$ and $\pm 2$, give $\kappa_{xy} = \mp 0.5$ and $\mp 1$, respectively, as shown in Fig. 2(b). However, $\kappa_{xy} = 0$ whenever $C_{\text{tot}} = 0$, irrespective of whether the superconducting phase possesses a nontrivial Zak phase or not. Furthermore, it should be noted that the sign of $\kappa_{xy}$ can be changed without altering the nature of the TSC, namely the BdG band inversion momentum ($K_{\text{BdG}}^{\text{inv}}$), by taking $\tau \rightarrow -\tau$ for example. Thus a full characterization of TSCs also demands a smoking gun probe of $K_{\text{BdG}}^{\text{inv}}$.

**Edge band structure.** The topological nature of the superconductors and the associated $K_{\text{BdG}}^{\text{inv}}$ can be established from the band structure of $H_{\text{BdG}}(k)$ in a semi-infinite system with only $k_x$ or $k_y$ as a good quantum number. One-dimensional $|C_{\text{tot}}|$-fold degenerate edge modes then appear as dispersive states along $k_x$ or $k_y$, separated from the bulk states. See Fig. 3. Furthermore, the edge modes cross the zero energy exactly at $K_{\text{BdG}}^{\text{inv}}$. We find that TSC with $C_{\text{tot}} = -2$ (+2) supports doubly-degenerate edge states with the BdG band inversion at the $\Gamma$ (M) point. The $C_{\text{tot}} = \pm 1$ TSCs replicate this outcome. But the edge modes are then non-degenerate. The paired state with $C_{\text{tot}} = 0$ supports counter-propagating edge modes, crossing the zero energy at $k_x$ or $k_y = 0$ and $\pi$, only when it possesses a nontrivial Zak phase. Next we show that dislocation lattice defects probe $K_{\text{BdG}}^{\text{inv}}$.

**Edge dislocation.** Two dimensional edge dislocations are constructed from the so-called Volterra cut-glue procedure. The main idea is to cut a line of atoms up to a site, called the dislocation core as a first step. Subsequently, the sites across the cut are glued. This way, the system regains translational symmetry everywhere except near the dislocation core, where the missing translation characterizes the defect in terms of the Burgers vector ($b$). Due to this, when a BdG fermion encircles the defect core, it picks up a hopping phase $\exp[i\Phi_{\text{dis}}]$, governed by the $K \cdot b$ rule [38–49], where $\Phi_{\text{dis}} = K_{\text{BdG}}^{\text{inv}} \cdot b$ (modulo $2\pi$). Following this principle, we find that TSCs with $C_{\text{tot}} = -1$ (+2) support one (two) pair(s) of zero energy dislocation modes. Furthermore, the TCS with $C_{\text{tot}} = 0$, but a nontrivial Zak phase features two zero energy defect modes. See Fig. 4. In all these phases $\Phi_{\text{dis}} = \pi$ (nontrivial) when $b = a\hat{e}_x$ or $a\hat{e}_y$, as $K_{\text{BdG}}^{\text{inv}} = (\pi, \pi)$ therein, resulting in edge modes crossing the zero energy at $k_x$ or $k_y = \pi$ [Fig. 3]. For all the other paired states $\Phi_{\text{dis}} = 0$ (trivial). None of them thus hosts any zero energy dislocation mode.

These observations can be supported from an alternative explanation. Notice that the two edges, introduced during the cut procedure, support counter-propagating edge modes. Once these two edges are glued, the associated edge modes hybridize and suffer level repulsion. When $n$ number of edge modes cross the zero energy at momentum $\pi$ or $0$, such a level repulsion can be modeled by a domain wall or uniform Dirac mass, acting on the edge subspace. Then the Jackiw-Rebbi mechanism applies [50], and in the former situation the dislocation core supports $n$ pairs of localized Majorana zero modes.

**Discussions.** From a paradigmatic toy square lattice model, featuring $T$-breaking TIs with distinct topological invariant ($C$) and $K_{\text{inv}}^{\text{Td}}$, here we argue that their proximal NIs with band gap minima at $K_{\text{min}}^{\text{Td}} = K_{\text{inv}}^{\text{Td}}$ can be distinguished, but only when TSCs develop in the system. In particular, $\kappa_{xy}$ and the response to the dislocation lattice defects inside the paired states (governed by $K_{\text{BdG}}^{\text{inv}} = K_{\text{NI}}^{\text{NI}}$) unambiguously distinguish parent NIs with different $K_{\text{NI}}^{\text{NI}}$. A generalization of this proposal possibly rests on the answer to the following question.

*Can two NIs realized in the limits $m_0 \rightarrow \pm \infty$ be adiabatically connected?* In these two limits the kinetic energy becomes unimportant and NIs can be modeled by a simple Hamiltonian $H_{\text{NI}} = m_0 \Gamma_{2N}$, where $\Gamma_{2N}$ is a $2N$-dimensional traceless Hermitian matrix and $2N$ is the total number of bands in the system, with $N = 1$ in our study. At half-filling, there are $N$ filled valence and $N$ empty conduction bands, with a band gap $2m_0$ between them. Irrespective of the representation, eigenvalues of $\Gamma_{2N}$ are $+1$ and $-1$ (named generalized parity eigenvalues), and each of them is $N$-fold degenerate. The corresponding wavefunctions are parity eigenstates. When $m_0 \rightarrow \infty$, the conduction (valence) band is constituted by positive (negative) parity eigenstates. In the $m_0 \rightarrow -\infty$ limit, the situation is exactly the opposite. See, for example, Fig. 1(a). As the parity eigenstates are orthogonal to each other, two atomic insulators in the limits $m_0 \rightarrow \pm \infty$ therefore cannot be smoothly deformed into each other. This proof allows us to at least conjecture that our proposal to distinguish trivial atomic insulators by inducing TSCs should be applicable to systems of arbitrary dimensionality (above one) belonging to arbitrary symmetry class, as long as it can support distinct TIs with different $K_{\text{inv}}^{\text{Td}}$. A further rigorous mathematical proof of this statement (if exists) is beyond the scope of the present work.

Nature harbors a plethora of TIs with the hallmark
band inversion at various points in the BZ [3–21]. In these systems, TI-NI quantum phase transitions can be triggered by changing the quantum well width [51] or via chemical substitutions [52–56] or by applying a hydrostatic pressure [57, 58]. When doped these quantum materials typically accommodate TSCs [59]. Here only for the sake of simplicity, we set the chemical potential to zero. Our proposal holds even when the insulating systems are doped, which favors nucleation of TSCs by forming a Fermi surface. Therefore, the task is to induce TSCs in doped topological materials with different $K_{\text{inv}}$ after driving the system into a NI. While the thermal Hall conductivity is intimately tied with the breaking of the $T$ in the paired state (class D), responses to dislocation modes can be detected via scanning tunneling microscope [66, 67]. Therefore, our proposal to distinguish NIs from the responses of their proximal TSCs can be tested in well-characterized topological quantum materials with existing experimental tools.

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