Local invariants identify topological metals

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Although topological band theory has been used to discover and classify a wide array of novel topological phases in insulating and semi-metal systems, it is not well-suited to identifying topological phenomena in metallic or gapless systems. Here, we develop a theory of topological metals based on the system’s Clifford pseudospectrum, which can both determine whether a system exhibits boundary-localized states despite the presence of a degenerate bulk bands and provide a measure of these states’ topological protection. Moreover, the Clifford pseudospectrum yields a set of invariants that are locally defined at a given position and energy while still being rigorously connected to the system’s $K$-theory. We demonstrate the generality of this method in two systems, a Chern metal and a higher-order topological metal, and prove the topology of these systems is robust to relatively strong perturbations. The ability to define invariants for metallic and gapless systems allows for the possibility of finding topological phenomena in a broad range of natural and artificial materials which have not been previously explored.

Topological band theory has enabled enormous progress in the discovery and classification of novel states of matter. The preponderance of these developments have been predicted and realized in insulators and semi-metals, where these systems’ topological features are easily identified due to their isolation in energy and wavevector ($E, \mathbf{k}$)-space. However, in metals and other materials lacking a bulk band gap, any states of topological origin are degenerate with bulk states, generally resulting in hybridization between the two sets of states. This hybridization makes it difficult to say whether a particular set of states remains localized to the system’s boundaries, or retains any of the other topological properties that they would possess in an insulating system. Moreover, even if boundary-localized states could be identified, the absence of a bulk band gap means that traditional topological band theories would be unable to predict whether these states would be robust to perturbations, or quantify the strength of that protection. Although detailed studies in particular metallic and gapless systems have demonstrated the existence of some topological behaviors, a general theory for predicting topological phenomena in any metallic or gapless system has remained elusive.

Theories of topological materials predicted upon diagonalizing a system’s Hamiltonian to determine its topology possess an inherent challenge when considering metals or other gapless materials. In general, the Hamiltonians, $H$, of topologically non-trivial systems do not commute with position operators, $X$, i.e., $[H, X] \neq 0$. Thus, it is impossible to find eigenstates of both operators simultaneously. In insulators and semi-metals, where any energy eigenstates of topological origin can be spectrally isolated, position expectation values provide a measure of the state’s location and localization. However, in metals or gapless systems, any potential topological energy eigenstate is a member of a large degenerate subspace consisting primarily of bulk states, which renders position expectation values meaningless without some other discriminant between possible choices of basis within this subspace. Instead, this argument suggests that a theory of topological metals should be pursued using real-space definitions of topology that do not require diagonalizing the Hamiltonian. Such real-space topological theories have recently been used to identify distinct phases in aperiodic systems, such as quasicrystals, amorphous structures, and fractal lattices.

Here, we develop a general theory of topological metals and other gapless materials defined using local invariants derived from the system’s Clifford pseudospectrum. This theory has three inherent features that allow it to directly solve the difficulties facing any topological theory of gapless systems: First, as the Clifford pseudospectrum treats the system’s Hamiltonian on equal footing with its position operators, it is able to simultaneously identify the approximate energy and position of the system’s states. Second, in the absence of a state, the Clifford pseudospectrum returns a measure of the strength of the perturbation required to find a state at that location and energy — in particular, one can calculate the Clifford pseudospectrum in the immediate vicinity of a boundary-localized state to determine the strength of its protection against disorder. Third, the Clifford pseudospectrum is mathematically proven to be connected to the system’s $K$-theory and thus can be used to define local invariants that classify the system’s topological phase at a given energy and position. To demonstrate the generality of this method, we explicitly determine the topological character and quantify the strength of its protection in two disparate models, a Chern metal and a higher-order topological metal. As part of this study, we also provide a definition of a local, real-space invariant for higher-order topological phases. The theory we present here provides the groundwork for classifying the topology of metals and...
other gapless systems of any dimension in any symmetry class [78, 81].

To illuminate how the Clifford pseudospectrum can be used to classify topological metals, we first consider a 2D Chern insulator with an added intervening band that is degenerate with the Chern insulator’s chiral edge states. A minimal tight-binding model for this system can be formed using a Haldane honeycomb lattice coupled to a single-band triangular lattice whose vertices are located in the center of each honeycomb [51, 52], schematically illustrated in Fig. 1b. In the Haldane lattice, \( t_1 \) is the amplitude of the nearest neighbor coupling, \( t_C \) and \( \phi \) set the amplitude and phase of the next-nearest neighbor couplings and are oriented along the arrows in Fig. 1b, and the on-site energy difference between the honeycomb sublattices is \( 2M \). The coupling strength within the triangular lattice is \( t_2 \), with on-site energy \( M_2 \). The coupling strength between the two lattices is \( t_3 \). In the absence of coupling between the two lattices, \( t_3 = 0 \), the Haldane model exhibits topological and trivial insulating phases separated by semi-metal phases and protected by the Chern number, \( C \), see Fig. 1b, while the triangular lattice exhibits a single band centered around \( E = M_2 \). When the coupling between the two lattices is turned on, \( |t_3| > 0 \), the intervening band from the triangular lattice prohibits the unique identification of chiral edge states within its extent. Nevertheless, previous numerical studies have shown that this system still exhibits some unusual transport properties that are robust against disorder, even for choices of the Fermi energy for that are within the extent of the middle band for any choice of edge and \( k \) along that edge (for example, \( E = 0 \) in Fig. 1b) [51, 52].

Here we prove that boundary-localized states exist in the Chern metal, even for energies within the extent of the middle band, and quantify their topological protection. To do so, we first construct the “localizer,” a matrix composed of both the system’s Hamiltonian and the locations of its lattice sites [78, 80]. For a \( d \)-dimensional system, the localizer is

\[
L_\lambda(X_1, \ldots, X_d, H) = \sum_{j=1}^{d} \kappa(X_j - \lambda_j I) \otimes \Gamma_j + (H - \lambda E I) \otimes \Gamma_{d+1},
\]

where \( I \) is the identity matrix and the matrices \( \Gamma_j \) form a non-trivial Clifford representation, \( \Gamma_j^I = \Gamma_j, \Gamma_j^J = I \), and \( \Gamma_j \Gamma_l = -\Gamma_l \Gamma_j \) for \( j \neq l \). The diagonal position matrices \( X_j \) specify the coordinate of each lattice site in the \( j \)th dimension, while \( \kappa > 0 \) is a scaling coefficient that ensures \( X_j \) and \( H \) have compatible units and a small commutator, \([H, \kappa X_j] \approx 0 \). Rigorously, \( \lambda \in \mathbb{R}^{d+1} \) is a member of the system’s Clifford pseudospectrum, \( \lambda \in \Lambda_\epsilon(X_1, \ldots, X_d, H) \), if at least one of the localizer’s eigenvalues is within some neighborhood \( \epsilon \) of 0, i.e.,

![FIG. 1. (a) Schematic of the combined tight-binding model for a Haldane honeycomb lattice, green and orange circles, coupled to a trivial lattice, blue triangles. Some couplings are only shown in a portion of the system for clarity. (b) Haldane model phase diagram, with the topological (red) and trivial (blue) systems considered marked. (c-f) Simulations of a topological Chern metal, with \( M/t_1 = 0, t_C/t_1 = 0.5, \phi = \pi/2, M_2/t_1 = -0.35, t_2/t_1 = 0.2 \) and \( t_3/t_1 = 0.3 \). (d) Strip band structure with two zig-zag edges. Chiral edge states can be identified outside of the intervening band at \( E = 0 \). \( \Delta E \) is the gap between the top and bottom bands. (d) The local density of states at \( E = 0 \). Each lattice site is represented as a 2D Gaussian with radial width \( r_0 = 0.5a_c \). (e) 2D localizer gap, \( \min(|\sigma(L_\lambda(X, Y, H))|)/\Delta E \) at \( \lambda = (x, y, E = 0) \) with \( \kappa = 1 \). The colored overlay shows the local Chern number, \( C_L(x, y, 0) \). (f) Full localizer spectrum along the line shown in green in (e). The eigenvalue which yields a change in topology is highlighted in magenta. (g-j) Same as (c-f), except for a trivial metal, with \( M/t_C = 4\sqrt{3} \).]
min(|\sigma(L_\lambda)|) \leq \epsilon$, where $\sigma(L_\lambda)$ denotes the spectrum of $L_\lambda$. Physically, it is more intuitive to view this process constructively, by first choosing coordinates in position and energy $\lambda = (x, E)$ and then solving for the “localizer gap,” $\min(|\sigma(L_\lambda)|)$; localizer gaps near zero indicate that the system possesses a state approximately at $x$ and with energy $E$, while large localizer gaps indicate that a shift in $x$ or $E$ (or both) is required to find a state with strong support near this $(x,E)$.

Alternatively, one could close the localizer gap at a given $(x,E)$ by adding a perturbation to the system. Thus, the localizer gap at $(x,E)$ is a direct measure of the strength of disorder required to move the closest state to this position and energy, and, as such, quantifies the robustness of any nearby topological features.

In particular, it has been proven that a symmetry preserving perturbation to the Hamiltonian, $\delta H$, is unable to change the topology of the system $(x,E)$ so long as $|\delta H| < \min(|\sigma(L_\lambda)|)$. Moreover, this measure of the strength of the topological protection inherently includes the possibility of correlated disorder that is “designed” to defeat the system’s topology. Thus, in most systems, the localizer gap will underestimate the strength of the system’s topological robustness for uncorrelated fabrication disorder. Additionally, there has been recent progress in understanding the effects of perturbations that only approximately respect the system’s symmetry class $[82]$.

As the localizer provides a route to approximately diagonalizing a system’s Hamiltonian and position operators simultaneously, it is able to identify the approximate presence (or absence) of a state at a given position regardless of other degenerate states elsewhere in the system. Thus, whereas conventional analysis methods that give preference to the system’s Hamiltonian, such as the local density of states, have difficulty distinguishing topological and trivial metals (Figs. 1l and h are similar), the difference between these systems can be immediately seen in the localizer gap of these two systems (Figs. 1i and i). Here, the presence of the chiral edge states in the topological metal causes the localizer gap to close around the entire perimeter of the system regardless of whether these states hybridize. Moreover, the sizeable localizer gap just inside this closing indicates that these boundary-localized states are robust against disorder despite the absence of a bulk band gap.

For every symmetry class, the localizer is mathematically connected to the system’s $K$-theory $[78,80,82]$, which can only change when the corresponding localizer gap vanishes, $\min(|\sigma(L_\lambda)|) = 0$. In particular, the topological invariant at any $\lambda = (x,y,E)$ for 2D systems in symmetry class A is given by

$$C_L(x,y,E) = \frac{1}{2} \text{sig}(L_{(x,y,E)}(X,Y,H)) \in \mathbb{Z}, \quad (2)$$

assuming that the localizer gap is non-zero, and in which sig denotes a matrix’s signature, the number of positive eigenvalues minus the number of negative eigenvalues. Thus, this formulation of the local Chern number is necessarily an integer, even for finite systems. Calculating this invariant for the system in Figs. 1f proves it is topological, with a non-trivial local Chern number in its bulk even for energies residing within the extent of the middle band. Furthermore, the non-trivial bulk topology can be viewed as forcing the localizer gap to close around the Chern metal’s entire edge, as the local Chern number must be trivial far away from the system and, thus, the localizer gap along any path connecting the system’s interior and exterior must close for one of the localizer’s eigenvalues to switch signs, see Figs. 1f.

To our knowledge, other methods of defining a local or global index all rely on some notion of a gap in the bulk spectrum, perhaps a mobility gap, and are not designed to work in a metallic setting. Indeed, the localizer index was initially designed to work in the presence of a bulk gap, since a bulk gap causes a localizer gap $[78,80]$. Nevertheless, we have found that useful localizer gaps can still appear even in the absence of a bulk gap, due to the spatial separation between degenerate states that can be revealed using pseudospectrum-based methods. This feature allows the Clifford pseudospectrum to unambiguously identify non-trivial topology in metals and other gapless systems.

As the Clifford pseudospectrum yields a set of local, real-space definitions for finding boundary-localized states and determining topological invariants, the entire mathematical machinery of the localizer is immediately applicable in the presence of disorder without alteration. Thus, we can show that the topology of the Chern metal is robust against perturbations that do not close the gap between the systems first and third bands, $\Delta E$ in Fig. 1h, i.e., those bands which originate from the Haldane honeycomb lattice. To demonstrate this, we add on-site disorder to the system with strength $W$, such that
each vertex has an independent, uniformly distributed random on-site energy in the range $[-W/2, W/2]$. For $W < \Delta E$, the topological character of the system remains unchanged with the entire bulk still possessing a non-trivial local Chern number, an example of one disorder realization is shown in Fig. 2a. As the strength of the disorder is further increased, $W > \Delta E$, the system begins to revert to a trivial phase, with an example system shown in Fig. 2b. Nevertheless, even at this strength of disorder, regions within the system can still be in a topological phase, and these regions can be identified using the local Chern number.

To demonstrate the generality of using the Clifford pseudospectrum to identify topological metals, we prove the existence of robust higher-order topological metallic phases with in-band corner-localized states and find the associated local topological invariant. Here, we consider a 2D chiral and $C_{4h}$ symmetric lattice with four sites per unit cell, whose tight-binding model is schematically shown in Fig. 3a, and in which $v$ and $w$ are the intra- and inter-unit cell couplings, respectively. When a magnetic flux is uniformly threaded through this system, it becomes an insulator with a bulk bandgap at $E = 0$, and when the system is in its topological phase, $w > v$, localized states appear at each corner of the system with energies pinned to $E = 0$ due to the system’s chiral symmetry $[28, 31]$. Without this flux, the middle two bulk bands of this system are degenerate and centered at $E = 0$, as shown in Fig. 3b. Previous studies of this flux-less system with $w > v$ have shown that so long as $C_{4h}$ (and chiral) symmetry are preserved, corner-localized states exist that are prohibited from hybridizing with the degenerate bulk states $[57, 58]$, and are associated with a non-trivial fractional corner charge invariant $[59]$. However, these arguments do not hold in the absence of $C_{4h}$ symmetry, nor do they readily generalize to other gapless systems at $E = 0$ suspected of exhibiting higher-order topological behaviors.

Here, we can first use the 2D Clifford pseudospectrum to see that the topological corner-localized states must remain approximately localized to the corners until any added disorder is strong enough to close this gap, information which is not available in the system’s local density of states, Figs. 3c,d. However, the metallic system in Fig. 3b is in symmetry class AIII, so the 2D localizer is not connected to a non-trivial topological invariant for this system $[81, 83, 84]$. Instead, we can leverage the real-space construction of the localizer and project the system into a single spatial dimension to make use of class AIII’s 1D integer invariant, $[78, \S 4.1]$. To do so, we construct a position operator that effectively flattens the lattice along one of its diagonals, $D = (X + Y)/2$, a choice which spatially isolates two of the system’s corners while obscuring the other two with overlapping bulk vertices. The local topological index along this diagonal coordinate is then

$$\nu_{D} \left( \frac{x+y}{2} , 0 \right) = \frac{1}{2} \text{sgn} \left( Q_{1} L \left( \frac{x+y}{2} , 0 \right) (D, H) Q_{2} \right) \in \mathbb{Z},$$

where $Q_{1} = [0, I]$, $Q_{2} = [I, 0]^{T}$, $H$ is the system’s chiral operator, $\Pi H \Pi = -H$, and again we assume that the localizer gap is non-zero $[78, 79]$. For a true 1D system, $\nu_{D}$ is a local version of the 1D winding number, while for higher-order topological phases in higher dimensional systems it is a local version of the corresponding multipole winding number $[53]$.

Calculating Eq. 3 along the diagonal of the metallic system in Fig. 3b reveals that it is a higher-order topological metal: the system acquires a non-trivial invariant after the localizer gap first closes at the corner of the system, indicating the presence of a corner-localized state, cyan curves in Fig. 3. Moreover, this corner-localized state is protected by a large localizer gap, preventing it from moving into the system’s bulk for disorder strengths $W < 0.5\Delta E$. (Here, $\Delta E$ is the bandgap between the bottom and middle bands, or equivalently the gap between the middle and top bands.) Thus, even though the corner-localized states will hybridize with the bulk for any strength of disorder, the system’s Clifford pseudospectrum identifies that these states must maintain strong support on the system’s corners until the disorder is strong enough to close the localizer gap. Finally, we can explicitly confirm this topological protection by

FIG. 3. (a) Schematic of the tight-binding model for a higher-order topological metal with intra-unit cell couplings $v$, and inter-unit cell couplings $w$. (b) Bulk band structure with $w/v = 3$. $\Delta E/v = 2$ is the bandgap between the top (or bottom) band and the middle bands. (c) Local density of states at $E = 0$. Each lattice site is represented as a 2D Gaussian with radial width $r_{0} = 0.5a$. (d) 2D localizer gap, $\min(|\sigma(K_{x}(x, y, H))|)/\Delta E$ at $x = (x, y, E = 0)$ with $\kappa = 0.1$. 

two bulk bands of this system are degenerate and centered at $E = 0$, as shown in Fig. 3b. Previous studies of this flux-less system with $w > v$ have shown that so long as $C_{4h}$ (and chiral) symmetry are preserved, corner-localized states exist that are prohibited from hybridizing with the degenerate bulk states $[57, 58]$, and are associated with a non-trivial fractional corner charge invariant $[59]$. However, these arguments do not hold in the absence of $C_{4h}$ symmetry, nor do they readily generalize to other gapless systems at $E = 0$ suspected of exhibiting higher-order topological behaviors.

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adding disorder to the system which breaks all crystalline symmetries and time-reversal symmetry, where we numerically observe the ensemble averaged localizer gap to remain open and the topological index to remain pinned to $v_L = 1$ with little variance even for $W = 1.5 \Delta E$. This provides numerical evidence for the notion that, in practice, for uncorrelated disorder the localizer gap is usually an underestimate of the strength of the topological protection in a system.

In conclusion, we have developed a general theory for assessing a metallic or gapless system’s topology using its Clifford pseudospectrum, even in the presence of disorder. This theory is able to both demonstrate the existence of boundary-localized modes despite a degenerate background continuum, and yields a measure of the strength of the topological protection these modes possess. Although we have only explicitly demonstrated this theory for Chern and higher-order topological metals, this theory should extend without difficulty to all symmetry classes and for systems in any dimension $d$ [78–80]. As such, this theory should enable the discovery of novel topological phases of matter in natural and artificial metals and other gapless materials.

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