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Teleportation of Berry curvature on the surface of a Hopf insulator

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The paradigm of topological insulators asserts that an energy gap separates conduction and valence bands with opposite topological invariants. Here, we propose that equal-energy bands with opposite Chern invariants can be spatially separated, onto opposite facets of a finite crystalline Hopf insulator. On a single facet, the number of Berry-curvature quanta is in one-to-one correspondence with the bulk homotopy invariant of the Hopf insulator; this originates from a bulk-to-boundary flow of Berry curvature which is not a type of Callan-Harvey anomaly inflow. In the continuum perspective, such nontrivial boundary states arise as nonchiral, Schrödinger-type modes on the domain wall of a generalized Weyl equation, describing a pair of opposite-chirality Weyl fermions acting as a dipolar source of Berry curvature. A rotation-invariant regularization of the generalized Weyl equation manifests a generalized Thouless pump, which translates charge by one lattice period over half an adiabatic cycle, but reverses the charge flow over the next half.

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The Hopf insulator [1] is the prototype of a topological insulator that is neither a stable topological insulator in the tenfold way [2,3], nor a fragile topological insulator[4–6] in topological quantum chemistry [7,8]. Having a $k$-dependent Hamiltonian that is only a sum of Pauli matrices, the Hopf insulator is conceptually the simplest topological insulator. As originally touted by Moore, Ran, and Wen [1], the Hopf insulator is the first-known three-dimensional (3D) magnetic bulk-insulator with topological surface states, as illustrated in Fig. 1(a). Contrary to some expectations [9–11], we will demonstrate that all surfaces can be made insulating while preserving the bulk gap [cf., Fig. 1(b)]. What then is “topological” about such surface states which can be spectrally disconnected from the bulk states?

We will show that the faceted Chern number—defined as the first Chern number of all bands localized to a single surface facet, independent of their filling—is in one-to-one correspondence with the integer-valued, bulk homotopy invariant $\chi$. $\chi$ classifies maps from the 3D Brillouin zone (BZ) to the Bloch sphere of pseudospin-half wave functions [11,12], and is given by a BZ integral of the Abelian Chern-Simons three-form [1,13]:

$$\chi = -\frac{1}{4\pi^2} \int_{BZ} A \cdot \nabla \times A d^3k,$$

(1)

with $A(k) = \langle u|i\nabla_k u \rangle$ the Berry connection of the energy-nondegenerate band [14]. The above integral is gauge invariant only if the first Chern number vanishes on any 2D cut of the BZ; this triviality of the first Chern class [15] is assumed throughout this work.

In the geometric theory of polarization [16–18], the charge polarization is proportional to $\int_{BZ} A$; analogously, one may view $\int_{BZ} A \cdot \nabla \times A$ as proportional to a real-space polarization of Berry curvature [19–21]. Just as the charge polarization is revealed by the charge that accumulates at a surface termination [22], a Berry-curvature polarization of $\chi$ contributes $(-\chi/2)e^2/h$ to the geometric component ($\sigma_{xy}^g$) of the surface anomalous Hall conductance (SAHC) [23–25]. Crucially, the bulk conduction and valence bands individually and equally contribute $(-\chi/2)e^2/h$, owing to the fundamental antisymmetry of all Pauli-matrix Hamiltonians: $\sigma_{xy}^g(k) = -\sigma_{xy}(k)$ for all bands. In the Hilbert space are accounted for, the net contribution to $\sigma_{xy}^g$ should vanish [24], hence there should exist surface band(s) which contribute $\chi e^2/h$ to $\sigma_{xy}^g$. This argument is confirmed numerically in Fig. 1(c) and will be demystified in this work.

FIG. 1. (a) The red line depicts the 001-surface states of the Hopf insulator in the Moore-Ran-Wen tight-binding model [1] with $\chi = 1$ and open boundary conditions. (b) The surface band of (a) is detached by modifying the surface Hamiltonian, as detailed in the Supplemental Material [26]. (c) For a 50-cell-tall 001 slab, we plot the layer-resolved SAHC [Eq. (12) in Ref. 19] of the bulk valence band (blue), bulk conduction band (red), and surface band (black) illustrated in (b). Summing the layer-resolved SAHC over ten layers approximates $\sigma_{xy}^g[e^2/h]$ to exponential accuracy.
It will be shown that such nontrivial surface bands originate from a bulk-to-boundary flow of Berry curvature, at the critical point between the trivial and Hopf insulator. Such flow does not occur via the Callan-Harvey anomaly inflow mechanism [27,28], which is understood through chiral zero modes of the Dirac equation with a mass coupling to a domain wall [29,30]. Instead, the surface states of the Hopf insulator arise as nonchiral, Schrödinger-type modes on the domain wall of a generalized Weyl equation, describing a pair of opposite-chirality Weyl fermions acting as a dipolar source of Berry curvature. A single surface facet of a Hopf-insulating crystal is undescirbable by a 2D lattice model of a Chern insulator, because the conjugate surface states (with opposite Chern number) lie on the opposite facet of a finite slab, realizing a nonlocal “teleportation” of Berry curvature.

I. FACETED CHERN NUMBER AS A TOPOLOGICAL INVARIANT

We propose the faceted Chern number $C_f$ as a topological invariant for any three-space-dimensional Hamiltonian that is a two-by-two matrix at each $k \in \text{BZ}$, with a spectral gap (at each $k$) separating a low-energy and high-energy bulk band with trivial first Chern class. For such category of Hamiltonians which include the Hopf insulator, we consider a surface termination whose reduced Brillouin zone (rBZ) is a 2D cut of the BZ. Throughout this work, “bulk” objects refer to the crystalline interior which has the symmetry of a 3D space group, up to exponentially weak corrections due to a surface termination.

The triviality of the first Chern class implies any surface-localized mode is continuously deformable to a flat-band dispersion [31,32] and is therefore detachable from bulk bands. To “detach” means to energetically separate a surface band from bulk bands while preserving all crystallographic spacetime symmetries of the surface, such that the projector to the surface-band wave function is continuous throughout rBZ, as illustrated in Figs. 1(a) and 1(b). (In contrast, the surface states of a 3D Chern insulator [33] are undetachable [34]). The conceptually simplest formulation of the faceted Chern number is as a rBZ integral of the Berry curvature $\mathcal{F}$ of the surface-band wave function:

$$
C_f := \frac{1}{2\pi} \int_{\text{rBZ}} \text{Tr}[\mathcal{F}(k) \cdot \hat{n}] d^2 k, \tag{2}
$$

with $\hat{n}$ the outward-normal vector for a chosen facet, and Tr a trace over all surface bands, independent of electron filling. The second half of this work will present a more general formulation of $C_f$ that is well defined without need of detachment.

Let us demonstrate that $C_f$ is invariant under continuous deformation of the surface-terminated Hamiltonian, so long as both bulk gap and bulk translational symmetries are maintained. Since surface bands are detachable, their wave function is exponentially localized to the surface, and therefore their net Chern number cannot change under a bulk deformation alone. What remains is to prove the absence of a continuous deformation between two Hamiltonians with the same bulk but with distinct faceted Chern numbers: $C_f > C_f'$. Assume to the contrary that such a deformation exists and is parametrized by $\lambda \in [0, 1]$. It is simplest to view $C_f$, $C_f'$ as applying to the top facet of a finite slab, with periodic boundary conditions in two surface-parallel directions. As $\lambda$ is varied, we hypothesize that $(C_f - C_f')$ quanta of Berry curvature can leave the top facet and enter the bulk [20,21]. Since the bulk Hamiltonians at $\lambda = 0$ and $\lambda = 1$ are indistinguishable, this Berry curvature must finally end up at the bottom facet of the slab. There must then exist an adiabatic cycle for a bulk Hamiltonian $H(k, \lambda)$ that is periodic in $\lambda$, such that $(C_f - C_f')$ quanta of Berry curvature are translated by a surface-normal lattice vector over one cycle. If this translation occurs through the low-energy (resp. high-energy) band of $H(k, \lambda)$, then $(C_f - C_f')$ is identifiable as the second Chern number $C_2$ of the low-energy (resp. high-energy) band; $C_2$ is defined [35] as the $(k, \lambda)$ integral of the second Chern character. The wrongness of our hypothesis becomes self-evident, because $C_2$ necessarily vanishes for any band spanned by a single Bloch function [of $(k, \lambda)$] that is analytic with respect to $k$ [36].

The above argument relied on identifying $C_2$ as the number of Berry-curvature quanta pumped by one lattice vector in an adiabatic cycle. Indeed, if $H(k, \lambda)$, with trivial first Chern class and $C_2 \neq 0$, were diagonalized with open boundary conditions in the $z$ direction, then the boundary theory describes $(3+1)$D Weyl fermions with a net chiral charge [37] equal to $C_2$, in the three-dimensional, momentum-like space of $(k_1, k_2, \lambda)$ [21]. (These Weyl fermions may be derived from a continuum model, as chiral zero modes of the $(4+1)$D Dirac equation with a domain wall [27,35]). Let us view the boundary theory as $(2+1)$D fermions tuned by $\lambda$: over one $\lambda$ cycle, $C_2$ quanta of Berry curvature must be transferred at critical closings of the boundary energy gap. Since the full Hamiltonian (that operates on both boundary and bulk Hilbert spaces) is periodic in $\lambda$, there must be a compensating pump of curvature through the bulk to exactly cancel the transfer of curvature at the boundary. Such a cancellation occurs between two systems of differing dimensionality, and has the same origin as the Callan-Harvey anomaly inflow [27,28,38]. We have proved that $C_2 \neq 0$ implies a Berry-curvature pump in the bulk; the converse statement, that a pump implies $C_2 \neq 0$, has been proved by formulating the Chern-Simons magnetoelectric polarizability in terms of “hybrid Wannier sheets” [20,21].

Our argument for the invariance of $C_f$ shows the Callan-Harvey effect does not explain the Berry curvature on the Hopf-insulator surface. (In contrast, the Callan-Harvey effect is responsible for the SAHC of the “layered Haldane model” [21].) Understanding the Hopf insulator not only reveals a new mechanism for a bulk-to-boundary flow of Berry curvature, but also leads to the bulk-boundary correspondence $\chi = C_f$.

II. BULK-TO-BOUNDARY FLOW OF BERRY CURVATURE

In the continuum perspective, the advertised mechanism may be understood in terms of nonchiral domain-wall modes of a generalized Weyl equation: $(i\partial_t - H)\psi = 0$ with

$$
H(k) = -B \cdot \sigma \ B(k) = z^\prime \sigma z^\prime; \quad \sigma := (\sigma_1, \sigma_2, \sigma_3) \\
z(k) = (z_1, z_2)^T = (k_1 + ik_2, k_3 + i\phi)^T; \quad \phi \in \mathbb{R}. \tag{3}
$$
This equation describes the critical transition between a trivial and a Hopf insulator, in analogy with how the Dirac equation describes the critical point for an insulator without nontrivial Chern class [35]. If \( \phi = 0 \), both bands disperse quadratically in all momentum directions, and they touch at a point which acts as a dipolar source of Berry curvature, illustrated in Fig. 2(a) as a unit positive (resp. negative) Berry flux out of the southern (resp. northern) hemisphere. Such a Berry dipole contrasts with linearly dispersing Weyl points that act as monopole sources [39]. The dipole moment lies parallel to the \( k_3 \) axis, which is also an axis of rotation:

\[
U_\theta H(k)U^{-1}_\theta = H(k', k_2, k_3), \quad U_\theta = e^{i\theta a1/2}
\]

with \( k'_1 = k_1 \cos \theta - k_2 \sin \theta \), and \( U_\theta \) a spinor matrix representation with spin operator \( a1/2 \). For \( \phi \neq 0 \), \( \phi \| z/||z|| \) \( \to B/||B|| \) exhibits the standard Hopf map from \( S^3 \) \( \to S^2 \), and the continuum analog of the Hopf invariant equals

\[
\frac{1}{4\pi^2} \int_{\mathbb{R}^3} A \cdot \nabla \times A d^3k = \frac{1}{2} \text{sgn} [\phi], \quad (5)
\]

for both the low-energy wave function (\( z/||z|| \)) and its orthogonal complement (\( \sigma z/||z|| \)). \( \phi = 0 \) is thus the critical point for a unit change in \( \chi \) for both low- and high-energy bands. Away from criticality, the spin texture of the low-energy (resp. high-energy) band is skyrmionic (resp. antiskyrmionic) over the \( k_1k_2 \) plane, as illustrated in Fig. 2(c). (In comparison, the meronic spin texture [40] of a \( (2+1)D \) massive Dirac fermion is “half” of a skyrmion.)

To manifest the nontrivial boundary mode that develops at criticality, we solve Eq. (3) with \( k_3 \to -i\partial_3 \) and \( \phi(r_3) \) having a domain-wall profile. It is analytically convenient to choose \( \phi(r_3) = \phi' r_3 \) that is linear in the interval \( r_3 < \Lambda \) (with \( \Lambda \gg |\phi'|^{-1/2} \)), with \( \phi' \) tapering off to a constant outside this interval, as depicted in Fig. 2(b). Then a Gaussian-localized, spin-polarized mode \( \psi_n \) exists with a Schrödinger-type dispersion \( \epsilon_n \):

\[
\psi_n = k_s e^{-i\omega \epsilon_n^2/2}, \quad \epsilon_n = -\eta (k_1^2 + k_2^2 - |\phi'|),
\]

with \( \sigma k_{\pm} = \pm k_{\pm} \). The mass and spin depend on \( \text{sgn} [\phi'] := -\eta \); we refer to modes with positive (resp. negative) mass with respect to \( (k_1, k_2) \) as electron-like (resp. hole-like).

The contrasting spin textures—constant for the domain-wall mode but (anti)skyrmionic for the bulk modes—imply that the integrated Berry curvature vanishes for both electron- and hole-like domain-wall modes, but equals \( +2\pi \) (resp. \(-2\pi \)) for the electron-like (resp. hole-like) bulk mode. We will see that the differential curvature—between electron-like bulk and electron-like domain-wall modes—is maintained upon regularizing our continuum model on a lattice. The Hopf insulator is a lattice regularization satisfying that all bulk modes have trivial first Chern number; this would imply that the regularized domain-wall mode has a nontrivial first Chern number \( (= \eta) \) which depends on the orientation of the domain wall, like how the facet number depends on the facet orientation \( \hat{n} \) [cf., Eq. (2)].

Since \( \phi = 0 \) describes a Berry dipole and not a monopole, a regularization can be found without any fermion doubling [37], meaning that the energy gap of the lattice model closes at a single isolated wave vector (the BZ center) when \( \phi = 0 \). A lattice regularization satisfying the above-stated properties is given by the Moore-Run-Wen tight-binding model [1], though they did not emphasize the dipole picture that is presented here. Their lattice Hamiltonian has the form of Eq. (3) with \( z_1 = \sin k_1 + i \sin k_2, z_2 = \sin k_3 + i(\phi + \sum_{j=0}^3 \cos k_j - 3) \). The tight-binding Hilbert space may be viewed as comprising spin-half particles \( (\sigma_i = \pm 1) \) in each unit cell of a tetragonal lattice.

### III. BULK-BOUNDARY CORRESPONDENCE

If \( \chi = C_f \) is proved for the Moore-Run-Wen model, the correspondence would extend to the entire homotopy class of translation invariant, two-by-two Hamiltonians. This is because \( \chi \) and \( C_f \) are individually invariant under any continuous, bulk-gap-preserving deformations that preserve the bulk-translational symmetry; this fact is well known for \( \chi \) [1,12] and has been proved above for \( C_f \). Hamiltonians with nonzero \( \chi \) may have any non-translational symmetry that does not invert the pseudoscalar: \( \chi \to -\chi \). Particularly, the Moore-Run-Wen regularization retains an order-4 rotational symmetry [cf., Eq. (4)], which not only allows us to utilize our rotation-symmetric domain-wall analysis, but also manifests several topologically robust features unique to rotation-invariant Hopf insulators.

For sufficiently negative \( \phi \), \( H(k) \approx \phi^2 \sigma \), implies that both low- and high-energy bands are spin polarized and the Hopf invariant vanishes. It is instructive to represent both bands by basis functions that are extended as Bloch functions with wave vector \( (k_1, k_2) \in \mathbb{B}Z \), but exponentially localized in the \( z \) direction as Wannier functions [41-43]. In units of the lattice period, the positional center \( Z \) of a hybrid function is related [16] to the Berry phase as \( Z(k_1, k_2) = \int_0^{2\pi} A.\epsilon d\bar{k}/2\pi \). Owing to the discrete translational symmetry along \( z \), the hybrid centers \( Z \) are arranged as a Wannier-Stark ladder [44-46] with unit spacing between adjacent rungs. The low-energy band having only spin-down character implies the Berry connection can be trivialized, implying \( Z = 0 \) (modulo integer) for all \( (k_1, k_2) \). For finite \( \phi < 0 \), the low-energy band acquires some spin-up character except at the four rotation-invariant \( (k_1, k_2) \) points [denoted as \( \Gamma, X, Y, M \) in Fig. 3(a), where distinct rotational representations cannot mix; each hybrid function retains the topology of a “flat sheet” which is pinned to integer values at the rotation-invariant \( (k_1, k_2) \) points.
The unit gain of angular momentum for the top-surface band introduces an irremovable twisting of the wave function [49] that is quantified by the Chern number \( C_f = 1 \). Bearing in mind that the surface-normal vector \( \hat{n} \) flips between top and bottom surfaces [cf., Eq. (2)\], we arrive at \( C_f = \chi = 1 \) for both surfaces. The generalization to \( C_f = \chi = N \) is attained by substituting \( k_3 \to N k_3 \) (\( N \in \mathbb{Z} \)) in the Moore-Ran-Wen model, such that \( \phi = 0 \) marks a critical point with \( |N| \) Berry dipoles. We remark that the full subspace of surface states (on a single facet) has a net Chern number \( = C_f \); in contrast, the full Hilbert space of any strictly 2D, tight-binding Hamiltonian must have vanishing net Chern number. The absence of a strictly 2D description also applies to \( \mathbb{Z}_2 \)-topological-insulating surface states, but in the latter case it is because an odd number of gapless, chiral fermions [27] violates the fermion-doubling theorem [37,50].

Our Chern-number analysis may be verified by detaching surface bands and numerically calculating \( C_f \) through Eq. (2). It is possible to formulate \( C_f \) without detaching surface bands, but requiring the milder condition that a spectral gap exists throughout the rBZ and separates two orthogonal subspaces \( P \) and \( Q \). Such a gap always exists for certain surface terminations of the considered class of Hamiltonians, because the surface bands are continuously deformable to hybrid Bloch-Wannier bands which disperse like “flat sheets” [31,48]. We consider a semi-infinite geometry that is periodic in \( x \) and \( y \), and with the position operator \( \hat{z} \) taking only negative values. Let us diagonalize the projected position operator \( \hat{\mathbf{P}}^2 \hat{P} \), and define \( C_f^p[n] \) as the first Chern number of the \( n \) Bloch-Wannier eigenbands whose eigenvalues lie closest to \( \hat{z} = 0 \). Viewed as a sequence in \( n \), \( C_f^p[n] \) has a unique accumulation point \( (\equiv C_f^p) \) because all bulk eigenbands have trivial first Chern class. Analogously defining \( C_f^Q \) as the accumulation point for the orthogonal subspace \( Q \), the faceted Chern number is then \( C_f = C_f^p + C_f^Q \). This formulation manifests the unique definition of \( C_f \); in particular, \( C_f \) is invariant if a Chern-insulating layer is adsorbed onto the surface.

What does \( \chi = C_f \) imply for the magnetoelectric response of the Hopf insulator? It is known that the geometric contribution to the frozen-lattice, orbital magnetoelectric polarizability[19,23,25,34,35,51] equals \((\theta/2\pi \mod 1)e^2/h\), with the “axion angle” [52] \( \theta \) equal to an integrated Chern-Simons three-form of the Berry connection [19,35]. For the considered class of Hamiltonians, \( \theta \) is gauge-invariant and simplifies to \( \pi \chi \), thus the Hopf insulator exemplifies the simplest axion insulator[19,34,35,53–55] with only a Pauli-matrix Hamiltonian. The possibilities for SAHC on different facets of a Hopf-insulator crystallate are rich, and depend on the energy dispersion of surface bands as well as the electrochemical potential; the latter is tunable by differential doping or gating. Partially filled surface bands on any facet behave like a 2D anomalous Hall metal [56]. The detachability of surface bands allows also for complete filling and depletion; e.g., if the topologically nontrivial surface band is completely filled on the 001 facets and completely depleted on the 010 and 100, then \(|C_f|\) number of chiral “hinge” modes [29,57–59] will run around the edges of the 001 facet, a manifestation of higher-order topology.

FIG. 3. Dispersion of the projected-\( z \) operator over a high-symmetry line in the rBZ, for a 50-cell-tall 001 slab. \( z \) is projected to the low-energy band of the Moore-Ran-Wen model in (a)–(c), and to the high-energy band in (d), \( \phi = -0.2 \) in (a), and \( = 1 \) in (b)–(d). (a) and (b) illustrate the bulk dispersion, while (c) and (d) depict the top and bottom surfaces respectively. The expected spin \( \langle \sigma_z/2 \rangle \) is depicted according to the color scheme on the right.

As negative \( \phi \) is tuned through zero, the spins of the bulk eigenstates of \( H(0) = \phi^2 \sigma_z \) are not inverted; nevertheless, the Hopf invariant increases by unity [cf., Eq. (1)]. Analogously, the Berry phase of the low-energy mode in the continuum model is \( \int_{\Gamma} A_z(0, 0, k_3)dk_3 = \pi \text{ sgn} [\phi] \), which implies a \( 2\pi \) quantum of Berry phase is transferred from the high- to low-energy band (at the rBZ center). Therefore, there must be a discontinuous change in the connectivity of the Wannier-Stark ladder, resulting in upward-protruding (resp. downward-protruding) sheets for the high-energy (resp. low-energy) band, as illustrated in Figs. 3(b) and 3(d). The triviality of the first Chern class ensures the periodicity of \( \text{Tr} \hat{\mathbf{W}} \). Despite the absence of a conventional Thouless pump [47], observe that the hybrid center is translated by exactly one lattice period at the halfway mark before returning to its original position. Such a returning Thouless pump implies that the Wannier function—obtained by two-dimensional Fourier transform of the hybrid Bloch-Wannier functions—cannot be localized to a single lattice site. (There is, however, no obstruction to exponentially localized Wannier functions respecting all crystallographic spacetime symmetries, according to a theorem in Ref. [32]).

The above-described connectivity of Wannier-Stark sheets holds for an infinite ladder, but is frustrated for a finite slab with rotation-invariant surface terminations, meaning that protrusions of the lowermost (resp. uppermost) sheet of the high-energy (resp. low-energy) band are incompatible with the confining surface potentials. These two frustrated sheets are continuously deformable to the surface bands of the finite-slab Hopf insulator [31,48]. For these surface bands, the spin at the rBZ center is determined by our domain-wall analysis, which asserts that the electron-like (resp. hole-like) mode localized to the bottom (resp. top) surface has spin down (resp. up); this is confirmed by a numerical calculation illustrated in Figs. 3(c) and 3(d). A colloquial interpretation is that the lowermost sheet of the high-energy band “acquires” a spin-down particle from the low-energy band, which has been “left over” at the bottom surface due to a returning Thouless pump in the upward direction. Effectively, there is a mutual exchange of rotational representations between surface bands localized to opposite facets of a finite slab, manifesting a symmetry “teleportation.”
IV. OUTLOOK

The first solid-state proposal of the Hopf insulator—on a distorted pyrochlore lattice with noncollinear magnetic order and strong spin-orbit coupling—has not been realized in twelve years [1]. It has not been recognized that the Moore-Ran-Wen tight-binding model is also compatible with an integer-spin representation of the black-white magnetic space group $P4mnm'$, which applies to a parity-breaking ferromagnet with negligible spin-orbit coupling; the two relevant orbitals (per unit cell) differ in angular momentum by $h$. We hope this observation helps to widen the search for solid-state Hopf insulators, which would complement existing ultracold-atomic platforms [60,61].

We leave to future work the generalization of the bulk-boundary correspondence to Hopf-Chern insulators, analogs of the Hopf insulator with nontrivial bulk Chern invariants [11]. It is interesting to speculate if the static bulk-boundary correspondence presented here has any analogies with the physics of (2+1)D topological insulators subject to a quench [62] or to a periodic drive [63,64], for which the Hopf invariant also provides a topological classification.

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