Three-dimensional quantum anomalous Hall effect in hyperhoneycomb lattices

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We address the role of short-range interactions for spinless fermions in the hyperhoneycomb lattice, a three-dimensional (3D) structure where all sites have a planar trigonal connectivity. For weak interactions, the system is a node-line semimetal. In the presence of strong interactions, we show that the system can be unstable to a 3D quantum anomalous Hall phase with loop currents that break time-reversal symmetry, as in the Haldane model.

We find that the low-energy excitations of this state are Weyl fermions connected by surface Fermi arcs. We show that the 3D anomalous Hall conductivity is \( e^2/(\sqrt{3}a\hbar) \), with \( a \) the lattice constant.

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Introduction. The quantum Hall conductivity describes dissipationless transport of electrons in a system that breaks time-reversal symmetry (TRS) due to an external applied magnetic field. In two dimensions (2D), the current is carried through the edges [1], and the Hall conductivity \( \sigma_{xy} \) is quantized in units of \( e^2/\hbar \). In three dimensions (3D), the Hall conductivity is not universal and has an extra unit of inverse length. As shown by Halperin [2], the 3D conductivity tensor on a lattice has the form \( \sigma_{ij} = e^2/(2\pi \hbar) \epsilon_{ijk} G_k \), where \( G \) is a reciprocal lattice vector (it could be zero). The realization of the 3D quantum Hall effect has been proposed in systems with very anisotropic Fermi surfaces [3–5], or else in node-line semimetals [6–9], where the Fermi surface has the form of a line of Dirac nodes [10–24].

Equally interesting would be to realize the 3D quantum anomalous Hall (QAH) effect [25–28], where the anomalous Hall conductivity emerges from the topology of the 3D band structure in the absence of Landau levels. The first proposal for a Chern insulator system was the Haldane model [29] on the honeycomb lattice, where loop currents break TRS and can produce a nonzero Chern number in the bulk states. Hyperhoneycomb lattices have the same planar trigonal connectivity of the honeycomb lattice [see Fig. 1(a)], and hence could provide a natural system for the emergence of a 3D QAH conductivity. While we are not aware of a concrete example of a material that realizes this lattice [30], this system may directly appeal to experimental groups working in the field of quantum simulation of topological phases. Very recently, the Haldane model was simulated with cold atoms [31] and in quantum circuits [32].

In this Rapid Communication, we describe the 3D QAH state that emerges from repulsive interactions in a hyperhoneycomb lattice with spinless fermions. This state competes with a CDW state, and produces a very anisotropic gap around a line of Dirac nodes in the semimetallic state. Due to a broken inversion symmetry, the QAH gap changes sign along the nodal line, forming Weyl points connected by Fermi arcs [33,34]. We show that the QAH conductivity of the surface states is \( e^2/(\sqrt{3}a\hbar) \), with \( a \) the lattice constant.

Lattice model. We start from the tight-binding model of the hyperhoneycomb lattice, which has four atoms per unit cell and planar links spaced by 120°, as shown in Fig. 1(a). The lattice has three vector generators \( a_1 = (\sqrt{3}, 0, 0) \), \( a_2 = (0, \sqrt{3}, 0) \), and \( a_3 = (-\sqrt{3}/2, \sqrt{3}/2, 0) \), and the corresponding reciprocal lattice vectors \( b_1 = (2\pi/\sqrt{3}, 0, -\pi/3) \), \( b_2 = (0, -2\pi/\sqrt{3}, \pi/3) \), and \( b_3 = (0, 0, 2\pi/3) \). For a model of spinless fermions, which could physically result from a strong Rashba spin-orbit coupling [35], the kinetic energy is \( H = -t \sum_{i,j} (a_i^\dagger a_j + \text{H.c.}) \), where \( a_i \) destroys an electron on site \( i \), \( t \) is the hopping energy, and \( (ij) \) denotes nearest-neighbor (NN) sites. In the four-sublattice basis, the Hamiltonian is a \( 4 \times 4 \) matrix [7]:

\[
H_0 = -t \begin{pmatrix}
0 & \Theta_x & 0 & e^{ik_z} \\
0 & 0 & e^{-ik_z} & 0 \\
e^{-ik_z} & 0 & \Theta_y & 0 \\
0 & e^{ik_z} & 0 & \Theta_x \end{pmatrix},
\]

where \( \Theta_y = 2e^{ik_z/2} \cos(\sqrt{3}k_z/2) \), with \( y = x, y, z \) and \( k \) is the momentum away from the center of the Brillouin zone (BZ). The electronic structure has a doubly degenerate zero energy line of nodes in the form of a Dirac loop at the \( k_z = 0 \) plane, \( k_{0}(s) \equiv [k_{x}(s), k_{y}(s), 0] \) in some parametrization that satisfies the equation \( 4\cos[\sqrt{3}k_{y}(s)/2] \cos[\sqrt{3}k_{z}(s)/2] = 1 \), as schematically depicted in Fig. 1(b). The projected low-energy Hamiltonian has the form

\[
H_{0,p}(q) = [v_{x}(s)q_{x} + v_{y}(s)q_{y}]\sigma_{x} + v_{z}(s)q_{z}\sigma_{y},
\]

where \( q \equiv k - k_{0}(s) \) is the momentum away from the nodal line, \( \sigma_{x}, \sigma_{y} \) are Pauli matrices, with \( v_{x}(s) = \frac{\sqrt{3}t}{2} \sin[\sqrt{3}k_{y}(s)/2]/(1 + \alpha^2) \), \( v_{y}(s) = \frac{\sqrt{3}t}{2} \alpha \sin[\sqrt{3}/2]/(1 + \alpha^2) \), and \( v_{z} = -3a\alpha/(1 + \alpha^2) \) the quasiparticle velocities, and \( \alpha(s) = 2\cos[\sqrt{3}/2] \). Hamiltonian (2) corresponds to the low-energy spectrum

\[
\epsilon(q) = \sqrt{(v_{x}q_{x} + v_{y}q_{y})^2 + v_{z}^2q_{z}^2},
\]

which is gapless along the nodal line.

The total Hamiltonian is \( H = H_0 + H_I \), where

\[
H_I = \sum_{\langle i,j \rangle} (\hat{n}_{i} - 1)(\hat{n}_{j} - 1) + \sum_{\langle i,j \rangle} (\hat{n}_{i} - 1)(\hat{n}_{j} - 1).
\]
is the interaction term, with \( \hat{n}_i = a_i^\dagger a_i \) the density operator on site \( i \), and \( V_1 \) and \( V_2 \) are the repulsion between NN and next-nearest neighbors (NNN) sites, respectively. For spinless fermions, one possible instability is a charge density wave (CDW) state that corresponds to a charge imbalance among the different sublattices. The CDW state is defined by the four-component order parameter \( \rho_\alpha = (a_i^\dagger a_i) - \rho_0 \) with \( i \in \alpha \) belonging to sublattice \( \alpha = A,B,C,D \), as shown in Fig. 2, and \( \rho_0 \) a uniform density. At the neutrality point, the local densities at the four sites of the unit cell add up to zero, \( \sum_{\alpha} \rho_\alpha = 0 \). The nodal line is protected by a combination of TRS and mirror symmetry along the \( z \) axis. The state where \( \rho_A = -\rho_B = \rho_C = -\rho_D \), namely, \( (\rho, -\rho, -\rho, -\rho) \), breaks the mirror symmetry and opens the largest gap among all possible charge neutral configurations of \( \rho_\alpha \). The more symmetric state \( (\rho, \rho, -\rho, -\rho) \) does not open a gap. Hence, the former state is the dominant CDW instability. We will not consider other possible states that enlarge the size of the unit cell [36], such as an \( n \)-site CDW state, with \( n > 4 \).

The other dominant instability is the QAH state, where complex hopping terms between NNN sites lead to loop currents in the \( xz \) and \( yz \) planes, as shown in Fig. 2. Each plane can have loop currents with opposite flux \( \Phi \), producing zero magnetic flux in the unit cell, in analogy with the 2D case in the honeycomb lattice [29]. The QAH order parameter is defined as \( \chi_{ij} = (a_i^\dagger a_j) \), where \( i \) and \( j \) sites are connected by NNN vectors [37]. We define the ansatz \( \chi_{ij} = e^{i\phi_{ij}} \) for \( i,j \in \{A,C\} \) sublattices and \( \chi_{ij} = e^{i\phi_{ij}} \) for \( i,j \in \{B,D\} \), where \( \phi \) is real. Due to particle-hole symmetry, \( \chi_{ij} \) is purely imaginary and hence \( \phi, \phi = \pm \frac{\pi}{2} \). The state that minimizes the free energy of the system has total zero flux in the unit cell, \( \Phi_1 = -\Phi_2 \) (see Fig. 2), when the magnetic flux lines can more easily close. The QAH order parameter is \( \chi_{ij} = \pm i \chi \) for NNN sites and zero otherwise, with the + sign following the convention of the arrows in Fig. 2.

We perform a mean-field decomposition of the NN interaction in the CDW state \( (\rho) \) and of the NNN repulsion in the QAH order parameter \( \chi_{ij} \). For simplicity, we absorb the couplings \( V_1 \) and \( V_2 \) in the definition of the order parameters, \( \rho V_1 \to \rho \) and \( \chi V_2 \to \chi \), which have units of energy from now on. The effective interaction in the four-sublattice basis is

\[
H^{\text{MF}}_i = \begin{pmatrix}
\chi g - 3\rho & -\chi f & 0 & 0 \\
-\chi f^* & \chi g - 3\rho & 0 & 0 \\
0 & 0 & \chi g - 3\rho & 0 \\
0 & 0 & 0 & -g\chi + 3\rho
\end{pmatrix},
\]

where

\[
g(k) = 2[\sin(\sqrt{3}k_x) + \sin(\sqrt{3}k_y)]
\]

and

\[
f(k) = [e^{i3k_x/2} \sin(\sqrt{3}k_x/2) + e^{-i3k_x/2} \sin(\sqrt{3}k_x/2)].
\]

The mean-field Hamiltonian \( H^{\text{MF}} = H_0^{\text{MF}} + H^{\text{MF}}_i \) has an additional constant energy term \( E_0 = 6\rho^2 / V_1 + 16\chi^2 / V_2 \) that is reminiscent of the decomposition of the interactions to quadratic form.

The phase diagram follows from the numerical minimization of the free energy \( F \) with respect to \( \rho \) and \( \chi \) at zero temperature, \( \partial F / \partial \rho = \partial F / \partial \chi = 0 \). The semimetal state is unstable to a CDW order at the critical coupling \( V_{1,c} = 0.41t \), and to a QAH phase at \( V_{2,c} = 1.51t \). The CDW and QAH states compete with each other, as shown in Fig. 3. Fluctuation effects are expected to be less dramatic in 3D compared to the more conventional 2D case [37–39]. Hence, the mean-field phase diagram is likely a reliable indication of the true instabilities of the fermionic lattice for the spinless case.

In real crystals, screening and elastic effects lead to a distortion of the lattice in the CDW state, in order to minimize the Coulomb energy due to electron-ion coupling, which can be high [40]. While the CDW appears to be the leading instability over the QAH state, the elastic energy cost to displace the...
ions and equilibrate the charge in the electron-ion system may hinder the CDW order and favor the QAH phase when $V_2 > V_{2c}$.

**Low-energy Hamiltonian.** Integrating out the two high-energy bands using perturbation theory, the effective low-energy Hamiltonian (2) of the nodal line becomes massive, as expected. The leading correction to Hamiltonian (2) around the nodal line to lowest order in $\rho$ and $\chi$ has the form of a mass term

$$H_{1,\rho}(\mathbf{q}) = -[3\rho + m(\mathbf{k}_0) + v'_s q_x + v'_y q_y] \sigma_3, \quad (8)$$

gives the QAH mass at the nodal line, with $v'_s(s) = 2\chi [\cos(\sqrt{3}q_y(s)) + \frac{1}{\sqrt{3}} \cos(\sqrt{3}q_x(s)/2)]$ and $\alpha(s)$ defined below Eq. (2). The low-energy spectrum is

$$\epsilon(\mathbf{q}) = \pm \sqrt{\epsilon_0^2(\mathbf{q}) + [3\rho + m(\mathbf{k}_0) + v'_s q_x + v'_y q_y]^2}, \quad (10)$$

which describes either a uniformly gapped state in the CDW phase ($\rho \neq 0, \chi = 0$) or a nonuniform QAH gap ($\rho = 0, \chi \neq 0$) with six nodes at the zeros of $m(\mathbf{k}_0)$, as indicated in Fig. 4.

The CDW state breaks mirror symmetry along the $z$ axis, but preserves the screw axis symmetry and hence creates a fully gapped state that is rotationally symmetric along the nodal line. The QAH state, on the other hand, breaks inversion symmetry. The mass term (9) changes sign at six zeros along the nodal line, as shown in Fig. 4(b). Two zeros are located along the diagonal direction of the nodal line, at the points $\pm \mathbf{Q}_1 = (\frac{2\pi}{\sqrt{3}}, -\frac{2\pi}{\sqrt{3}}, 0)$. The other four zeros of $m(\mathbf{k}_0)$ are symmetrically located around that direction, at $\pm \mathbf{Q}_2 = \mp(\mathbf{Q}_+, \mathbf{Q}_-, 0)$ and $\pm \mathbf{Q}_3 = \pm(\mathbf{Q}_-, \mathbf{Q}_+, 0)$, as shown in Fig. 4, with $Q_x = \frac{1}{\sqrt{3}} \arccos(\frac{-1}{\sqrt{3}}) = \frac{1}{\sqrt{3}} \arccos(\frac{-2}{3})$. The position of the nodal points extracted from the low-energy Hamiltonian (8) is in agreement with the values calculated numerically from Hamiltonians (1) and (5) in the regime where $\chi < \chi_c$. For larger values of $\chi$, the nodal points $\pm \mathbf{Q}_1$ and $\pm \mathbf{Q}_3$ can move in the $k_z = 0$ plane, as the position of the nodal line is renormalized by the interactions. The two nodal points in the diagonal $\pm \mathbf{Q}_1$ remain fixed.

Expanding the mass term around the zeros of $m(\mathbf{k}_0)$, the low-energy quasiparticles around the nodes are Weyl fermions. Performing a rotation of the quasiparticle momenta into a new basis $\tilde{p}_x = (q_x - q_y)/\sqrt{2}$, $p_y = -q_x$, and $p_z = (q_x + q_y)/\sqrt{2}$, the expansion around the nodes at $\pm \mathbf{Q}_1$ gives the low-energy Hamiltonian

$$H_{\pm \mathbf{Q}_1}(\mathbf{p}) = \mathbf{h}_{\pm \mathbf{Q}_1}(\mathbf{p}) \cdot \mathbf{\sigma} = \sum_{i=x,y,z} \epsilon_{0,i}(\mathbf{p}_0) p_i \sigma_i, \quad (11)$$

with $\mathbf{p}$ the momentum away from the nodes and $\epsilon_{0,i} = \pm \sqrt{2}/4$, $v_{0,y} = 3t/2$, and $v_{0,z} = \sqrt{3}3\chi$ the corresponding velocities in the rotated basis. The equation above describes two Weyl points with opposite helicities $\gamma = (2\pi)^{-1} \int_{Q_0} d^2 p \tilde{p} \cdot (\partial_{p_i} \tilde{h} \times \partial_{p_j} \tilde{h}) = \pm 1$, and hence brokenTRS, with $\tilde{h} = \mathbf{h}/|\mathbf{h}|$ a unitary vector and $\Omega$ the surface of a small sphere enclosing each node. Similarly, the expansion around the nodes $\pm \mathbf{Q}_2$ and $\pm \mathbf{Q}_3$ give Hamiltonians of Weyl fermions with helicities $\pm 1$, as indicated in Fig. 4(b).

**Anomalous Hall conductivity.** The Weyl points delimit a topological domain wall between slices of the BZ parallel to the (110) plane. Each slice in the light-gray region in Fig. 4(b) crosses the nodal line twice and has a well-defined Chern number $v = +1$. The slices in the dark-gray regions across the domain walls have opposite Chern number $v = -1$, as the QAH mass changes sign simultaneously at the two Weyl points (with the same helicity) where each domain wall intersects the nodal line. The BZ slices in the light-blue region do not cross the nodal line and have zero Chern number.
The 3D QAH conductivity is defined as\[\sigma_{ij} = \langle e^2 / h \rangle (2\pi)^{-3} \oint_{kz} d^3k \sum_{\ell \in \text{filled}} \frac{\partial}{\partial k_{\ell}} \epsilon_{ijk} \nu_{ij}(k_0)\]

where $\nu_{ij}(k_0) = 0, \pm 1$ is the Chern number of a slice of the BZ oriented in the $j$ direction, intersecting the nodal line $k_{s}(s)$ at two points, and $C \in [k_{j,\text{min}}(s), k_{j,\text{max}}(s)]$. Therefore, we find that
\[\sigma_{yz} = \sigma_{zx} = e^2 / (3\hbar a),\]

while $\sigma_{xy} = 0$. In the 3D QAH phase, the bulk of the system is a semimetal with topologically protected Weyl quasiparticles [25], while charge currents spontaneously emerge on the $[100]$ and $[010]$ surfaces of the crystal.

**Surface states.** The presence of Weyl points in the QAH state implies the existence of Fermi arcs on the surfaces of the lattice, connecting nodes with opposite helicities. In Fig. 5(a), we numerically calculate the Fermi arcs in the (001) surface Brillouin zone, as shown in the solid blue lines. The nodes at $\pm Q_2$ are connected by a Fermi arc crossing the center of the BZ, while the pair of nodes at $Q_1, -Q_3$ and $-Q_1, Q_3$ are connected by short Fermi arcs directed along the nodal line.

In Fig. 5(b), we scan the energy spectrum of the $k_z = 0$ plane along the $k_x$ axis along three paths indicated by the dotted horizontal lines in panel (a). Line 1 [$k_y = 3\pi / (4\sqrt{3})$] intersects a Fermi arc close to the node at $Q_1$, as indicated by the arrow in the left panel of Fig. 5(b), which has a zero energy crossing in the vicinity of a node. The scan on line 2, at $k_y = \pi / (2\sqrt{3})$, does not intercept a Fermi arc, as shown in the center panel of Fig. 5(b). The third path at $k_y = \pi / (10\sqrt{3})$ crosses the Fermi arc near the center of the zone, as indicated by the zero energy mode shown in the right panel of Fig. 5(b).

**Conclusions.** We have shown that hyperhoneycomb lattices with spinless fermions may host a 3D QAH effect, which competes with a CDW state. The 3D anomalous Hall conductivity is $e^2 / (\sqrt{3}\hbar a)$. Due to the symmetry of the mass term, which spontaneously breaks inversion symmetry around the nodal line, the low-energy excitations of the QAH state have a rich structure, with Weyl fermions in bulk and topologically protected surface states.

**Note added.** Recently, we became aware of a related work [42], which predicted the conditions for the emergence of Weyl points in nodal-line semimetals from symmetry arguments.

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[30] This geometry has been realized in honeycomb iridates as a spin lattice. See K. A. Modic et al., Nat. Commun. 5, 4203 (2014). The metallic version of it, which is a nodal-line semimetal, requires s-wave orbitals and may in principle be realized in optical lattices with cold atoms.