Chiral magnetic conductivity and surface states of Weyl semimetals in topological insulator ultra-thin film multilayer

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Abstract
We investigate an ultra-thin film of topological insulator (TI) multilayer as a model for a three-dimensional (3D) Weyl semimetal. We introduce tunneling parameters $t_S$, $t_L$, and $t_D$, where the former two parameters couple layers of the same thin film at small and large momenta, and the latter parameter couples neighbouring thin film layers along the $z$-direction. The Chern number is computed in each topological phase of the system and we find that for $t_S, t_D > 0$, the tunneling parameter $t_L$ changes from positive to negative as the system transits from Weyl semi-metallic phase to insulating phases. We further study the chiral magnetic effect (CME) of the system in the presence of a time dependent magnetic field. We compute the low-temperature dependence of the chiral magnetic conductivity and show that it captures three distinct phases of the system separated by plateaus. Furthermore, we propose and study a 3D lattice model of Porphyrin thin film, an organic material known to support topological Frenkel exciton edge states. We show that this model exhibits a 3D Weyl semi-metallic phase and also supports a 2D Weyl semi-metallic phase. We further show that this model recovers that of 3D Weyl semimetal in topological insulator thin film multilayer. Thus, paving the way for simulating a 3D Weyl semimetal in topological insulator thin film multilayer. We obtain the surface states (Fermi arcs) in the 3D model and the chiral edge states in the 2D model and analyze their topological properties.

Keywords: Weyl semimetal, quantum anomalous conductivity, chiral magnetic conductivity, topological insulator thin film, porphyrin thin film

(Some figures may appear in colour only in the online journal)
been discovered experimentally in photonic crystals [17]. The experimental realization of Weyl semimetal in TaAs has also been reported using angle-resolved photoemission spectroscopy [18–20]. In a lattice model, it is possible to generate massless Dirac fermions with chirality in 2 dimensions. Such systems have been dubbed 2D Weyl semimetals [21]. They appear as chiral relativistic fermions [21] and exhibit an additional hidden discrete symmetry represented by an anti-unitary operator. The degeneracy of the resulting Weyl nodes are protected provided that there exists an anti-unitarity operator that commutes with the Hamiltonian whose square is equal to \(-1\) at the degenerate points. This is reminiscent of time-reversal symmetry protected Dirac points in graphene.

In this paper, we study two ultra-thin film models. Firstly, we study an ultra-thin film of TI multilayer by utilizing the explicit expression of the conventional 2D TI ultra-thin film Hamiltonian [23–26], which contains quadratic corrections in its low-energy Hamiltonian, with tunneling parameters \(t_z, t_s\). As a customary procedure, we construct a 3D version of this model by sandwiching a normal insulator between layers of TI thin film with tunneling parameter \(t_D\) and a magnetic field along the z-direction. The resulting 3D model exhibits topological properties similar to Burkov and Balents model [1]. However, in the present model we compute the explicit expressions for the Chern numbers in all the topological phases and show that when \(t_z, t_D > 0\), the tunneling parameter \(t_z\) changes sign as the system transits from Weyl semi-metallic phase to insulating phases. We further study the low-temperature dependence of the chiral magnetic effect (CME) by computing the explicit expressions for the response function in the presence of a time-dependent magnetic field. In this case, the model does not possess any analytical solution. We numerically show that the chiral magnetic conductivity exhibits plateaus which separate three distinct phases of the system even though it is not an integer quantized quantity.

Secondly, we study a simple lattice model using the layers of porphyrin thin films [22]—an organic material that can be synthesized in the laboratory. We present a detailed analysis of this model in both 2 and 3 dimensions. In particular, we show that this lattice model captures a 2D Weyl semi-metallic phase, whose nodes are protected by an anti-unitary operator. In addition, our model also captures a 3D Weyl semi-metallic phase, which appears as an intermediate phase between a 3D quantum anomalous Hall (QAH) insulator and a normal insulator (NI). It is also shown that the porphyrin lattice model can be used as a tight binding model for topological insulator thin film multilayer. We use this model to simulate the chiral edge states of the 2D system and the surface states (Fermi arcs) of the 3D system in all the nontrivial topological phases of the system.

### 2. Topological insulator ultra-thin film multilayer

In 2D topological insulator ultra-thin film, the hybridization between the top and the bottom layers gives rise to a massive Dirac fermion [23–26]. Here, we work from this 2D low-energy Hamiltonian and construct a 3D model for Weyl semimetal by inserting insulator spacer layers between TI thin films and introduce a tunneling parameter that couples neighbouring layers of the ultra-thin film. The Hamiltonian for this multilayer is given by

\[
H = \sum_{k, j} c_{k,j}^\dagger H_{ij} c_{k,j},
\]

where

\[
H_{ij} = v_F (\vec{\sigma} \cdot \vec{k}) \delta_{ij} + \left( \frac{t_s}{2} - t_z k_z^2 \right) \tau_i \sigma_i \delta_{ij} + \gamma \sigma_i \delta_{ij} + \frac{t_D}{2} (\delta_{i,j+1} + \delta_{i,j-1}) \tau_i \sigma_i.
\]

The difference between this Hamiltonian and that of Burkov and Balents [1] is that equation (2) is quadratic in the momentum variables and the couplings are diagonal in the pseudo spin space. It also has an advantage in that the surface states can be simulated through a lattice model and the Chern numbers can be obtained explicitly in all the topological phases of the system.

The Pauli matrices \(\sigma\) denote the real spin space and \(\tau\) are the *which surface* pseudo spins; \(k_i = (k_x, k_y)\) is a 2D momentum vector in the BZ. The indices \(i, j\) label distinct thin film layers and \(v_F\) is the Fermi velocity; \(t_z\) and \(t_s\) are the tunneling parameters that couple the top and bottom surfaces of the same thin film layer for small \(k_z\), and large \(k_z\), respectively, and \(\gamma = g \mu_B B\) is the Zeeman splitting which can be induced by magnetic doping or directly applying a magnetic field; \(t_D\) is the tunneling parameter that couples the top and bottom surfaces of neighbouring thin film layers along the growth z-direction. The parameters \(\gamma, t_z, t_s, t_D\) depend on the thickness of the thin film, \(t_z\) and \(t_s\) have been determined both numerically [24–26] and experimentally [28, 29]. The new parameter \(t_D\) can also be determined by growing the multilayer above. In the 2D model, the energy gap in the TI ultra-thin film can be enhanced by using a thinner film. Thus, the thickness of the film can change the topology of the system. In the present model, a smaller thickness should also enhance the Weyl semimetallic state induced by the interlayer coupling \(t_D\) and the magnetic field. Without loss of generality we assume all the parameters to be positive; \(b, t_s, t_D > 0\). However, as will be shown in the subsequent sections, \(t_s\) can be positive or negative when moving from the Weyl semi-metallic phase to other phases of the system.

It is expedient to Fourier transform the Hamiltonian along the growth z-direction. We obtain

\[
\hat{H}(k) = v_F (\vec{\sigma} \cdot \vec{k}) \cdot \vec{\kappa} + [\gamma + \hat{\Delta}(k)] \sigma_z,
\]

where

\[
\hat{\Delta}(k) = \left[ \frac{t_s}{2} - t_z k_z^2 + \frac{t_D}{2} \cos(k_z d) \right] \tau_z.
\]

The Hamiltonian (equation (3)) breaks \(T\)-symmetry due to the magnetic field, but inversion symmetry is preserved \(T: \hat{H}(k) \rightarrow \tau_z \sigma_z \hat{H}(-k) \tau_z \sigma_z\). The eigenvalues of \(\hat{\Delta}(k)\) are \(\pm \Delta(k)\), where \(\Delta(k) = \frac{t_s}{2} - t_z k_z^2 + \frac{t_D}{2} \cos(k_z d)\) and the corresponding eigenspinors are

\[
|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |u\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]
Hence, the Hamiltonian can be written as a $2 \times 2$ massless Dirac equation (Weyl equations) given by

$$H(k) = \nu_F (\hat{\sigma} \cdot k + m_0 k)\sigma_z,$$

where $m_0 = \gamma + s\Delta(k)$ and $s = \pm \uparrow, \downarrow$. The form of the $\Delta$ function for this model affects the phases that emerged when $\gamma = 0$. For the present model, equation (6) with $\gamma = 0$ describes a 3D Dirac semimetal which possesses time-reversal and inversion symmetries. It exhibits a phase with two Dirac nodes along the $k_z$-direction when $t_k < t_0$ and an insulating phase (3D QSH phase) for $t_k > t_0$. In the insulating phase, the $Z_2$ topological number is $(-1)^\nu = -\text{sign}(t_k - t_0)$, where $\nu = 1$ characterizes a nontrivial phase. The semi-metallic phase and the insulating phase are separated by a saddle point at $k_s = k_z = 0$, $k_r = \pi/d$, with energy $\pm |t_k - t_0|/2$.

To obtain a nontrivial Weyl semi-metallic phase, $T$- or $I$-symmetry must be broken as mentioned above. This requires that $\gamma \neq 0$. The corresponding energy eigenvalues of equation (6) are given by

$$\epsilon_{\lambda}(k) = \lambda \sqrt{1 + \frac{m_0(k)}{c_0(k)}} - i\lambda \epsilon_0 k \sqrt{1 - \frac{m_0(k)}{c_0(k)}},$$

where $\lambda = \pm$ labels the conduction and valence bands respectively, and the eigenvectors are

$$|\psi_{\lambda}^\pm(k)\rangle = \begin{pmatrix} |\psi_0^\pm\rangle \\ 0 \end{pmatrix}; \quad |\psi_{\lambda}^\pm(k)\rangle = \begin{pmatrix} 0 \\ |\psi_0^\pm\rangle \end{pmatrix}.$$

Two Weyl nodes are realized in the $H(k)$ block of the Dirac equation (equation (6)). This corresponds to the solutions of $m_0(k) = 0$, where $m_0(k)$ never changes sign. The Weyl nodes are located at $k_s = k_0 = 0$, $k_\pm = \pi/d \pm k_w$, where

$$k_w = d \arccos \left(1 - \frac{2}{t_0}(\gamma - \gamma_\pm)\right).$$

with $\gamma_\pm = (t_k \pm t_0)/2$ and $\gamma_\pm > \gamma$.

The phase diagram in figure 1 comprises an ordinary insulator phase for $\gamma < \gamma_\pm$, and a 3D QAH phase for $\gamma > \gamma_\pm$. A 3D Weyl semimetal with two Weyl nodes appears in the regime $\gamma < \gamma < \gamma_\pm$, and a pair annihilation occurs exactly at the boundaries. As in all theoretical models, a 3D Weyl semimetal phase always appears as an intermediate state between an ordinary insulator and a 3D quantum anomalous Hall insulator. The Hall conductivity is given by

$$\sigma_y^\pm(k) = \frac{e^2}{h} \sigma^\pm(k).$$

In the present model, we can calculate the Chern number explicitly by treating $k_s$ as a parameter, thus reducing the problem to an effective 2D model. Hence, the Chern number is computed with the same formula [27]

$$\sigma^\pm(k) = \int \frac{dk}{\lambda} \frac{\partial^2 A_{\lambda}^\pm}{\partial k^2},$$

where

$$A_{\lambda}^\pm = i \langle \psi^\pm | \partial k \cdot \hat{a}^\dagger \rangle.$$
Thus, \( k_y \) and \( k_z \) are good quantum numbers and \( k_z \) is replaced by \( k_z \rightarrow -i \partial_z \). The Hamiltonian can be written as

\[
H_- = i\sigma_y v_F \partial_t \sigma_y \sigma_z \partial_t + v_F \sigma_y k_y - \sigma_y t_z k_z^2 + m_{-(k_z, x)} \sigma_y.
\]

(18)

We first consider \( k_y = 0 \) and solve for the zero energy solution of the Schrödinger equation \( \mathcal{H}_- \Phi (k_z, x) = 0 \),

\[
[v_F \partial_t + t_z \sigma_y \sigma_z \partial_t - m_{-(k_z, x)} \sigma_y] \Phi (k_z, x) = 0,
\]

(19)

where \( \Phi(k_z, x) \) is a 2-component spinor and we have multiplied through by \(-i\sigma_y\). We seek for a solution of the form

\[
\Phi_\lambda (k_z, x) = \xi_\lambda e^{i\omega t},
\]

(20)

where \( \xi_\lambda = \lambda \xi_\lambda \), \( (\lambda = \pm 1) \) and \( \omega \) solves the equation

\[
v_F \omega + \lambda \omega \omega^2 - \lambda m_{-(k_z, x)} = 0.
\]

(21)

The allowed solution that obey the boundary conditions of the wavefunction \( \Phi (k_z, 0) = \Phi (k_z, \infty) = 0 \) is given by

\[
\Phi_\lambda (k_z, x) = \frac{\mathcal{C}}{\sqrt{2}} \left( \frac{1}{\lambda} \right) (e^{-\omega t} - e^{-\omega t}),
\]

(22)

where \( \mathcal{C} \) is a normalization constant, and \( \omega \) are the positive solutions of equation (21). The surface Hamiltonian is obtained by projecting equation (18) onto the surface states

\[
\mathcal{H}_{\text{surf}} (k_z, k_y) = \Phi_\lambda^\dagger \mathcal{H}_- \Phi_\lambda = v_F k_y \sigma_y.
\]

(23)

### 3. Magnetic field response

In the previous section, we derived the phase diagram, anomalous Hall conductivity, and surface states of an ultra-thin film of TI Hamiltonian with quadratic momentum corrections. In this section, we study the response of the system to an orbital magnetic field through the vector potential, \( \mathbf{A} = e \mu_B B \mathbf{B} \), which corresponds to a magnetic field along the growth \( z \)-direction.

The Hamiltonian is given by

\[
\mathcal{H}_\mathbf{e} (\mathbf{k}) = v_F (\xi \times \sigma) \cdot (-i \nabla + e \mathbf{A}) + m_{\mathbf{k}}(\mathbf{k}) \sigma_y.
\]

(24)

We introduce the operator \( \mathbf{\pi} = -i \nabla + e \mathbf{A} \), and define the creation and annihilation operators:

\[
a = \hat{l}_0 (\pi_\mathbf{x} + i \pi_\mathbf{y}) \sqrt{2}; \quad \hat{a}^\dagger = \hat{l}_0 (\pi_\mathbf{x} + i \pi_\mathbf{y}) \sqrt{2}, \quad \text{where} \quad \hat{l}_0^2 = (e \mu_B B)^{-1}
\]

is the magnetic length. In terms of \( a \) and \( \hat{a}^\dagger \), the Hamiltonian becomes

\[
\mathcal{H}_\mathbf{e} (\mathbf{k}_z) = i \omega_0 \sqrt{2} \left( \sigma^+ a - \sigma^- a^\dagger \right) + m_{\mathbf{k}}(\mathbf{k}_z) \sigma_y,
\]

(25)

where \( \sigma^\pm = (\sigma_x \pm i \sigma_y) / 2 \) and \( m_{\mathbf{k}}(\mathbf{k}_z) = \gamma + s \Delta (k_z) \), where \( \Delta (k_z) \) is given by

\[
\Delta (k_z) = \left[ \frac{\hbar s}{2} + \frac{\hbar d}{2} \cos (k_x d) - \omega_0 \left( \frac{\hbar a}{2} + 1 \right) \right].
\]

Here, \( \omega_0 = v_F / \hbar B \) is the magnetic frequency and \( \omega_0 = 2 \gamma / \hbar B \) is the harmonic oscillator frequency. The eigenvector of each \( 2 \times 2 \) block may be written as

\[
\mathcal{U}_m = \left( \begin{array}{c} \alpha_{m}^* \alpha_{m-1} \alpha_{m}^2 \alpha_{m} \end{array} \right),
\]

(27)

where \( \alpha_{m}^* \alpha_{m}^2 \) are constants to be determined. The operators satisfy

\[
u_F \omega + \lambda \omega \omega^2 - \lambda m_{-(k_z, x)} = 0.
\]

(21)

The eigenvalues of equation (28) are given by

\[
\epsilon^\prime_{n, \lambda} (k_z) = \frac{\omega_0}{2} + \lambda \sqrt{2n \omega_0^2 + m_{\mathbf{k}}^2 (k_z)}, \quad n \geq 1,
\]

(30)

\[
\epsilon^0 (k_z) = -m_{\mathbf{k}} (k_z), \quad n = 0.
\]

(31)

The corresponding eigenvectors are

\[
\left| \psi^\prime_{n, \lambda} \right> = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 + \lambda m_{\mathbf{k}} (k_z) \epsilon^\prime_{n, \lambda} (k_z) \epsilon^\prime_{n, \lambda} (k_z) \\ -i \lambda \left( 1 - \lambda m_{\mathbf{k}}^2 (k_z) \epsilon^\prime_{n, \lambda} (k_z) \epsilon^\prime_{n, \lambda} (k_z) \right) \end{array} \right)^T
\]

(32)

\[
\left| \psi^0 \right> = (0, 1)^T.
\]

(33)

For \( \gamma = 0 \), the zero Landau levels crosses at \( B_c = (\hbar s + \hbar d \cos (k_x d)) / 2e \mu_B \mathbf{B} \), which vanishes at the Dirac nodes \( k_z^\pm = \pi / d \pm k_w \). At the transition point \( k_z = \pi / d \), \( B_c = 0 \). For

Figure 1. The phase diagram of the TI multilayer comprising a normal insulator (NI), Weyl semimetal (WSM), and quantum anomalous Hall (QAH) insulator along the magnetic field line. The values of the corresponding Chern numbers are indicated by \( \mathcal{C} \).
The regime $B < B_c$ corresponds to a 3D QSH phase and $B > B_c$ corresponds to trivial phase. The Landau level for $\gamma = 0$ is shown in figure 2, which evidently captures the appearance of two Weyl nodes in the vicinity of the bulk gap.

3.1. Chiral magnetic effect

Chiral magnetic effect is the response of a system to a time-dependent magnetic field. This phenomenon is well-known in high energy physics as the chiral magnetic conductivity. For instance, gluon field configurations with nonzero topological charges exhibit this effect [34]. It has been shown to occur in Weyl semimetals [5, 33]. In this subsection, we investigate the low-temperature dependence of the chiral magnetic conductivity on the TI ultra-thin film Hamiltonian. We will derive the expressions for our model, which do not possess any analytical solution. We also show that the chiral magnetic conductivity captures the appearance of the three distinct phases of the system though it is not integer quantized like the quantum anomalous Hall conductivity. In the linear response theory, the current operator is given by

$$J_I (\mathbf{q}, \omega) = \Pi_I (\mathbf{q}, \omega) A_I (\mathbf{q}, \omega),$$

where $\Pi_I (\mathbf{q}, \omega)$ is the current–current correlation function. The chiral magnetic effect (or conductivity) arises in the presence of a time-dependent magnetic field along the $z$-direction. In the Landau gauge we adopt here, the magnetic field is only related to the $A_z$ component of the gauge field, that is $\mathbf{B}_z = \partial_t A_z (x)$. Assuming $A_z (x) = A_z (x, \omega) e^{i\omega t - \omega t}$, we have $\mathbf{B}_z (\mathbf{q}, \omega) = iq A (\mathbf{q}, \omega)$. The response of the system to a time-dependent magnetic field gives rise to an induced current given by

$$J (\mathbf{q}, \omega) = \sigma (\mathbf{q}, \omega) B_z (\mathbf{q}, \omega).$$

Thus, the chiral magnetic conductivity is

$$\sigma (\mathbf{q}, \omega) = -\frac{i}{q} \Pi (\mathbf{q}, \omega).$$

The response function $\Pi (\mathbf{q}, \omega)$ is in general antisymmetric. The most convenient way to calculate the response function is from the imaginary time path integral of equation (24) minimally coupled to a vector potential,

$$S = \int \! d\tau d^3 r \psi^\dagger (\mathbf{r}, \tau) [\partial_\tau - \mu + i e A_0 (\mathbf{r}, \tau) + \mathcal{H}_r] \psi (\mathbf{r}, \tau).$$

After integrating out the fermion degree of freedom, the response function is given by [33]

$$-i \Pi (\mathbf{q}, \omega) = \frac{i e^2 V}{\nu_F} \sum_{s, \lambda, \lambda'} \sum_k f \{ \xi_{s, \lambda} (\mathbf{k}) \} - f \{ \xi_{s, \lambda} (\mathbf{k} + \mathbf{q}) \}
\times \left\langle \psi_{s, \lambda} \psi_{s, \lambda'}^\dagger \right\rangle \left\langle \psi_{s, \lambda} \sigma \cdot \mathbf{q} \psi_{s, \lambda'}^\dagger \right\rangle,$$

where $i \Omega = \omega + i \tau$ and $f \{ \xi_{s, \lambda} (\mathbf{k}) \} = [e^{\xi_{s, \lambda} (\mathbf{k})/\tau} + 1]^{-1}$ is the Fermi function, with $\xi_{s, \lambda} (\mathbf{k}) = \epsilon_{s, \lambda} (\mathbf{k}) - e \mathbf{q} \cdot \mathbf{A}$. Without loss of generality we assume $e \mathbf{q} > 0$. The spatial contribution only comes from the Landau gauge choice, thus we take $\mathbf{q} = q \hat{e}$. There are two contributions to the response function—the interband with $\lambda = \lambda'$ and the intraband with $\lambda = \lambda'$. We are interested in the low-frequency and long wavelength limits $\Omega \rightarrow 0$ (second limit) $q \rightarrow 0$ (first limit) and $q \rightarrow 0$ (second limit) $\Omega \rightarrow 0$ (first limit). However, the two limits are not commutative so the order in which the limits are taken is very crucial. The former limit is the direct current (DC) limit of a transport coefficient, while the latter is the static limit. For the interband case, both order of limits contribute to the response function, so we can start with $i \Omega = 0$. In this case all other terms in equation (39) are finite as $q \rightarrow 0$ except $\left\langle \psi_{s, \lambda} \sigma \cdot \mathbf{q} \psi_{s, \lambda}^\dagger \right\rangle$.

Hence, we will expand this term to first order in $q$. Since the pseudo spin scalar product produces a term $\left\langle \mathbf{u}^\dagger \mathbf{u} \right\rangle = \delta_{\mathbf{u} \mathbf{u}}$, we have

$$\left\langle \psi_{s, \lambda} \sigma \cdot \mathbf{q} \psi_{s, \lambda}^\dagger \right\rangle = \delta_{\mathbf{u} \mathbf{u}} \frac{q}{2 \nu_F} \frac{\epsilon_{s, \lambda} (\mathbf{k})}{\epsilon_{s, \lambda} (\mathbf{k})} \left[ \pm 2 k \xi_{s, \lambda} (\mathbf{k}) \right]$$

$$+ \frac{q^2}{2 \nu_F} \left[ -i k \xi_{s, \lambda} (\mathbf{k}) \right] \left[ k \xi_{s, \lambda} (\mathbf{k}) \right] [k, \mathbf{m}_\mathbf{k} (\mathbf{k})],$$

(40)

(41)

Plugging equations (40) and (41) into equation (39), the terms containing $k$, $\xi_{s, \lambda}$ vanish by angular integration, we obtain

$$-i \Pi^{\text{inter}} (\mathbf{q}, \Omega) = -\frac{e^2 q}{8 \pi^2} \sum_k \int_{-\pi/d}^{\pi/d} \! d \xi \int_0^\infty \! dx \Omega_{s, \lambda} (x, k_x) \int_0^\infty \! dx \Omega_{s, \lambda} (x, k_x) \times \left[ 1 - f \left( \sqrt{x^2 + m_x^2 (x, k_x)} - e \mathbf{q} \right) \right].$$

Performing the angular integration, we obtain

$$-i \Pi^{\text{inter}} (\mathbf{q}, \Omega) = -\frac{e^2 q}{8 \pi^2} \sum_k \int_{-\pi/d}^{\pi/d} \! d \xi \int_0^\infty \! dx \Omega_{s, \lambda} (x, k_x) \int_0^\infty \! dx \Omega_{s, \lambda} (x, k_x) \times \left[ 1 - f \left( \sqrt{x^2 + m_x^2 (x, k_x)} - e \mathbf{q} \right) \right].$$

(44)
where $x = \sqrt{2}k^2$, and

$$\Omega_{12}^z(x, k_z) = -\frac{m_t(x, k_z)}{2[x + m_s^2(x, k_z)]^{1/2}}.$$  
$$\Omega_{22}^z(x, k_z) = \frac{i\hbar m_s^2(x, k_z)}{2[x + m_s^2(x, k_z)]^{1/2}},$$

$$m_t(x, k_z) = \gamma + k_z \left[ \frac{F_s}{2} - \frac{\gamma_0}{2} \cos(k_d) \right].$$  

(45)

with $\tilde{l}_z = t_z/\sqrt{F}$. Now for the intraband case $\lambda = \lambda_t$, the response function vanishes in the DC limit $\Omega \to 0$; $q \to 0$, i.e. if we take long-wavelength limit first. However, in the static limit $q \to 0$, $\lambda_t \to 0$, it is nonzero. In this case, we have

$$f[\xi_{\lambda t}(k + q)] = f[\xi_{\lambda t}(k)] + q \frac{\partial \xi_{\lambda t}(k)}{\partial q} q \frac{\partial \xi_{\lambda t}(k)}{\partial q} + \ldots$$

(46)

$$\xi_{\lambda t}(k + q) = \xi_{\lambda t}(k) + q \frac{\partial \xi_{\lambda t}(k)}{\partial q} + \ldots$$

(47)

The intraband response function is given by

$$-i\Pi^{\text{intra}}(q, i\Omega) = \frac{e^2 q}{2} \sum_s \int \frac{d \bf{k}}{(2\pi)^3} \left[ \frac{\partial \xi_{\lambda t}(k)}{\partial q} M_s(k) \right] \frac{1}{\epsilon_s^2(k)}.$$  

(48)

In the present model, the integrations (equations (44) and (48)) cannot be done analytically. We can reduce the problem in a way that is amenable to numerical integration by performing the angular integration. We obtain

$$-i\Pi^{\text{intra}}(q, i\Omega) = -\frac{e^2 q}{8\pi^2} \sum_s \int \frac{d \bf{k}}{\pi} \int_0^\infty \frac{d q}{q} \sum_s \left[ 4T \cosh^2 \left( \sqrt{x + m_s^2(x, k_z)} - \epsilon_F \right) \right]^{-1},$$

(49)

where

$$\tilde{\Omega}_{12}^z(x, k_z) = -\frac{m_t(x, k_z)}{2[x + m_s^2(x, k_z)]}; \quad \tilde{\Omega}_{22}^z(x, k_z) = \frac{i\hbar m_s^2(x, k_z)}{2[x + m_s^2(x, k_z)].}$$

(50)

The conductivity is given by equation (37). In the two non-commutative limits we obtain two conductivities given by

$$\sigma_{\chi} = \lim_{\Omega \to 0, q \to 0} -\frac{i}{q} \Pi^{\text{inter}}(q, i\Omega),$$

(51)

$$\sigma_{\chi} = \lim_{q \to 0, \Omega \to 0} -\frac{i}{q} \Pi^{\text{inter}}(q, i\Omega) + \Pi^{\text{intra}}(q, i\Omega).$$

(52)

The first limit (equation (51)) is the chiral magnetic effect (CME). As mentioned above, this is nothing but the chiral magnetic conductivity, a phenomenon well-studied in high energy physics [34]. The second limit (equation (52)) is a thermodynamic equilibrium quantity corresponding to the static limit; we will focus on equation (51).

Figure 3 shows the plot of the chiral magnetic conductivity against the magnetic field $\gamma$. Note that the sign of $t_z$ is irrelevant because the two masses $m_\pm(k)$ contribute in the $z$-direction. The $2D$ Hamiltonian of a porphyrin thin film is given by [22]

$$H_{2D} = \sum_{m, n} \left[ \mathcal{J}_2(e^{i\phi}a^\dagger_m b_{m+n\delta_x} + e^{-i\phi} a^\dagger_m b_{m-n\delta_x}) \right. + \left. \mathcal{J}_2(e^{-i\phi}a^\dagger_m b_{m+n\delta_x} + e^{i\phi} a^\dagger_m b_{m-n\delta_x}) + \text{h.c.} \right]$$

$$+ J_{\perp} \sum_m [a^\dagger_m a_{m+\delta_y} - b^\dagger_m b_{m+\delta_y} + \text{h.c.}]$$

$$+ \mu_{\perp} \sum_m [a^\dagger_m a_m - b^\dagger_m b_m].$$

(53)

The nearest neighbour (NN) sites are along the diagonals with coordinates $\delta_x = (\delta_x + \delta_y)/2$ and $\delta_y = (-\delta_x + \delta_y)/2$, and complex hopping parameters, $\mathcal{J}_2$, where $l = 1, 2$; $\delta_x = (1, 0)$ and $\delta_y = (0, 1)$; $\Phi$ is a phase factor, which can be regarded as a
magnetic flux treading the lattice. The total flux on a square plaquette vanishes just like in Haldane model [30]. The next nearest neighbour (NNN) sites are along the horizontal and vertical axes with real hopping parameter $J_z$. The last term in equation (53) is the staggered onsite potential with a tuneable parameter $\mu$. Next, we introduce an interlayer coupling between the porphyrin thin film layers along the $z$-direction. The Hamiltonian is given by

$$H_{\text{lat}} = J_0 \sum_{m} [a_m^\dagger a_{m+z} - b_m^\dagger b_{m+z} + \text{h.c.}] + \mu \sum_{m} [a_m a_m - b_m^\dagger b_m].$$

(54)

Here, the staggered onsite potential is along the $z$-direction with tuneable parameter $\mu$, and $J_0$ is a real coupling constant. Performing the Fourier transform of the lattice model we obtain $\mathcal{H} = \sum_k (a_k, b_k)^T \mathcal{H}(k) (a_k, b_k)^T$, where

$$\mathcal{H}(k) = \left[ \begin{array}{c} \rho_1 \cos(k_x - \Phi) + \rho_2 \cos(k_y - \Phi) \sigma_x - \rho_1 \cos(k_x + \Phi) + \rho_2 \cos(k_y + \Phi) \sigma_y + \mu \nu_1 - 2\nu_2 \cos(k_x + k_y) + \cos(k_x - k_y) \end{array} \right] \sigma_z - \frac{t_0}{2} \cos(k_y d) + \cos(k_x d) \sigma_y. \quad (55)$$

The above Hamiltonian equation (55) is obtained with the rescaled parameters $J_z \to -J_z$, $J_0 \to -J_0/4$, and we have fine-tuned the staggered potential to $\mu = J_0 \cos(k_y d)$. We also set the lattice constants $a_1 = a_2 = 1$, and $d = 1$, where $d$ is the separation of the porphyrin thin film layers. $k_{\pm} = (k_x \pm k_y)/2$, $\rho_1 = 2.5 J_0$, $\rho_2 = 2 J_0$, $\rho_2 = 2 J_0$, and $\rho_2 = 2 J_0$, where $\prod$ and $\bigwedge$ denote real and imaginary parts of the complex hopping terms $J_z$. The model equation (55) can be simplified by taking $J_1 = J_2^*$, which implies that $\rho_1 = \rho_2 = \rho$ and $\rho_1 = -\rho_2 = \rho$. This is a reasonable simplification and will be adopted throughout our analysis.

5. 2D Weyl semimetal

As mentioned above, 2D Weyl semi-metals can be constructed from a lattice model [21]. In this section, we show how it emerges from the porphyrin thin film layer. In the 2D limit $t_1 = t_0 = 0$, the Hamiltonian equation (55) has the form

$$\mathcal{H}(k) = \rho \cos(k_+ + \Phi) \cos(k_+ - \Phi) \sigma_x - \rho \cos(k_+ - \Phi) \cos(k_+ + \Phi) \sigma_y. \quad (56)$$

For $\Phi = 0$ or $\pi$, equation (56) can be written as

$$\mathcal{H}_{\Phi=0} = \rho \cos\left(\frac{k_x}{2}\right) \cos\left(\frac{k_y}{2}\right) \sigma_x + \rho \sin\left(\frac{k_x}{2}\right) \sin\left(\frac{k_y}{2}\right) \sigma_y, \quad (57)$$

where $\mathcal{H}_{\Phi=\pi} = -\mathcal{H}_{\Phi=0}$. As shown in figure 5, the energy band has four degenerate points located at $W_1 = (0, \pm \pi)$ and $W_2 = (\pm \pi, 0)$. However, the degeneracy of an energy band does not guarantee a Weyl semi-metallic phase. To obtain a nontrivial topological semimetal, symmetry consideration must be taken into account. For the Hamiltonian in equation (57), time-reversal symmetry ($k \to -k$; $\sigma \to -\sigma$) is broken but inversion symmetry ($k \to -k$) is preserved. For 2D systems, however, there is an additional hidden discrete symmetry with an anti-unitary operator [21]. More generally, if a system is invariant under the action of an anti-unitary operator and the square of the operator is not equal to 1, there must be degeneracy protected by this anti-unitary operator [21]. In the present model, there is an anti-unitary operator for which the Hamiltonian (equation (55)) is invariant. It is given by $U = \sigma_y K T_{\prod 2+\bigwedge 2}$, where $K$ is complex conjugation and $T_{\prod 2+\bigwedge 2}$ translates the lattice by $\pi/2$ and $\pi/2$ along the $x$- and $y$-directions. It is easy to check that $U^* H_{\Phi=0} U = \mathcal{H}_{\Phi=0}$. It follows that $U^* \mathcal{H}_{\Phi=\pi} U = -\mathcal{H}_{\Phi=0}$. Thus, the theorem stated above is only valid at the $U$-invariant points. The four degenerate points in the energy band have Fermi energy for several temperatures $T = 0.001$ (solid); $T = 0.1$ (dotted); $T = 0.5$ (dotted). The parameters are in units of $0.001$ (solid); $0.5$ (dotted). The chiral magnetic conductivity as a function of the Fermi energy for several temperatures $T = 0.001$ (solid); $T = 0.1$ (dotted); $T = 0.5$ (dotted). The parameters are in units of $0.001$ (solid); $0.5$ (dotted). The chiral magnetic conductivity as a function of the Fermi energy for several temperatures $T = 0.001$ (solid); $T = 0.1$ (dotted); $T = 0.5$ (dotted). The parameters are in units of $0.001$ (solid); $0.5$ (dotted). The chiral magnetic conductivity as a function of the Fermi energy for several temperatures $T = 0.001$ (solid); $T = 0.1$ (dotted); $T = 0.5$ (dotted). The parameters are in units of $0.001$ (solid); $0.5$ (dotted). The chiral magnetic conductivity as a function of the Fermi energy for several temperatures $T = 0.001$ (solid); $T = 0.1$ (dotted); $T = 0.5$ (dotted). The parameters are in units of $0.001$ (solid); $0.5$ (dotted).
Spectrum is consistent with Nielsen–Ninomiya theorem [31], which states that Weyl points must occur in pair(s) with opposite helicity in a lattice model. Near these points, the Hamiltonian is linearized as
\[ \mathcal{H}(q) = v_F(\mp q_x \sigma_x \pm q_y \sigma_y), \]
where \( q = k - W_{1,2} \) and \( v_F = \rho/2 \).

The Hamiltonian has the general form \( \mathcal{H}(q) = \sum_{ij} v_{ij} q_i \sigma_j \), where \( v_{ij} \) form a \( 2 \times 2 \) matrix. The chirality of the Weyl points is given by
\[ \chi_{\pm} = \text{sign}(\text{det}(v_{ij})). \]

From equations (58) and (59) we obtain \( \chi_{\pm} = \pm 1 \) for the whole system, which signifies the topological nature of the system. As a massless Dirac fermion with chirality, the system above can be regarded as a 2D Weyl semi-metal which hosts a 2D Weyl fermion. In figure 5, opposite chirality is assigned to neighbouring Weyl points in cyclic order. Moreover, in 2D Weyl semimetal there is a chiral edge state propagating in the intermediate region between the Weyl points. This can be explicitly shown by considering a semi-infinite system with periodic boundary conditions along the \( k_y \) direction and open boundary condition along the \( k_x \) direction [32]. The bulk band is shown in figure 6 along the \( k_y \) direction. The bulk gap vanishes at the locations of the Weyl points along the \( k_y \)-axis consistent with figure 5. However, topological protected flat-band chiral edge states emerge in-between the Weyl nodes. These chiral edge states connect the Weyl points with opposite chirality along the \( k_y \)-direction.

6. 3D Weyl semimetal

In this section, we study the possibility of 3D Weyl semimetallic phase in the proposed lattice model. The goal is to utilize this model to simulate the TI multilayer surface states (Fermi arc). In 3 dimensions we must have \( t_\theta \equiv 0 \); a 3D Weyl semimetal can be obtained with a judicious choice of \( \Phi \). In particular, for \( \Phi = \pi/2 \) and \( J_1 = J_2 \), equation (55) has the form \( \mathcal{H} = \mathcal{H}_{\Phi = \pi/2} + \mathcal{H}_\gamma \), where
\[ \mathcal{H}_{\Phi = \pi/2} = 2v_F \cos(k_x \frac{2}{2}) \sin(k_y \frac{2}{2}) \sigma_x - 2v_F \cos(k_y \frac{2}{2}) \sin(k_x \frac{2}{2}) \sigma_y, \]

**Figure 6.** The bulk energy band (pink) and the chiral edge states (blue) of equation (57) along the \( k_y \) direction.

**Figure 7.** The evolution of the energy along \( k_y = 0 \) at \( \Phi = 4\pi/2 \) with \( \mu_{xy} = 4t_\perp \). The four regimes are: the insulating phase. (a) \( \gamma < \gamma_c \), Weyl semi-metallic phase. (b) \( \gamma_c < \gamma < \gamma_c \), phase transition point. (c) \( \gamma = \gamma_c \), and the 3D QAH phase. (d) \( \gamma \geq \gamma_c \).

**Figure 8.** The evolution of the energy along \( k_y = 0 \) at \( \Phi = 0 \) or \( \Phi = \pi \) with \( \mu_{xy} = 0 \). The parameters are the same as figure 7.
\[ \mathcal{H}_t = \left[ \mu_{t_z} - 2 t_z (\cos k_x + \cos k_y) - \frac{t_0}{2} (\cos (k_d) + \cos (k_{wd})) \right] \sigma_z. \]  

(61)

It is easy to see that with a fine-tuned \( \mu_{t_0} = 4 t_L \), the partial continuum limit of equations (60) and (61) is exactly the inner 2 \times 2 block of equation (6) and the Weyl nodes are located at the same points \( \mathbf{W} = (0, 0, k_z^\pm) \), with \( k_z^\pm = \pi/d \pm k_W \). Thus, the porphyrin thin film multilayer lattice model recovers that of TI thin film multilayer in the partial continuum limit. The evolution of the energy bands in the BZ are shown in figure 7. Near the Weyl points the Hamiltonian is given by

\[ \mathcal{H}(\mathbf{q}) = v_F q_x \sigma_x - v_F q_y \sigma_y + v_F q_z \sigma_z, \]  

(62)

where \( \mathbf{q} = \mathbf{k} - \mathbf{W} \), and \( v_F = t_0 d \sin(k_{wd})/2 \).

The Hamiltonian still has the general form \( \mathcal{H}(\mathbf{q}) = \sum_\gamma v_\gamma q_\gamma \sigma_\gamma \), only that \( v_\gamma \) is now a 3 \times 3 matrix with components \( v_x = v_F, v_y = -v_F, v_z = \pm v_F \). The chirality of the Weyl points is the same \( \chi_z = \pm 1 \). In this case, the nontrivial topology of equation (55) stems from the fact that equation (55) preserves inversion symmetry but breaks time-reversal symmetry, when \( \Phi = \pi/2 \). Another judicious choice of \( \Phi \) is \( \Phi = 0 \) or \( \pi \). The resulting Hamiltonian in this case is given by \( \mathcal{H} = \mathcal{H}_{\Phi=0} + \mathcal{H}_c \), but it is different from that of TI thin film. However, the system still preserves inversion symmetry and breaks time-reversal symmetry; thus a Weyl semi-metallic phase can be obtained. There are four Weyl points in the BZ, each pair is located at \( \mathbf{W}_1 = (0, \pi, k_z^\pm) \) and \( \mathbf{W}_2 = (0, -\pi, k_z^\pm) \), where \( k_z^\pm = \pi/d \pm k_W \) and \( k_W = \frac{\pi}{2} \arccos[\cos(k_{wd}) - \mu_{t_3}/t_0], \) with \( \mu_{t_3} = 2 \mu_{t_3}/t_0 \). The energy bands are shown in figure 8. The Hamiltonian near the Weyl points is a combination of equation (58) and the last term in equation (62).

Now, we study the surface states evolution of the Weyl semi-metallic phases above. This is an important feature of 3D Weyl semimetals [7, 9] and it is what is observed in most experiments [17–20]. In our lattice model, these states can be solved explicitly for any surface not perpendicular to the \( z \)-axis. In fact, they are nothing but the edge states of the effective 2D model for fixed values of \( k_z \). We have shown the evolution of the states for \( \Phi = \pi/2 \) in figures 9(a)–(f), which corresponds exactly to the ultra-thin film of TI multilayer studied above. The top panel describes the Weyl semi-metallic phase bounded by two gapless bulk bands at the location of the Weyl points. For \( k_z \in (k_z^-, k_z^+) \), there exist dispersive surface states propagating in the vicinity of the bulk gap only when \( t_L > 0 \). They are gapless at \( k_z = 0 \) exactly at zero energy. In the bottom panel we show the insulating phases after the Weyl nodes annihilate and a gap opens at \( k_z = 0 \) or \( k_z = \pi/d \). In this case, the surface states still capture the appearance of the two insulating phases—3D QAH and NI only when \( t_L < 0 \). These results are consistent with our previous analysis and the energy dispersion in figure 7. For other choices of \( \Phi \) such as \( \Phi = 0, \pi \), the situation is a little bit different. The gapless surface states only occur at \( k_z = \pm \pi \), when \( k_z \in (k_z^-, k_z^+) \), but \( k_z = 0 \) is gapped in this case and we observe that there exist gapped surface states propagating in this vicinity (not shown).

7. Conclusion

In this paper, we have presented a detail analysis of two thin film models of Weyl semimetals. We showed that in an ultra-thin film of topological insulator multilayer the parameters of the system can change sign as the system transits from one topological phase to another. In this model, we presented the low-temperature dependence of the chiral magnetic...
conductivity, induced by a time-dependent magnetic field. We showed that the topological phases of the system can, indeed, be captured by the plateaus of the chiral magnetic conductivity. We also proposed and studied a simple lattice model of porphyrin thin film. We showed that this model embodies many Weyl semi-metallic phases for a specific gauge choice, which acts as a magnetic flux treading the lattice. We obtained a 2D Weyl semi-metallic phase in the $\sigma_x - \sigma_y$ space. We showed that the degeneracy of the Weyl nodes is protected by an anti-unitary operator. Our model also realized a 3D Weyl semi-metallic phase, which can be regarded as the lattice model for an ultra-thin film of topological insulator (TI) multilayer. Thus, it paved the way to numerically study the surface states of the TI multilayer. We obtained the edge states and the surface states in two and three dimensions respectively, as well as in all the non-trivial topological phases of the TI multilayer in three dimensions. As the porphyrin thin film is an organic material that can be grown in the laboratory, the proposed model can perhaps be studied experimentally or in 2D optical lattices. As shown in this paper, the porphyrin thin film is also a candidate to search for chiral relativistic fermions in two dimensions.

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References

[1] Burkov A A and Balents L 2011 Phys. Rev. Lett. 107 127205
[2] Burkov A A, Hook M D and Balents L 2011 Phys. Rev. B 84 235126
[3] Halasz G B and Balents L 2012 Phys. Rev. B 85 035103
[4] Zyuzin A A, Hook M D and Burkov A A 2011 Phys. Rev. B 83 245428
[5] Zyuzin A A, Wu S and Burkov A A 2012 Phys. Rev. B 85 165110
[6] Klinkhamer F R and Volovik G E 2005 Int. J. Mod. Phys. A 20 2795
[7] Volovik G E 2003 The Universe in a Helium Droplet (Oxford: Oxford University Press)
[8] Murakami S 2007 New J. Phys. 9 356
[9] Witzczak-Krempa W and Kim Y B 2012 Phys. Rev. B 85 045124
[10] Liu C-X, Ye P and Qi X-L 2013 Phys. Rev. B 87 235306
[11] Yang K-Y et al 2011 Phys. Rev. B 84 075129
[12] Chen C-Z et al 2015 Phys. Rev. Lett. 115 246603
[13] Lu H-Z, Zhang S-B and Shen S-Q 2015 Phys. Rev. B 92 045203
[14] Delplace P, Li J and Carpentier D 2012 Europhys. Lett. 97 67004
[15] Jiang J-H 2012 Phys. Rev. A 85 033640
[16] Slager R J et al 2015 (arXiv:1509.07705)
[17] Lu L et al 2015 Science 349 622
[18] Xu S-Y et al 2015 Science 349 613
[19] Lv B Q et al 2015 Phys. Rev. X 5 031013
[20] Lv B Q et al 2015 Nat. Phys. 11 724
[21] Hou J-M 2013 Phys. Rev. Lett. 111 130403
[22] Yuen-Zhou J et al 2014 Nat. Phys. 10 1026
[23] Lu H-Z et al 2010 Phys. Rev. B 81 115407
[24] Li H et al 2010 Phys. Rev. B 82 165104
[25] Li H, Sheng L and Xing D Y 2012 Phys. Rev. B 85 045118
[26] Shan W-Y, Lu H-Z and Shen S-Q 2015 New J. Phys. 12 043048
[27] Owerre S A and Nsofini J 2015 Solid State Commun. 218 35
[28] Sakamoto Y et al 2010 Phys. Rev. B 81 165432
[29] Zhang Y et al 2010 Nature 6 584
[30] Haldane F D M 1988 Phys. Rev. Lett. 61 2015
[31] Nielsen H B and Ninomiya M 1981 Phys. Lett. 105 219
[32] Qi X-L and Zhang S-C 2011 Rev. Mod. Phys. 83 1057
[33] Burkov A A 2014 Phys. Rev. B 89 155104
[34] Kharzeev D E and Warringa H J 2009 Phys. Rev. D 80 034028