Weyl semimetal from the honeycomb array of topological insulator nanowires

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Abstract — We introduce a topological semimetal phase with four isolated Weyl nodes in momentum space from a honeycomb arrangement of topological insulator nanowires. This realizes a Weyl semimetal phase in which the topological charge response is absent due to the opposite separation of two pairs of Weyl nodes in the Brillouin zone (BZ). The topological nature of the system manifests itself in the non-zero transverse “valley” current which is proportional to the length of the Weyl nodes’ separation vector. In the end, we show that anomalous Hall current can also emerge by considering the Haldane term, i.e., the next-nearest-neighbour inter-wire hopping of the electrons in the presence of a modulating magnetic flux.

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Introduction. — New topological phases of matter have been discovered recently highlighting the fact that the topological structures formed by the underlying electronic states are as important [1] as the symmetries involved and can be closely related to some interesting physically observable phenomena [2–12]. A recently discovered example in two and three dimensions is the time-reversal–invariant topological band insulator phase which can be formed by the electronic states in crystals with strong spin-orbit couplings and has been fully classified in terms of well-defined topological invariants [13,14]. In a strong topological insulator (TI) phase, the quantum states have been formed in a nontrivial fashion so that the system belongs to a different topological class than the ordinary insulator (OI) meaning that there is no fully gapped deformation path in the phase space of the Hamiltonians that connects the Hamiltonian of the system to that of an ordinary insulator preserving the time-reversal symmetry [15]. Any phase space path connecting two topologically distinct points in the phase space would contain a point where the associated Hamiltonian is gapless. This intuitively explains the presence of the robust topological surface states at the interfaces between these systems and ordinary insulators. It can be understood from the fact that one can establish a mapping between any path connecting a point in the bulk of a topological insulator to a point in the vacuum and the phase space paths which respect time-reversal symmetry connecting two topologically distinct regions and therefore it must contain a critical point where the system is locally gapless and all such points span the metallic surface. Therefore, any local perturbation on the surface that respects the time-reversal symmetry cannot destroy the gapless surface modes. These gapless surface modes are then protected by the coexistence of time-reversal symmetry on the surface and the nontrivial topological structure in the bulk of the system.

The topological protection is not restricted to just one- and two-dimensional metallic systems. Indeed one can generalize this idea to find a three-dimensional metallic system where the band crossing is protected by the underlying nontrivial topological structure of the quantum states rather than discrete symmetries such as the inversion or the time-reversal. Recently, experimentally feasible proposals to realize such 3D metallic phases has been made where linear energy crossings (Weyl points) exist in the band dispersion and are protected by global topological properties of the electronic states [16–20]. In this case there is no discrete symmetry involved in protecting the Dirac point from the gap opening as opposed to the 2D case on the surface of topological insulators where we still need to keep the time-reversal symmetry in order to maintain the band crossings [21,22]. The existence of this nontrivial topological structure associated with the
isolated linear touching points would lead to some interesting transport phenomena in the bulk and on the surface of such systems. A topological axion term with a nonuniform axion field is predicted to emerge in the effective electromagnetic Lagrangian which explains the chiral anomaly in these systems [23–28]. When such topological protection of band touching exists, the system is in a topological semimetal phase even in the presence of weak disorder or other types of interactions that preserve the momentum conservation. These band crossing points in the BZ can only exist in pairs [29]. Near an isolated Weyl point, the low-lying states can be described by a 2-by-2 Dirac Hamiltonian. Therefore, any local perturbation that does not violate the momentum conservation can only shift the position of such a point in the BZ and is not sufficient to gap out the spectrum unless it is strong enough to merge two such points with opposite chirality and make the system unstable towards becoming an insulator. These points can be thought of as topological defects in the fibre bundle formed by the electronic states in the BZ as the base manifold and are the magnetic monopoles of the pseudo-magnetic field (Berry curvature) associated with the gauge field defined for the Bloch states. Only the pairwise annihilation of such points with opposite chirality is possible as one can define a well-defined charge for these monopoles which is a conserved quantity in the regime where the crystal momentum is still a good quantum number.

In theory, it is possible to choose a physical parameter to adiabatically drive a system to a topological insulator phase starting from an ordinary insulator or vice versa by tuning such a parameter. As one fine-tunes such a parameter to the critical point where the gap closes, which is inevitable when we have time-reversal symmetry, the system becomes an unstable bulk metal if the time-reversal and inversion symmetry is preserved at the same time. At this critical point, the system would be in an unstable 3D metallic phase with degenerate bands near the crossing points. This gapless metallic phase is susceptible to local perturbations and instabilities that drive the system to either topological or ordinary insulator phases. Now if another parameter in the Hamiltonian is tuned in such a way that it separates the degenerate bands at the crossing points in the BZ by breaking the inversion and/or the time-reversal symmetry then the system would be in a topological semimetal phase with gapless modes dispersing in three spatial dimensions which are “robust” against momentum-conserving perturbations. The topological nature of the phase reflects itself in the appearance of a nontrivial term in the effective Lagrangian of the electromagnetic fields [26–28,30]. This topological term is an Abelian axion term with a nonhomogeneous axion field

\[ S_{\text{axion}} = C \int \theta(x) F \wedge F, \]

where \( C \) is a constant and \( \theta(x) \), for a Weyl semimetal phase in a lattice system, modulates only in space [30] with a wave vector that depends on the separation of the Weyl nodes in momentum and for a single pair of Weyl nodes it is given by \( \theta(x) = q \cdot x \) in which \( q \) is a vector of the separation of the pair of the Weyl nodes in the crystal momentum. This topological term in the effective electromagnetic Lagrangian is closely related to the topological transport phenomena that is present in these systems. It turns out that a system with more than one pairs of Weyl fermions might have zero net anomalous Hall conductivity since pairs can have total cancelling contributions due to the exactly opposite separations of them in momentum space (see fig. 1(a)) as we discuss in the “Results” section.

In the rest of this paper we introduce a lattice model made by arranging parallel TI nanowires in a honeycomb fashion with a lattice spacing which is small enough to allow a significant hopping of the electrons between these wires and then we discuss how one can achieve a time-reversal-invariant topological semimetal phase with a transverse valley current response from this arrangement.

**The building block: TI nanowires.** – The surface modes of a cylindrical topological insulator system can be described by a Dirac Hamiltonian in a curved space [31]
\( (h = 1) \)

\[
H_k = \frac{\hbar^2}{2R} \mathbf{n} \cdot \mathbf{\nabla} + \mathbf{n} \cdot (\mathbf{p} \times \mathbf{\sigma}) + (\mathbf{p} \times \mathbf{\sigma}) \cdot \mathbf{n},
\]

(2)

where \( \mathbf{\sigma} \) is the Pauli matrix vector which acts on the spin Hilbert space, \( \mathbf{p} = -i \mathbf{\nabla} \) is the momentum operator and \( \mathbf{n} \) is the unit vector normal to the surface. For a cylinder of radius \( R \) along \( \hat{z} \) axis we have \( \mathbf{n} = \cos \phi \mathbf{x} + \sin \phi \mathbf{y} \). The Hamiltonian that governs the TI surface modes in the presence of a sufficiently thin magnetic flux, \( \phi = \eta \phi_0 \), can then be written as

\[
H_k = \frac{1}{2R} + \left( \frac{i}{\hbar} \left( \frac{i \partial \phi + \eta}{ik_2} \right) \right) e^{-ik_2} \cdot \mathbf{e}^{i\varphi} - \left( \frac{i}{\hbar} \left( \frac{i \partial \phi + \eta}{ik_2} \right) \right) e^{-ik_2} \cdot \mathbf{e}^{i\varphi}.
\]

(3)

We can simplify this Hamiltonian by a unitary transformation \( \tilde{H}_k = U^\dagger(\varphi) H_k U(\varphi) \) in which \( U(\varphi) \) is given by

\[
U(\varphi) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix},
\]

(4)

using this transformation we can get rid of the phase in the off-diagonal components of the Hamiltonian matrix

\[
H_k = \begin{pmatrix} \frac{i}{\hbar} \left( \frac{i \partial \phi + \eta - \frac{1}{2}}{ik_2} \right) & -ik_2 e^{-i\varphi} \\ -ik_2 e^{i\varphi} & \frac{i}{\hbar} \left( \frac{i \partial \phi + \eta - \frac{1}{2}}{ik_2} \right) \end{pmatrix}.
\]

(5)

The eigenstates of this Hamiltonian are given by \( \psi_{kl}(\varphi) = e^{ik_2} \psi_{kl} \), where \( \psi_{kl} \) are eigenstates of the \( H_{kl} \) defined as

\[
H_{kl} = k_2 \sigma_2 - \frac{1}{R} \sigma_3 \left( l + \frac{1}{2} - \eta \right),
\]

(6)

when there is a magnetic flux through the wire equal to the odd multiple of the half quantum of the magnetic flux \( \eta = n + 0.5 \) we get a nondegenerate gapless band for \( l = n \). Note that in this special case, the system is time-reversal symmetric since \( \pi \) and \( -\pi \) phases acquired by electrons are indistinguishable (modulus \( 2\pi \)). We assume that \( R \) is small enough in a way that there exist a significant energy range, \( \Lambda \), in which the gapless band does not overlap with other bands then we can use this energy band as a building block of the model to realize a Weyl semimetal phase.

**Model.** – When the distance between two parallel nanowires (see fig. 1(b)) is sufficiently small, there would be an overlap between electronic wave functions and this leads to a hopping between adjacent electronic states of the surface modes. This can also arise from the inter-wire electron-electron interactions in a mean-field approximation. Here we consider a honeycomb arrangement of these nanowires by considering the nondegenerate gapless modes of these wires that can be achieved by exposing them to a static magnetic field along the wires. We assume that the spin-momentum lockings that occur at the surface of topological insulators are in opposite directions for wires in the \( A \) and \( B \) sub-lattices. We should point out here that all the by far discovered topological insulators happen to have the same direction for the spin-momentum locking. In theory, one can get a system with an opposite spin-momentum locking by simply changing the sign of the spin-orbit coupling required to get the original topological insulator system. We also assume that the Dirac points for both \( A \) and \( B \) wires have the same energy, however, in the end we relax this assumption and we discuss how this is essential in order to get a Weyl semimetal phase. With these assumptions and by considering only the non-degenerate lowest-lying band in each wire in the energy range \( 2\Lambda \) we can split the Hamiltonian into two parts as follows:

\[
H = H_0 + H_1,
\]

(7)

in which \( H_0 \) sums up the gapless nondegenerate modes of each individual wire in a second quantized notation and it is given in terms of the Fourier components as

\[
H_0 = \int \frac{dk_2}{2\pi} \sum_{k_{\perp}} \psi_{k_{\perp}}^\dagger(k_z) (\psi_0(k_z, \tau_3, \sigma_2) \psi_{k_{\perp}}(k_z),
\]

(8)

where \( \tau_3 \) is the Pauli matrix acting on the sub-lattice Hilbert space, \( k_z \) is the momentum along the wire and \( k_{\perp} \) spans the honeycomb’s reciprocal lattice (similar to what one gets for graphene) and \( \Psi^i = (\psi^i_A, \psi^i_{A^*}, \psi^i_B, \psi^i_{B^*})^T \). The first (last) two components act on the spin space of the wire in the \( A \) (\( B \)) sub-lattice, \( \psi^i_A, A^* \) creates an electron in the \( \alpha \) branch of the \( A/B \) wire when it acts on the vacuum state. Using this representation, \( \tilde{H}_k \) which represents the direct hopping between nearest-neighbour wires, can be written as

\[
\int \frac{dk_2}{2\pi} \sum_{k_{\perp}} \psi_{k_{\perp}}^\dagger(k_z) \left[ \begin{array}{c} 0 \\ g(k_{\perp}) \end{array} \right] \otimes \mathbb{I} \psi_{k_{\perp}}(k_z),
\]

(9)

\[
g(k_{\perp}) = -t \sum_{\delta_i} e^{-ik_{\perp} \cdot \delta_i} \text{ and } \delta_i \text{ are three vectors that connect a site in honeycomb lattice to the three adjacent points. The energy spectrum of the total Hamiltonian would then be doubly degenerate}
\]

\[
\varepsilon_{\pm}(k_z, k_{\perp}) = \pm \sqrt{4t^2 + |g(k_{\perp})|^2},
\]

(10)

\[
\varepsilon_{\pm}(k_z, k_{\perp}) \text{ vanishes at two inequivalent points in the two-dimensional reciprocal lattice, i.e., at } \mathbf{K}^\pm \text{ and is linear near these points. Therefore, we get two degenerate three-dimensional Dirac points at } (k_z, k_{\perp}) = (0, \mathbf{K}^\pm).
\]

**Results.** – In general, in order to get a topologically protected semimetal phase one needs to break time-reversal and/or inversion symmetry in such a way that it separates the Dirac points. Breaking inversion symmetry can be easily realized by relaxing the assumption we had in the beginning, i.e., Dirac points at two sub-lattices now can have different energies. By revising \( H_0 \) to account for such an energy difference, \( V \), we get

\[
H_0 = \int \frac{dk_2}{2\pi} \sum_{k_{\perp}} \psi_{k_{\perp}}^\dagger(k_z)(\nu_0 k_z \tau_3, \sigma_2 + V \tau_3) \psi_{k_{\perp}}(k_z).
\]

(11)

In this case the degeneracy is lifted and we have four bands \( \varepsilon_{sr}(k_z, k_{\perp}) \) \((s, r = \pm)\) given by

\[
\varepsilon_{sr}(k_z, k_{\perp}) = r \sqrt{(\nu_0 k_z + sV)^2 + |g(k_{\perp})|^2}.
\]

(12)
This spectrum has two pairs of Weyl points in the three-dimensional BZ. Each pair consists of two Weyl points centred at $(k_z, k_{\perp}) = (0, K^\pm)$ which are separated along the $k_z$ axis by $Q = 2V/z_0$. It is important to note that although they are robust against local momentum-conserving perturbations, the peculiarity in the Hall response that is present in a system with only one pair of Weyl nodes with broken time-reversal symmetry does not exist here. The transverse conductivity in the presence of the applied magnetic field along the wires, $\sigma_{xy}$, is zero [16,32] since the two pairs contribute oppositely to the Hall conductivity as they are separated in the opposite way at two valleys considering their chirality. On the other hand, the topological nature of the system can be observed in the existence of a nonzero transverse valley current which can be defined from the anti-symmetric combination of the two valley contributions to the charge current which can be defined from the anti-symmetric combination of the two valley contributions to the charge current and can be computed by summing up the contributions from two-dimensional massive Dirac fermions at each $k_z$ [16]:

$$
\sigma_{xy}^{\text{valley}} = \sigma_x^+ - \sigma_x^- = \frac{2V e^2}{\hbar v_0},
$$

(13)

where $\sigma_{xy}^{\pm}$ is the contribution from the Weyl pair in the $K^\pm$ valley.

One can also consider the possibility of phase transition to an insulator phase due to the electron-electron interactions. One example arises in a mean-field treatment of the inter-rod electron-electron interactions. When the wire radius, $R$, is much smaller than the honeycomb lattice constant, $a$, the coulomb interaction between electrons in the adjacent wires can be written as

$$
H_{\text{c-e}} = U \int_{-L/2}^{L/2} dz \int_{-\infty}^{\infty} dn \frac{\hat{n}(R, z)\hat{n}(R + \delta, z + u)}{\sqrt{1 + \left(\frac{R}{a}\right)^2}},
$$

(14)

where $\hat{n}$ is the electronic density operator and $U = e^2/(4\pi e a)$. $R$, $\delta$ and $z$ have been defined in fig. 1(b). In this example we neglect the intra-wire electron-electron interaction assuming that the single TI surface massless Dirac mode is stable against this interaction at least when the dielectric constant is large. In a systematic approach to study the effects of interactions in a Weyl semimetall system one should consider the full interaction. In a mean-field treatment of the above term and by considering a Kekule-type modulating order parameter with a wave vector $G = K^+ - K^-$, it is possible to connect the Weyl points separated by $G$. This would then open up a gap and the system becomes an insulator. The critical coupling, $U_c$, at which such a phase transition to an insulator phase occurs can be computed for this system. It is a function of the potential difference, $V$, as well as the hoping strength, $t$, and is given by

$$
U_c = \frac{4\Lambda}{3} \left( 1 + \ln \frac{\alpha V(\Lambda - V)}{t} \right)^{-1},
$$

(15)

in which $\alpha = (8/\sqrt{3})^{1/2}$. This critical coupling would be of the order of the single wire's nondegenerate bandwidth $\Lambda$ whenever the hoping strength is significant enough. For $U < U_c$ the system would remain in the topological semimetal phase and for $U > U_c$ the system would become a three-dimensional version of the Kekule insulator which has been discussed previously in two dimensions for graphene [33]. It is worth mentioning that there is another type of instability with opposite nonzero average magnetization on the two sub-lattices which can only arise when $U > V$ and is a dominant phase over the Kekule insulator [34] in this case. However, for $U < V$, this instability does not exist as this type of ordering cannot gap out the spectrum and can only shift the position of the Weyl nodes. It is possible to make the system stable against such phase transition for all ranges of interactions at least in this mean-field channel by introducing a Haldane [32] term in the Hamiltonian which separates two Weyl nodes at each valley ($K^+$ and $K^-$) by a different amount. In this case the system becomes stable against the perturbation that connects two valleys since all the opposite chirality Weyl pairs would have incommensurate separation in momentum space after the addition of such a term. This term can be induced by considering next-nearest-neighbour inter-wire hopping of the electronic states. The hopping amplitude is imaginary considering a modulating magnetic flux with a zero net average through each hexagon (see fig. 1(c)). Such a term was first introduced for a honeycomb lattice to realize a quantum Hall phase in a system without a net uniform applied magnetic field [32]. The Hamiltonian for this next-nearest-neighbour hopping in the momentum space can be written as

$$
H' = -t' \sum_{k_\perp} \Psi_{k_\perp}^\dagger (k_z) (\mu(k_\perp) + V(k_\perp) \tau_3) \Psi_{k_\perp} (k_z),
$$

(16)

which is similar to the term which has been introduced in eq. (11) but here the $V$ which separates the Dirac nodes along $k_z$ is a function of the $k_z$ and takes different values at $K^+$ and $K^-$. The presence of $\mu(k_\perp)$ separates two pairs in energy since it also depends on $k_\perp$ and can take different values at two valleys. In the original Haldane’s [32] flux configuration $\mu(k_\perp)$ and $V(k_\perp)$ are given by

$$
V(k_\perp) = -2t' \sin \phi \sum_{i=1,2,3} \sin k_\perp \cdot b_i,
$$

(17)

and

$$
\mu(k_\perp) = 2t' \cos \phi \sum_{i=1,2,3} \cos k_\perp \cdot b_i,
$$

(18)

$\mu$ and $\phi$ have been defined in the caption of fig. 1(c) and $t'$ is the next-nearest-neighbour hopping amplitude.

Therefore, the distance between each pair of Weyl nodes is now an incommensurate wave vector since the separations of Weyl nodes at two valleys, i.e., $q_1 = 2V(K^+ - K^-) / 2\pi v_0$ and $q_2 = 2V(K^- - K^+) / 2\pi v_0$ are not exactly opposite. This makes the system stable against charge density perturbations that connect the quantum states of two valleys.

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for all ranges of the interaction strength. The axion field is not zero in this case as the separations are not exactly opposite and it modulates in space [26].

Therefore in the presence of the Haldane term the system breaks the time-reversal symmetry and it would have a nontrivial topological charge response. The net $\sigma_{xy}$ can be obtained by a summation over the contribution of all two-dimensional Dirac fermions labeled by $k_z$ and the valley index, i.e., 1 and 2

$$\sigma_{xy} = \frac{1}{\Lambda} \int_{-\Lambda}^{\Lambda} [\nu_1(k_z) - \nu_2(k_z)] \frac{dk_z}{2\pi} \frac{e^2}{\hbar}, \quad (19)$$

in which $\nu = \Theta(q_1 - |k_z|)$ and $\Theta(q_2 - |k_z|)$. Using eq. (17) the transverse conductivity becomes

$$\sigma_{xy} = \frac{6\sqrt{3}\hbar}{\pi} \sin \phi \frac{e^2}{\hbar}. \quad (20)$$

Finally, we point out that the growth of large-scale vertically aligned nanorods and nanopillars with various arrangements including honeycomb has already been achieved by experimentalists [35–37]. However, realizing a system for which one can observe the robust Weyl energy crossings seems to be experimentally challenging at this point. One can name a few obstacles on the way of its experimental realization. First, wires are multiband systems and the two-band model approximation used throughout this paper requires a significant gap for the other existing sub-bands in the nanowires. For the so far discovered topological insulators, the surface Fermi velocity $v_0$, is of the order of $10^5$ m/s ($5 \times 10^4$ m/s for Bi$_2$Se$_3$ [6]), therefore, the wire diameter required ($2R \lesssim 60$ nm) to get a significant gap ($\Delta \gtrsim 10$ meV) is still out of the experimentally feasible sub-micrometer ranges [35–37]. Finally, another challenge to realize such a system is to find two types of topological insulators with opposite spin-momentum lockings. We note that the direction of the spin-momentum locking is a material-dependent property and in the theoretical lattice models for the topological insulators in three dimensions, it is possible to change it on the surface by varying physical parameters in the bulk.

In summary, we have constructed a simple theoretical model for a topological semimetal phase with 4 separated Weyl nodes in BZ. We showed that it is possible to have a topologically protected Weyl phase in which the topological charge response is absent even when the Weyl nodes are separated in the BZ. As we discussed, the existence and the strength of the charge and valley anomalous Hall response depend on the relative separations of the two Weyl pairs.

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