Dirac and Weyl Semimetals

M. Franz
University of British Columbia
I. Surface states of 3D Topological Insulators

Topological classification of 3D band insulators contains a surprise: in addition to the expected 3 ‘layered’ invariants there exists a 4\textsuperscript{th}, uniquely 3-dimensional ‘strong invariant’ \cite{MooreBalents2007, FuKaneMele2007}

Prediction: “Strong topological insulator (STI)”\index{strong topological insulator (STI)}: bulk insulator with gapless Dirac surface states.
Surface Dirac cone seen by ARPES in Bi$_2$Se$_3$ crystals

... and by STM in Bi$_2$Te$_3$ crystals

Hsieh et al, Nature 2009

Alpichshev et al, PRL 2010
Families of 3D topological insulators:

- $\text{Bi}_{1-x}\text{Sb}_x$ alloys
- $\text{Bi}_2\text{Se}_3, \text{Bi}_2\text{Te}_3, \text{Sb}_2\text{Te}_3$ crystals
- ternary $\text{Bi}_2\text{Te}_2\text{Se}_2, \text{GeBi}_2\text{Te}_3$
- Heusler compounds ($\text{Li}_2\text{AgSb}, \text{NdPtBi}, \text{SmPtBi}, \ldots$)
- chalcogenides ($\text{TlBiTe}_2, \text{TlBiSe}_2$)
- pyrochlores ($\text{Pr}_2\text{Ir}_2\text{O}_7, \text{Cd}_2\text{Os}_2\text{O}_7$)
- perovskites & antiperovskites ($\text{Sr}_3\text{NBi}, \text{Sr}_3\text{NBi}$)

... more to come?
Absence of neutrinos on a lattice: (I). Proof by homotopy theory

H. B. Nielsen
M. Ninomiya

The Niels Bohr Institute and Nordita, Blegdamsvej 17, DK-2100, Copenhagen Ø, Denmark
Rutherford Laboratory, Chilton, Didcot, Oxon OX11 0QX, England

Abstract
It is shown, by a homotopy theory argument, that for a general class of fermion theories on a Kogut-Susskind lattice an equal number of species (types) of left- and right-handed Weyl particles (neutrinos) necessarily appears in the continuum limit. We thus present a no-go theorem for putting theories of the weak interaction on a lattice. One of the most important consequences of our no-go theorem is that it is not possible, in strong interaction models, to solve the notorious species doubling problem of Dirac fermions on a lattice in a chirally invariant way.

References

Two Dirac fermions located on opposite surfaces
Protected by time reversal symmetry

\[ \Theta = i \sigma_y K, \quad \Theta^2 = -1 \]

For Bloch Hamiltonians, time reversal symmetry implies

\[ [\mathcal{H}, \Theta] = 0 \implies \Theta \mathcal{H}(k) \Theta^{-1} = \mathcal{H}(-k) \]

This, in turn implies "Kramers degeneracy" at time-reversal invariant momenta (TRIM) \( \Gamma_j = G - \Gamma_j \)

\[ \Theta \mathcal{H}(\Gamma_j) \Theta^{-1} = \mathcal{H}(\Gamma_j - G) = \mathcal{H}(\Gamma_j) \]

All states at TRIM are doubly degenerate
The key observation (by Kane and Mele):

![Diagram of band structures](image)

- **Trivial surface states**
- **Topological surface states**

\[ \mathbb{Z}_2 \text{ topological classification} \]
Surface states are topologically protected: they cannot be destroyed by any $\mathcal{T}$-invariant perturbation.

Massless Dirac Hamiltonian

$$\mathcal{H} = \nu \left[ \sigma_y p_x - \sigma_x p_y \right],$$

Pauli matrices in spin space, satisfy

$$[\sigma_i, \sigma_j] = 2i \epsilon^{ijk} \sigma_k, \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij}$$

Apply $\mathcal{T}$ to the surface Dirac Hamiltonian:

$$(i\sigma_y K)[\sigma_y k_x - \sigma_x k_y](-i\sigma_y K) = -[\sigma_y k_x - \sigma_x k_y] = \mathcal{H}(-k)$$
Spectrum: \[ \mathcal{H} \Psi = E \Psi, \quad \Psi(\mathbf{r}) = \begin{pmatrix} \psi_{\uparrow}(\mathbf{r}) \\ \psi_{\downarrow}(\mathbf{r}) \end{pmatrix} \]

Assuming translational invariance take \[ \Psi(\mathbf{r}) = e^{i \mathbf{k} \cdot \mathbf{r}} \begin{pmatrix} \psi_{\uparrow \mathbf{k}} \\ \psi_{\downarrow \mathbf{k}} \end{pmatrix} \]

\[ \mathcal{H}_k = v [\sigma_y k_x - \sigma_x k_y], \]

To find the spectrum easy way square the Hamiltonian

\[ \mathcal{H}^2_k = v^2 [k_x^2 + k_y^2 - (\sigma_y \sigma_x + \sigma_x \sigma_y) k_x k_y] \]

\[ E_k = \pm v \sqrt{k_x^2 + k_y^2} \]

\[ \Psi_k = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ k_y \pm ik_x \end{pmatrix} \]
To open a gap one needs to add a term

$$\delta \mathcal{H} = m \sigma_z, \quad E_k = \pm \sqrt{v^2(k_x^2 + k_y^2) + m^2}$$

However, this necessarily breaks $\mathbb{T}$:

$$(i \sigma_y K)m \sigma_z(-i \sigma_y K) = -m \sigma_z = -\delta \mathcal{H}(-\mathbf{k})$$

Corresponds to depositing a ferromagnet on the surface of a TI

Gapless surface states are protected by $\mathbb{T}$
Massive Dirac Fermion on the Surface of a Magnetically Doped Topological Insulator


In addition to a bulk energy gap, topological insulators accommodate a conducting, linearly dispersed Dirac surface state. This state is predicted to become massive if time reversal symmetry is broken, and to become insulating if the Fermi energy is positioned inside both the surface and bulk gaps. We introduced magnetic dopants into the three-dimensional topological insulator dibismuth triselenide (Bi3Se3) to break the time reversal symmetry and further position the Fermi energy inside the gaps by simultaneous magnetic and charge doping. The resulting insulating massive Dirac fermion state, which we observed by angle-resolved photoemission, paves the way for studying a range of topological phenomena relevant to both condensed matter and particle physics.

Science, 2010

- Gap opens without bulk magnetic ordering.
- Could there be surface ordering?
- Could disordered magnetic moments open a gap?
II. Topology in gapless systems: Dirac & Weyl semimetals

- 3D solids with linear electron dispersion at low energy near some points in the BZ

\[ H_{\text{eff}} = v \sigma \cdot q = v(\sigma^x q_x + \sigma^y q_y + \sigma^z q_z) \]

\[ E(q) = \pm v|q| \]

- Because we used up all 3 Pauli matrices there is no possibility of adding a mass term:

The gapless spectrum is “absolutely stable”.
Chirality and the Fermi arcs

• The most general perturbation takes the form

\[ H_{\text{Weyl}} \to H_{\text{Weyl}} + \delta H, \quad \delta H = u_0 + v\sigma \cdot \mathbf{q}_0 \]

\[ E(\mathbf{q}) \to u_0 \pm v|\mathbf{q} + \mathbf{q}_0| \]

• More generally the dispersion will be anisotropic:

\[ H_{\text{Weyl}} = v_i \sigma^i q_i, \quad \chi = \text{sgn}(v_x v_y v_z) = \pm 1 \]

chirality

In a system defined on the lattice Weyl points always come in pairs with opposite chirality.
The only way to remove the Weyl points is by moving them to the same (high-symmetry) point in the BZ. One then obtains a doubly degenerate Dirac dispersion which can be gapped out:

\[
H_{\text{Dirac}} = \begin{pmatrix}
 v\sigma \cdot q & M \\
 M & -v\sigma \cdot q
\end{pmatrix}, \quad E(q) = \pm \sqrt{v^2q^2 + M^2}
\]

**Fermi arcs:**
- Protected surface states in a Weyl semimetal.
- Connect projections of the bulk Weyl points onto the surface BZ.
Fermi arc states in the surface BZ:

For a slab one finds a complete Fermi surface but its two segments are on the opposite sides:
Fermi arcs in Weyl semimetal TaAs
Dirac semimetals

- Occur when a pair of Weyl points coincide but cannot open a gap due to crystal symmetry.

\[
H_{\text{Dirac}} = \begin{pmatrix}
 v \sigma \cdot q & \mp \sqrt{v^2 q^2 + M^2} \\
- v \sigma \cdot q & \mp \sqrt{v^2 q^2 + M^2}
\end{pmatrix}, \quad E(q) = \pm \sqrt{v^2 q^2 + M^2}
\]

- We then have a gapless linear dispersion with doubly degenerate bands, protected by crystal symmetry.
- Less robust than a Weyl semimetal because the symmetry can be broken e.g. by crystal distortion.
The calculated electronic structures shown in Fig. 2 for Na$_3$Bi: (a) shows Fermi points and Fermi arcs for the pristine surface and surface with Na-vacancies. The band structures without and with spin-orbit coupling, respectively, suggest that the top valence and conduction bands are dominated by Bi-6 character. The orbital inversion around 0.5 eV can be further confirmed by the following evidences: (1) the band gap is lower than Bi-6, which has higher symmetry, in momentum space by breaking time-reversal or inversion symmetry, and (2) the spin texture of surface states has a helical structure (also to the projection of bulk Dirac points to the surface). The entire Fermi surface is closed, its derivative and Fermi velocity vanishes at the singular points. This kind of Fermi surface has Fermi arc structures. As shown in Fig. 2(d), they form honeycomb lattice layers. Na(2) is at 2$\Gamma$ = (0,0,$\pm$0.33) with the key difference that at the surface consists of two isolated Fermi points, which are located around the (0,0,0) and (0,0,0.15) Fermi surfaces has Fermi arc structures. As shown in Fig. 2(d), they form honeycomb lattice layers. Na(2) is at 2$\Gamma$ = (0,0,$\pm$0.33) with the key difference that at the surface consists of two isolated Fermi points, which are located around the (0,0,0) and (0,0,0.15) points. This fact makes Na$_3$Bi unique, because the Fermi surface of surface states will also due to the inverted band structure, but the magnitude of spin texture of surface states has a helical structure (also to the projection of bulk Dirac points to the surface). The two bands which cross each other along the $\Gamma$ point. This fact makes Na$_3$Bi unique, because the Fermi surface of surface states will also due to the inverted band structure, but the magnitude of spin texture of surface states has a helical structure (also to the projection of bulk Dirac points to the surface). The two bands which cross each other along the $\Gamma$ point. This fact makes Na$_3$Bi unique, because the Fermi surface of surface states will also due to the inverted band structure, but the magnitude of spin texture of surface states has a helical structure (also to the projection of bulk Dirac points to the surface). The two bands which cross each other along the $\Gamma$ point.
Dirac semimetal Cd₃As₂

Neupane et al., Nat. Comm. 2014
The chiral anomaly

- Effect first predicted in high-energy physics
- Transfer of charge between Weyl points induced by the application of electric and magnetic fields.

\[ \partial_t \rho_5 + \nabla \cdot j_5 = \frac{e^2}{2\pi^2 \hbar^2 c} E \cdot B, \quad \rho_5 = \rho_+ - \rho_- \]

chiral charge not conserved

Pikulin et al., PRX 2016
Quantum oscillations without magnetic field

\[ H^{\text{latt}} = \epsilon_{\mathbf{k}} + \begin{pmatrix} h^{\text{latt}} & 0 \\ 0 & -h^{\text{latt}} \end{pmatrix} \]

\[ h^{\text{latt}}(\mathbf{k}) = m_{\mathbf{k}} \tau^z + \Lambda(\tau^x \sin a_x k_x + \tau^y \sin a_y k_y), \]
\[ m_{\mathbf{k}} = t_0 + t_1 \cos k_z + t_2 (\cos k_x + \cos k_y) \]
Chiral anomaly in Nb$_3$Bi

- Chiral anomaly leads to anomalous contribution to the magnetoresistance

\[
\sigma_X = \frac{e^2}{4\pi^2\hbar c} \frac{\nu (eB\nu)^2}{E_F^2} \tau_I
\]

Xiong et al., Science 2015
Conclusions

• Topology offers interesting insights into both gapped and gapless electron systems in 3D.
• Topological insulators and Dirac/Weyl semimetals are examples of topological materials with protected surface states.
• Many interesting phenomena occur in these surfaces that are not permitted in standalone 2D systems.