Title: Topological Semimetals

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Abstract: I will describe our recent work on a new topological phase of matter: topological Weyl semimetal. This phase arises in three-dimensional (3D) materials, which are close to a critical point between an ordinary and a topological insulator. Breaking time-reversal symmetry in such materials, for example by doping with sufficient amount of magnetic impurities, leads to the formation of a Weyl semimetal phase, with two (or more) 3D Dirac nodes, separated in momentum space. Such a topological Weyl semimetal possesses chiral edge states and a finite Hall conductivity, proportional to the momentum-space separation of the Dirac nodes, in the absence of any external magnetic field. Weyl semimetal demonstrates a qualitatively different type of topological protection: the protection is provided not by the bulk band gap, as in topological insulators, but by the separation of gapless 3D Dirac nodes in momentum space. I will describe a simple way to engineer such materials using superlattice heterostructures, made of thin films of topological insulators.
References: arXiv:1110.1089; Phys. Rev. Lett. 107, 127205 (2011); Phys. Rev. B 83, 245428 (2011)."


Topological Semimetals
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Michael Hook (Waterloo)
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NSERC CRSNG
Perimeter Institute, November 25, 2011

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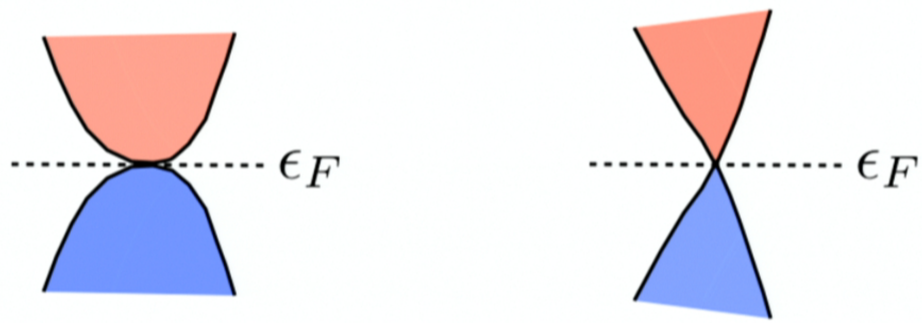
Outline

- Introduction: semimetals and topological semimetals.
- Weyl semimetal in a topological insulator multilayer.
- Anomalous Quantum Hall effect and chiral edge states in Weyl semimetal.
- Bulk transport in Weyl semimetals.
- Line node semimetals.

Semimetals

- Conduction and valence bands touch at isolated special points in the BZ.
- Neither a metal nor an insulator: no Fermi surface, but also no gap.



Herring, 1937   Halperin & Rice, 1968   Abrikosov, 1971

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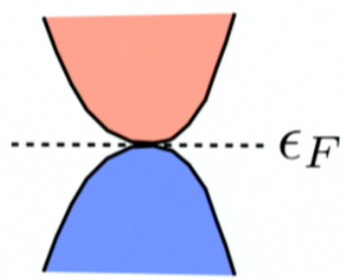

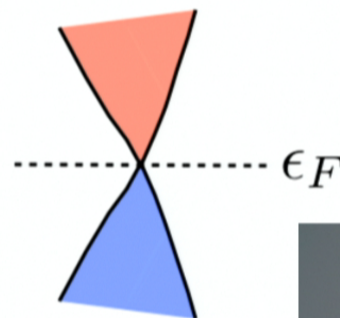

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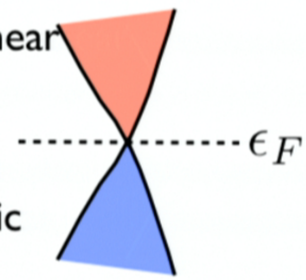
Topological Semimetals

- Has been realized recently that semimetals with linear band touching can be topologically nontrivial.



- We are used to (already) topologically-nontrivial insulators: insulators in the bulk, which have metallic surface states.
- The surface states are "protected" by the bulk gap (plus time-reversal in TR-invariant TI's).
- Some gapless semimetals also have protected metallic edge states, the nature of the protection distinct from topological insulators.

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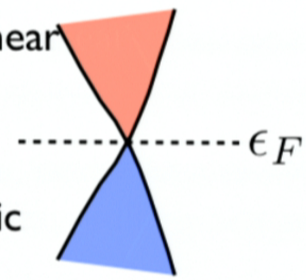

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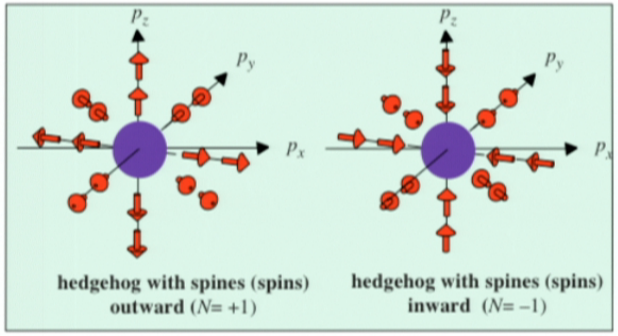
Accidental band touching: importance of dimensionality

- von Neumann & Wigner (1929): to make two levels cross need to tune 3 parameters.
- In a crystal band structure the only parameters available are components of the crystal momentum.
- Thus accidental band crossing can occur generically (without additional symmetry constraints: e.g. in graphene need time-reversal + inversion) only in 3 dimensions.

$$\mathcal{H} = h_x\sigma^x + h_y\sigma^y + h_z\sigma^z$$

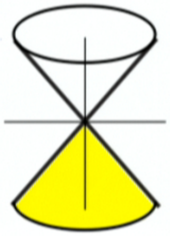
$$h_x = h_y = h_z = 0$$

Weyl nodes in 3D



$$\mathcal{H}(\mathbf{k}) = \pm v_F \boldsymbol{\sigma} \cdot \mathbf{k}$$

G.E. Volovik, 2003

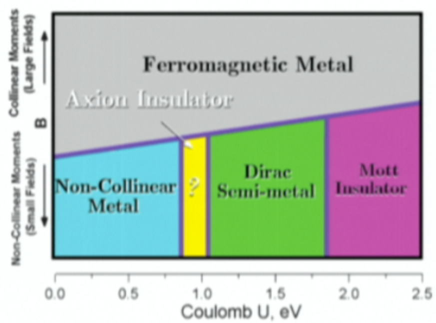


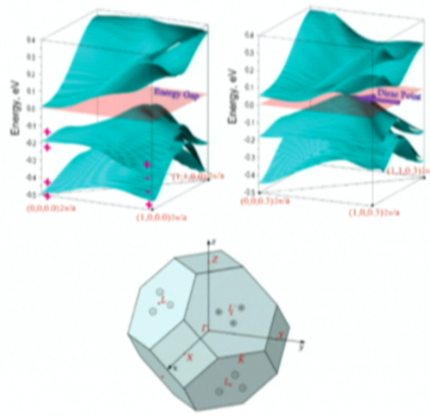
- An isolated Weyl node (can be visualized as a hedgehog in momentum space) is absolutely indestructible.
- The only way to get rid of a Weyl node is to annihilate it with an "antinode": a Weyl node of opposite chirality.
- Nielsen-Ninomiya theorem: Weyl fermions always appear in pairs of opposite chirality. Protection results from separating such pairs in momentum space.

How do we find Weyl nodes?

- Weyl nodes WILL occur generically in 3D bandstructures, so may stumble upon them accidentally: LDA+U calculation on a pyrochlore iridate material by X. Wan et al.

X. Wan et al., 2011 $Y_2Ir_2O_7$





Is there a systematic way?

- Yes! Weyl fermions occur generically at a critical point between an ordinary and a topological insulator in 3D.
- Physics of 3D TI: sign change of the mass of a 4-component Dirac fermion.
- The 4 components are 2 bands of opposite parity plus 2 spin directions.
- Mass = band gap, band inversion = change of sign of the mass.
- Dirac fermion = 2 Weyl fermions of opposite chirality.

3D topological insulators

- SO-driven inversion between two bands of opposite parity.
- k.p Hamiltonian near the Gamma-point:

$$|+\uparrow\rangle,\ |-\downarrow\rangle,\ |+\downarrow\rangle,\ |-\uparrow\rangle$$

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \Delta & iv_F k_- & 0 & iv_F k_z \\ -iv_F k_+ & -\Delta & -iv_F k_z & 0 \\ 0 & iv_F k_z & \Delta & -iv_F k_+ \\ -iv_F k_z & 0 & iv_F k_- & -\Delta \end{pmatrix}$$

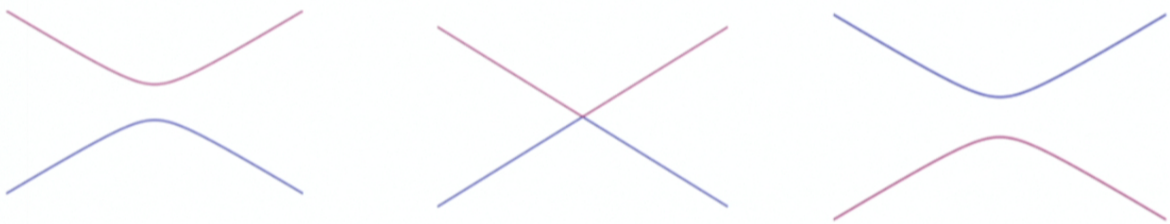
This is the Hamiltonian of a 4-component Dirac fermion

$$\epsilon(\mathbf{k})_\pm = \pm\sqrt{v_F^2\mathbf{k}^2 + \Delta^2}$$

3D topological insulators

- When both TR and I symmetries are present, bands are doubly-degenerate at every momentum.

$$|+\uparrow\rangle,\ |-\downarrow\rangle,\ |+\downarrow\rangle,\ |-\uparrow\rangle \quad \mathcal{H}(\mathbf{k}) = \begin{pmatrix} \Delta & iv_F k_- & 0 & iv_F k_z \\ -iv_F k_+ & -\Delta & -iv_F k_z & 0 \\ 0 & iv_F k_z & \Delta & -iv_F k_+ \\ -iv_F k_z & 0 & iv_F k_- & -\Delta \end{pmatrix}$$



$\Delta > 0$ $\Delta = 0$ $\Delta < 0$

Weyl fermions at the TI-NI critical point

- 4x4 Dirac fermion can always be decomposed into a pair of opposite-chirality Weyl fermions, which are hybridized when the mass is finite.
- Unhybridized only at a single point $\Delta = 0$, corresponding to TI-NI transition.
- This is because TR + I forces the two Weyl fermions to be at the same point in momentum space: this can not occur generically and requires fine-tuning.
- Break TR or I near the TI-NI critical point to separate Weyl fermions in momentum space: this will produce a stable Weyl semimetal phase.

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} v_F \boldsymbol{\sigma} \cdot \mathbf{k} & \Delta \\ \Delta & -v_F \boldsymbol{\sigma} \cdot \mathbf{k} \end{pmatrix}$$

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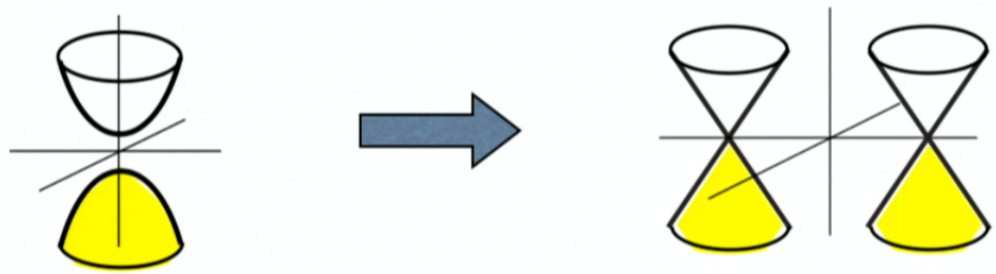
Breaking TR near the TI-NI critical point

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} v_F \boldsymbol{\sigma} \cdot \mathbf{k} + m\sigma^z & \Delta \\ \Delta & -v_F \boldsymbol{\sigma} \cdot \mathbf{k} + m\sigma^z \end{pmatrix} \qquad \epsilon_{\pm}(\mathbf{k}) = \pm\sqrt{v_F^2(k_x^2 + k_y^2) + [m - \sqrt{\Delta^2 + v_F^2 k_z^2}]^2}$$



Massive Dirac fermion   Two nondegenerate Weyl fermions at $k_z = \pm \frac{1}{v_F}\sqrt{m^2 - \Delta^2}$

Weyl nodes will stay unhybridized as long as $m > \Delta$

3D analog of graphene, only better!

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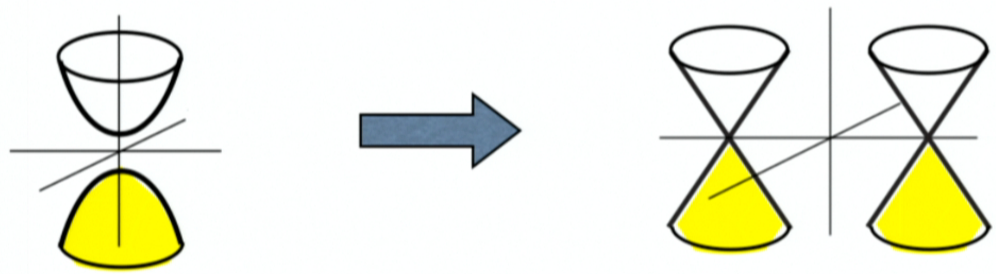

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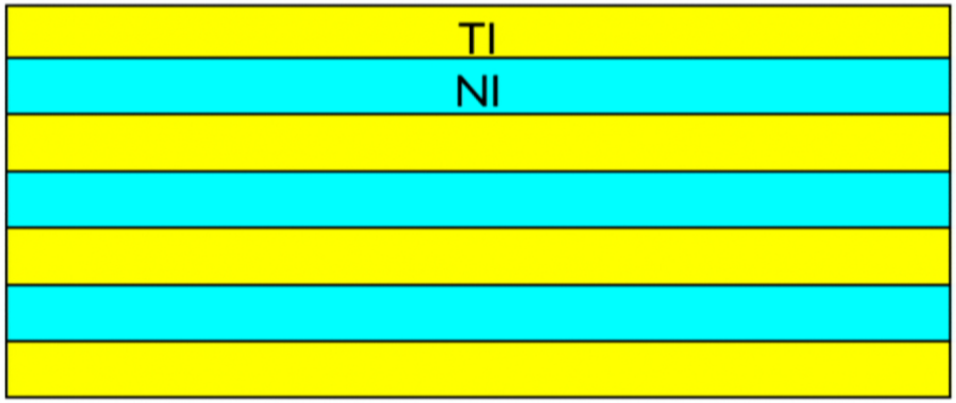
3D analog of graphene, only better!

How to realize this?

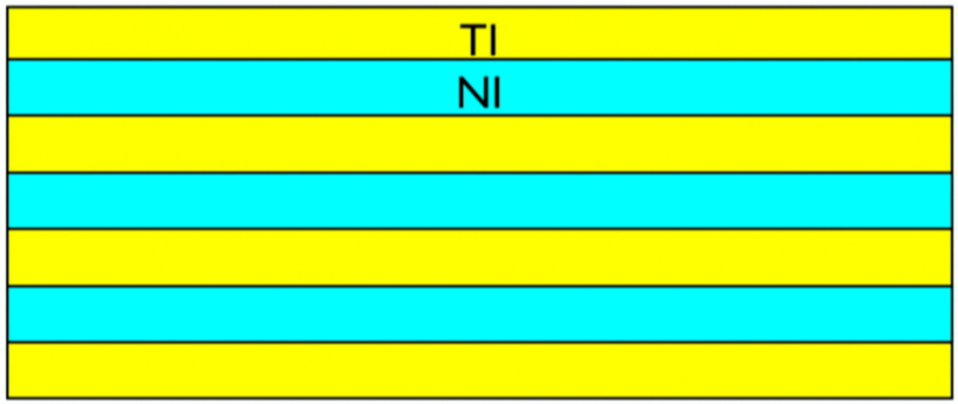
- Need a 3D material, which is close to a TI-NI critical point.
- Need TR-breaking of sufficient strength.
- Note: in 2D the first point is achieved by tuning the width of the HgTe quantum well in a HdTe/CdTe heterostructure (L. Molenkamp : better graphene).
- Our proposal: an even better graphene!

TI-NI multilayer heterostructure



- Layers are thin enough so electrons can tunnel across.
- Epitaxial growth of single thin TI films (BiSe or BiTe) has been demonstrated experimentally, shouldn't be a problem to grow a multilayer.

TI-NI multilayer heterostructure



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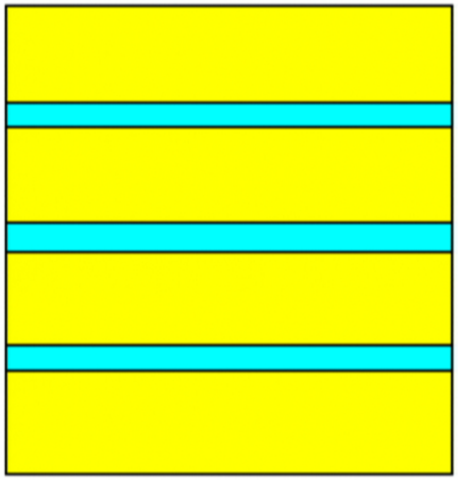
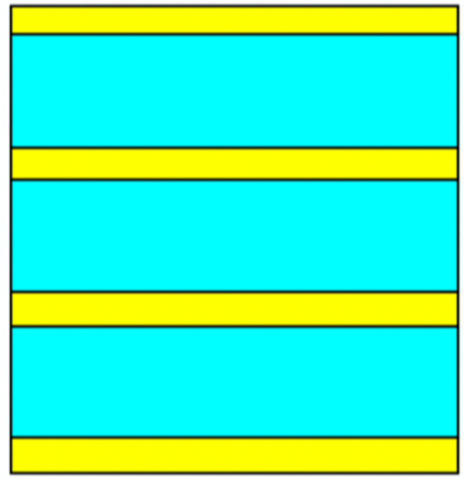
TI-NI phase transition



TI-NI phase transition in between

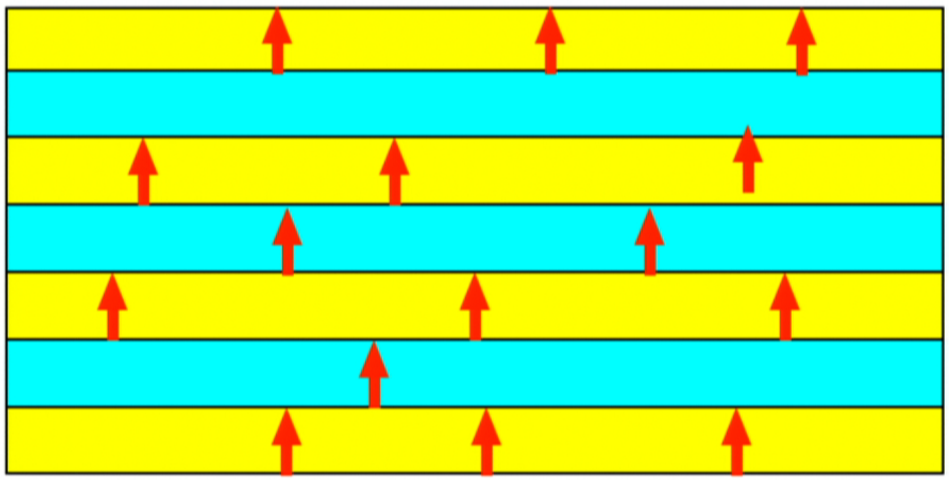


Thick TI layers, thin NI layers: strong 3D TI

Thin TI layers, thick NI layers: normal 3D insulator

Can tune the distance to the transition, much like in 2D HgTe/CdTe structures (Molenkamp et al.)

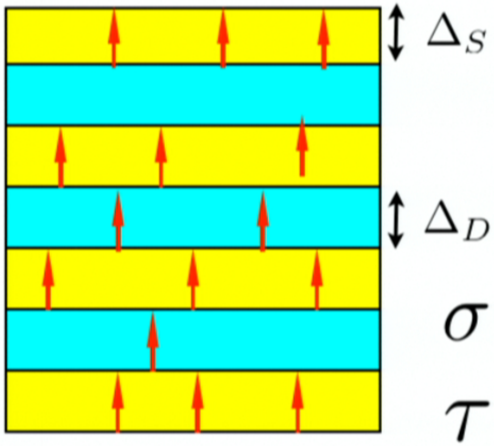
Breaking TR



- Dope with magnetic impurities, already achieved experimentally in Bi-based TI's.
- Assume at sufficient concentration impurities will order ferromagnetically, again has been demonstrated experimentally (C.Z. Chang et al, 2011)

Breaking TR

- Simplest theory: model in terms of TI film top and bottom surface states.



$$H = \sum_{\mathbf{k}_\perp, ij} \Big[v_F \tau^z (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k}_\perp \delta_{i,j} + m\sigma^z \delta_{i,j} + \Delta_S \tau^x \delta_{i,j} + \frac{1}{2}\Delta_D \tau^+ \delta_{j,i+1} + \frac{1}{2}\Delta_D \tau^- \delta_{j,i-1} \Big] c^\dagger_{\mathbf{k}_\perp i} c_{\mathbf{k}_\perp j}.$$

σ real spin

τ "pseudospin": describes the top-bottom surface in each TI layer

m is exchange energy due to magnetically-ordered impurities

i,j indices label different TI layers

$\Delta_S = \Delta_D$ TI-NI critical point at m=0

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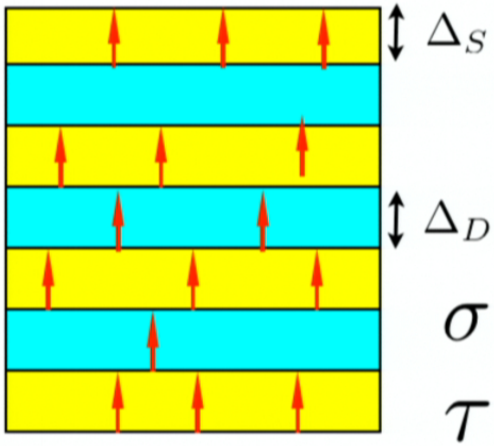

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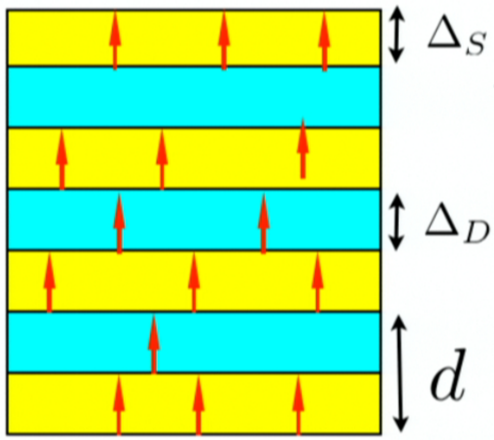
Bandstructure and Weyl nodes



$$\mathcal{H}_{\pm}(\mathbf{k}) = v_F k_y \sigma_x - v_F k_x \sigma_y + [m \pm \Delta(k_z)]\sigma^z$$

$$\Delta(k_z) = \sqrt{\Delta_S^2 + \Delta_D^2 + 2\Delta_S \Delta_D \cos(k_z d)}$$

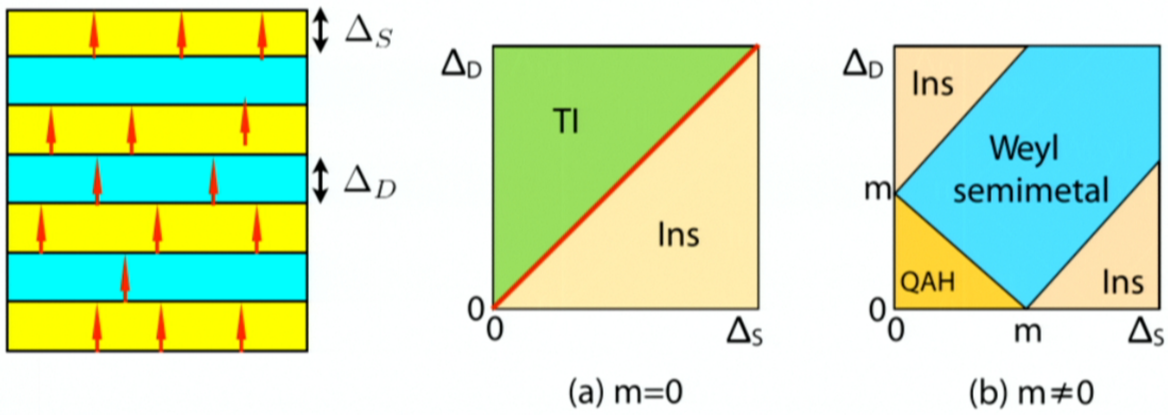
$$m = \Delta(k_z)$$

Get two Weyl nodes at $k_z = \pi/d \pm k_0$

$$k_0 = \frac{1}{d} \operatorname{arccos}\{1 - [m^2 - (\Delta_S - \Delta_D)^2]/2\Delta_S \Delta_D\}.$$

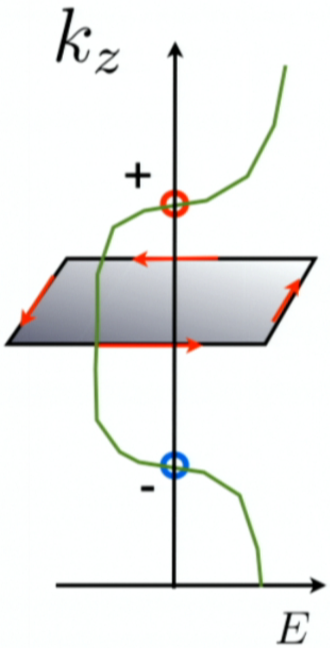
Nodes exist as long as: $m_{c1}^2 = (\Delta_S - \Delta_D)^2 < m^2 < m_{c2}^2 = (\Delta_S + \Delta_D)^2.$

Phase diagram



Direct TI-NI transition with TR symmetry is replaced by a Weyl semimetal phase when TR is broken.

Quantum Anomalous Hall Effect



2x2 block of the Hamiltonian, describing the Weyl nodes:

$$\mathcal{H}_-(\mathbf{k}) = v_F k_y \sigma_x - v_F k_x \sigma_y + m_-(k_z)\sigma^z$$

$$m_-(k_z) = m - \Delta(k_z)$$

Can regard this as Hamiltonian of 2D Dirac fermions with a parameter-dependent mass term.

$m_-(k_z)$ changes sign at the Weyl nodes.

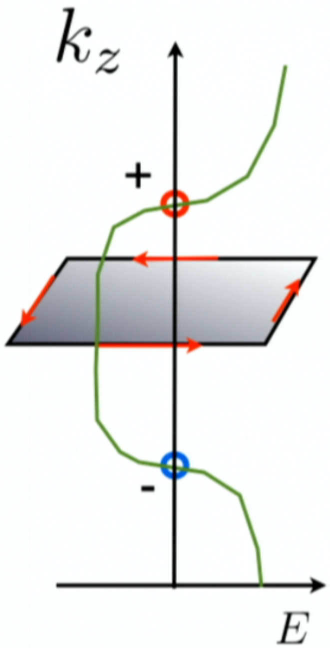
Mass sign change of 2D Dirac fermion = quantum Hall transition

Haldane, 1988

In a small external magnetic field along z, the zero-mode LL will dip below zero between the Weyl nodes.

Every momentum point between the nodes contributes a quantum of Hall conductance e^2/h

Quantum Anomalous Hall Effect



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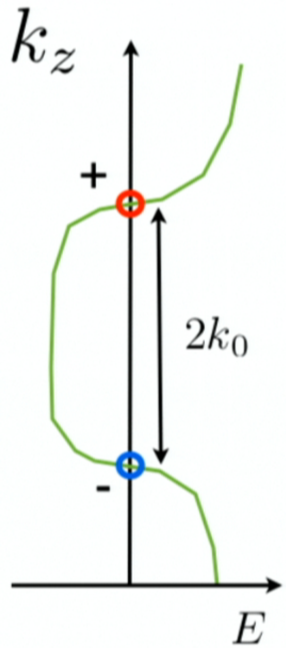
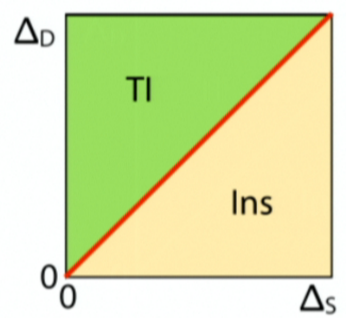
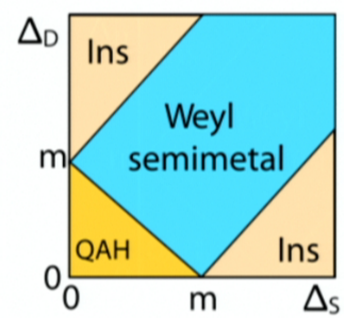


$$\sigma_{xy} = \int_{\frac{\pi}{d}-k_0}^{\frac{\pi}{d}+k_0} \frac{dk_z}{2\pi}\frac{e^2}{h} = \frac{e^2 k_0}{\pi h}$$ Weyl semimetal

$$2k_0 = 2\pi/d \Rightarrow \sigma_{xy} = \frac{e^2}{dh}$$ QAH insulator



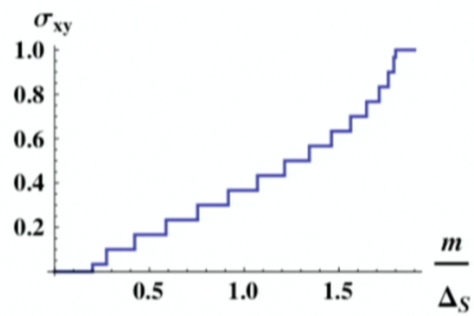
(a) m=0

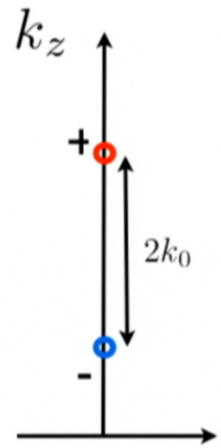


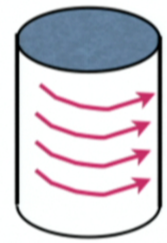
(b) m≠0

3D Quantum Anomalous Hall effect

$$\sigma_{xy} = \frac{e^2 k_0}{\pi h}$$







- Weyl semimetal is characterized by semi-quantized AHE.
- Chiral edge states, which exist in the subset of the surface BZ with kz between the Weyl nodes.
- The only known example of 3D state with (semi)-quantized Hall conductivity and chiral edge states.

Diagonal transport

- Bulk response is quantum-critical, due to lack of intrinsic energy scale.
- Graphene: disorder dominates e-e interactions.
- Weyl semimetal: interactions dominate at charge neutrality, transport properties significantly different from graphene, can observe quantum-critical response.

$$\sigma \sim \frac{e^2}{h}\frac{n}{\alpha^2 n_i} \qquad \sigma(n=0) \sim \frac{e^2}{h}$$

Diagonal transport: at neutrality

Scattering rate due to e-e interactions at neutrality: $\frac{1}{\tau(\epsilon)} \sim \alpha^2 max\{\epsilon, T\}$

This is much greater than the impurity scattering rate: $\frac{1}{\tau(\epsilon)} \sim \frac{u_0^2 n_i}{v_F^3}\epsilon^2$

DC conductivity at neutrality shows power-law insulating behavior: $\sigma_{DC} \sim \frac{e^2 T}{h\alpha^2 v_F}$

Unlike graphene, Weyl semimetal is an insulator.

Diagonal transport: away from neutrality

Sufficiently far from neutrality, transport properties are determined by scattering from charged donors, as in graphene:

$$\frac{1}{\tau_{tr}(\epsilon)} = \pi n_i g(\epsilon) \int_0^{\pi} d\theta \sin(\theta) |V(q)|^2 [1 - \cos(\theta)] \frac{1+\cos(\theta)}{2}$$

$$\sigma_{DC} \sim \frac{e^2 v_F^2}{h} g(\epsilon_F) \tau_{tr}(\epsilon_F)$$

$$\sigma_{DC} \sim \frac{e^2 n_i^{1/3}}{h f(\alpha)}$$

$$f(\alpha) = \frac{3\alpha^2}{\pi^2} \left[(1+\alpha/\pi) \text{atanh} \left(\frac{1}{1+\alpha/\pi} \right) - 1 \right]$$

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Diagonal transport: quantum critical scaling

The above two regimes can be captured by a single scaling function:

$$\sigma \sim \frac{e^2 k_F}{h} S(\epsilon_F/T)$$

$$S(\epsilon_F/T) \sim \frac{1}{f(\alpha)}, \; \epsilon_F \gg T$$

$$S(\epsilon_F/T) \sim \frac{T}{\alpha^2 \epsilon_F}, \; \epsilon_F \ll T$$

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Diagonal transport: quantum critical scaling

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Conclusions

- Weyl semimetal is a new "topological" state of matter: it has no gap, yet has topologically-protected edge states.
- Topological protection is provided by the separation of opposite-chirality Weyl nodes in momentum space.
- Characterized by semi-quantized Hall conductivity and chiral edge states (the only known 3D material with chiral edge states).
- Diagonal transport is quantum-critical.
- Can be realized in a magnetically-doped TI-NI multilayer heterostructure.
- Analogous to graphene, only better!