Weyl semimetals: the next (next) graphene?

Leon Balents, KITP, UCSB

Anton Burkov, U. Waterloo

Gabor Halasz, U. Cambridge

Outline

- Weyl fermions
- Where to find them
- TR-breaking and Hall effects
- I-breaking
- Graphene-like physics

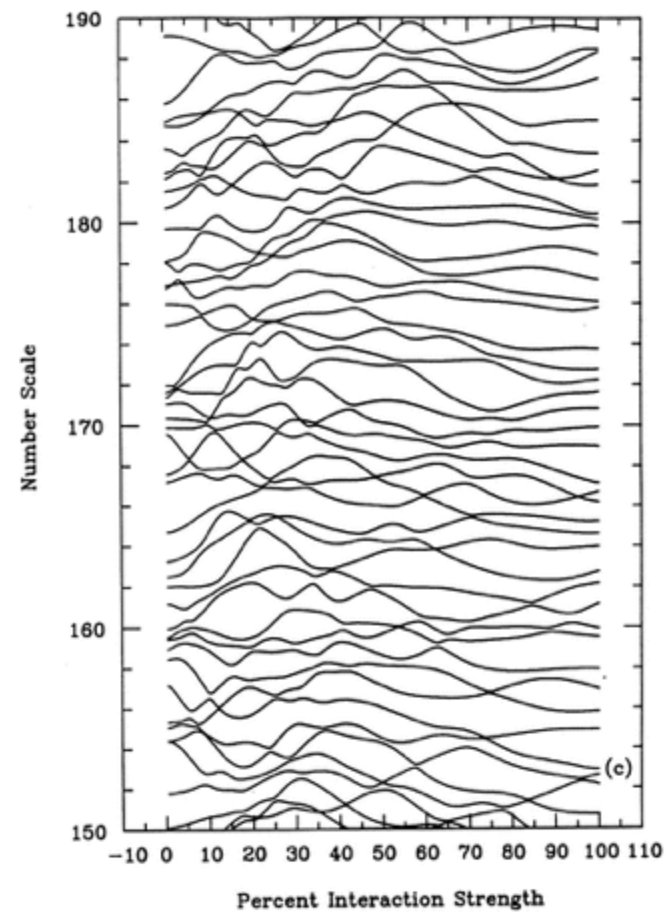
Weyl Fermion

- *Massless* Dirac fermion with fixed *handedness*
    - described by a 2-component spinor unlike 4-component (spin+particle/hole) Dirac spinor

$$H = v\vec{\sigma} \cdot \vec{k}$$

Level repulsion

- von Neumann and Wigner, 1929
    - In QMs, 3 parameters must be tuned to make 2 levels cross
    - led to a whole field of statistics of energy levels, quantum chaos,...



Weyl points in band theory

- In 3d band structures with non-degenerate bands - *lacking either inversion or TR* - this happens at isolated points
  - the non-degeracy of course requires breaking spin-rotation symmetry - typically by SOC

937 PHYSICAL REVIEW

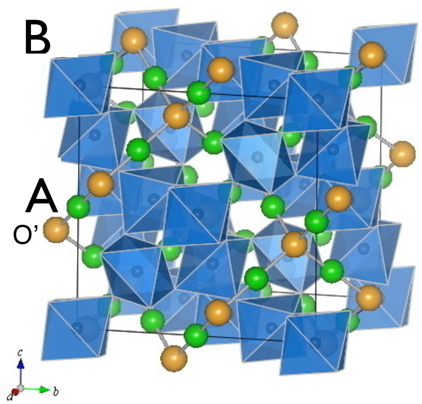
Accidental Degeneracy in the Energy Bands of Crystals

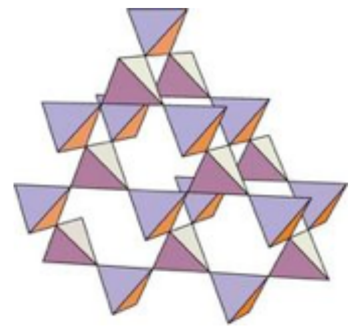
CONYERS HERRING
Princeton University, Princeton, New Jersey

(Received June 16, 1937)

For a crystal without an inversion center, the energy separation $\delta E(\mathbf{k}+\boldsymbol{\kappa})$ in the neigborhood of a point $\mathbf{k}$ where contact of equivalent manifolds occurs may be expected to be of the order of κ as $\kappa \rightarrow 0$, for all directions of $\boldsymbol{\kappa}$.

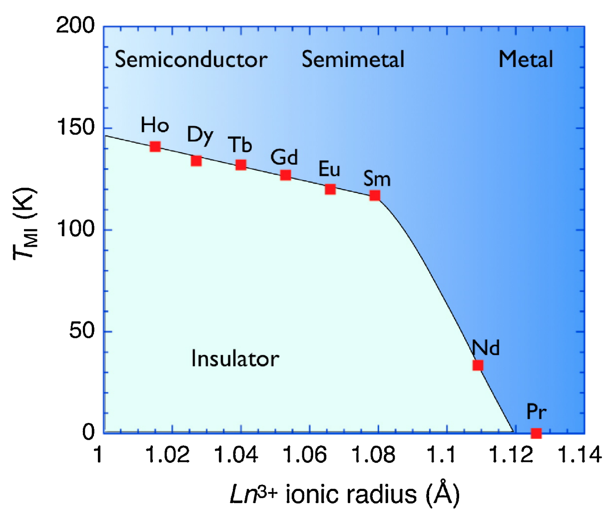
$Ln_2Ir_2O_7$ Pyrochlores





- Series of materials shows systematic MITs
- Ir^{4+} has $\lambda \approx 0.5$eV

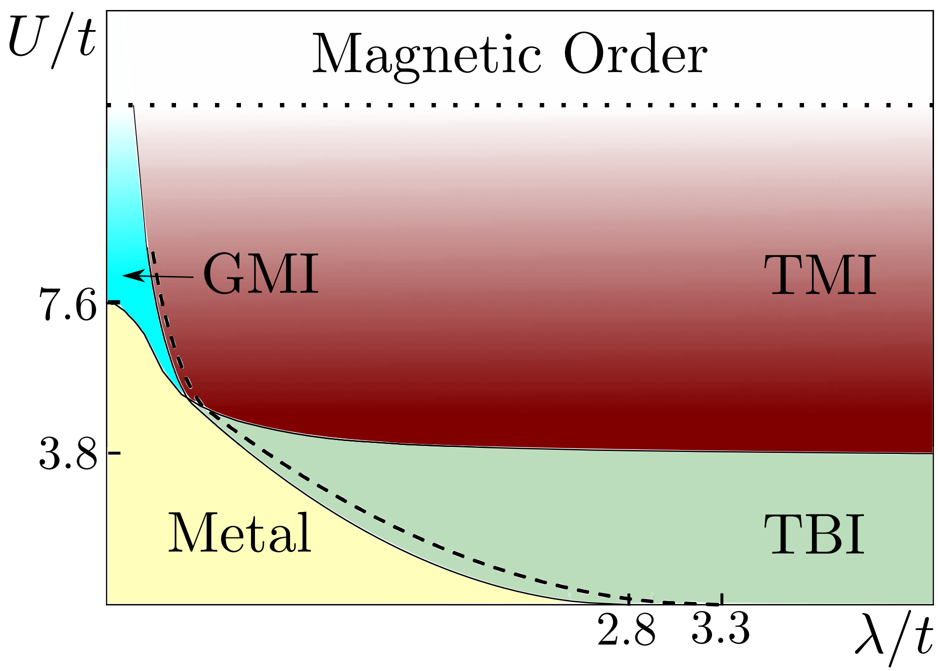
D. Yanagashima, Y. Maeno, 2001



K. Matsuhira *et al*, 2011

Exotic Possibilities

- Topological Mott Insulator?



D. Pesin+LB, 2010

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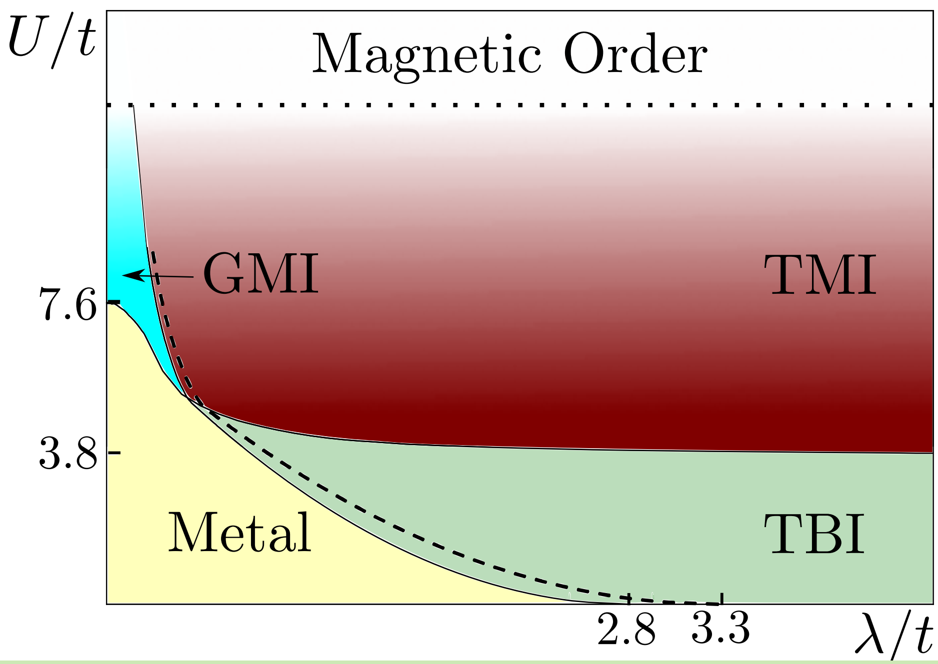


D. Pesin+LB, 2010

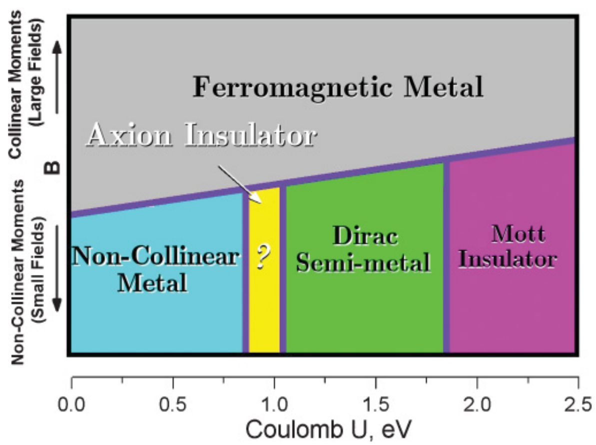
Probably not: commensurate magnetic order seen in μSR

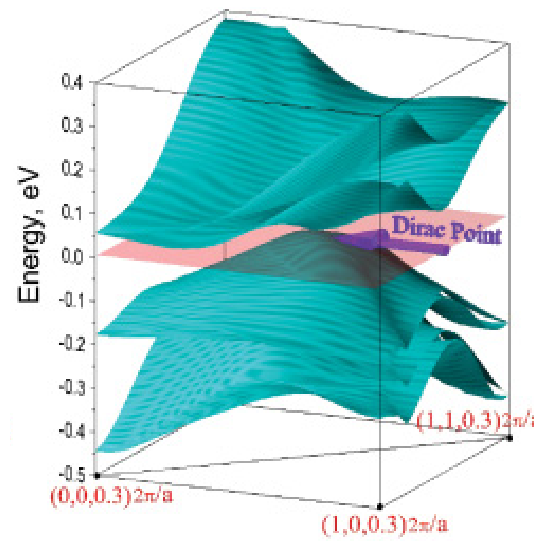
S. Zhao *et al*, 2011

Weyl semimetal?

X. Wan *et al*, 2011

- LDA+U calculations find Weyl state!

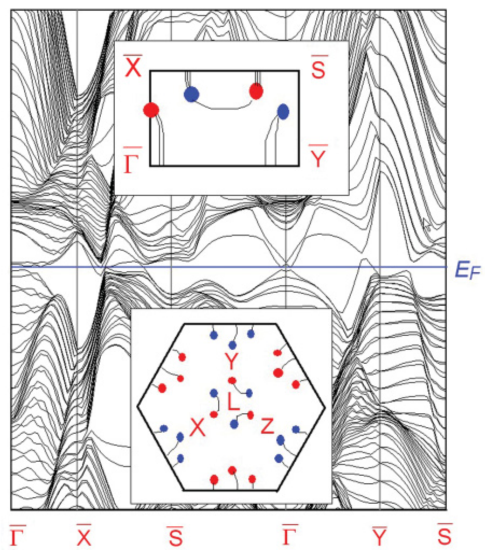




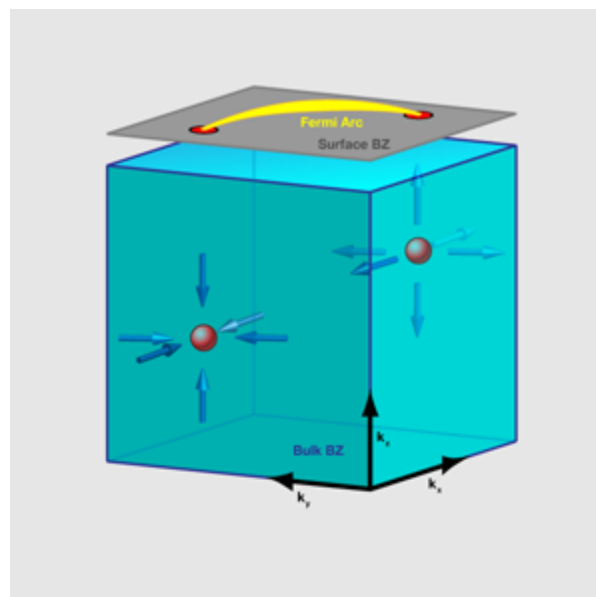
- They also pointed out very unusual surface states

Fermi Arcs

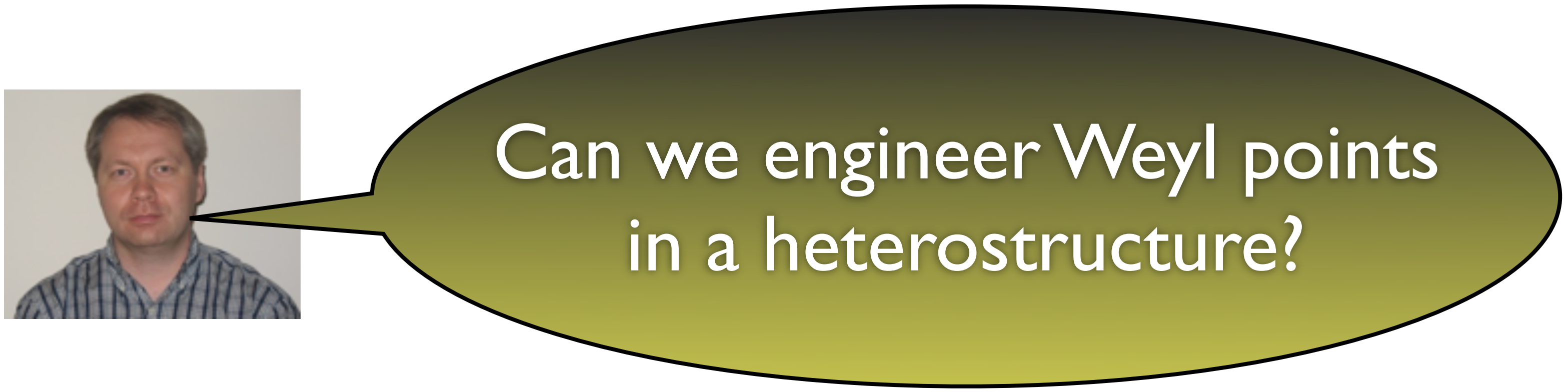
- On most surfaces, metallic Fermi surfaces *which are not closed* - "arcs" - terminate at the projections of the Weyl points



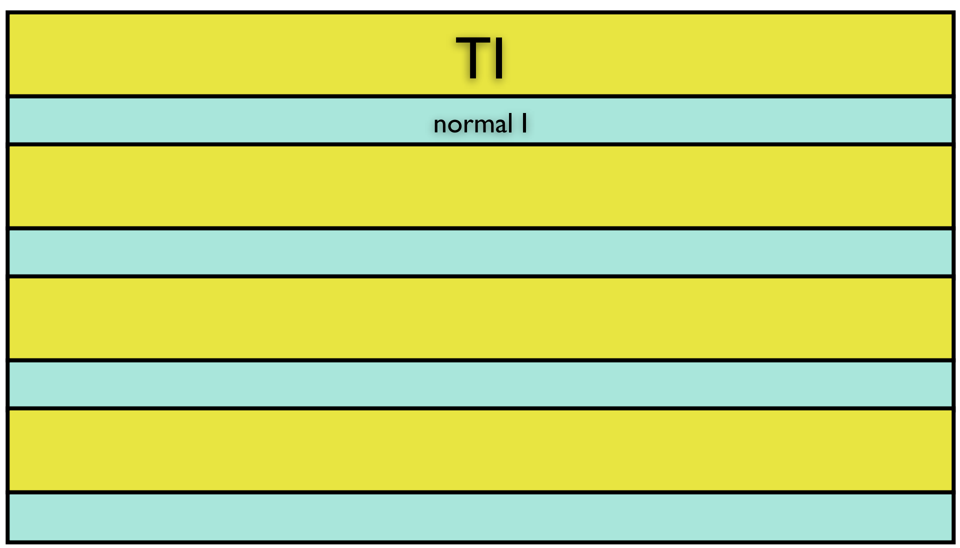
24 Weyl points predicted in $Y_2Ir_2O_7$



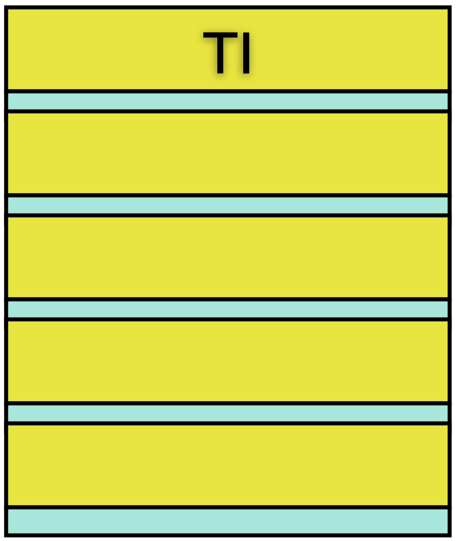
Heterostructuring

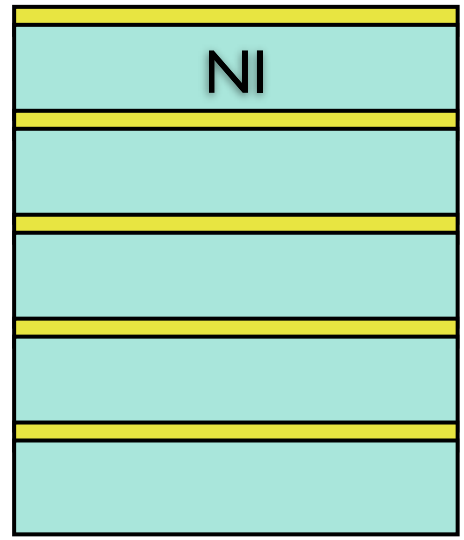


- A: yes! And you can do it with topological insulators



TI to NI transition

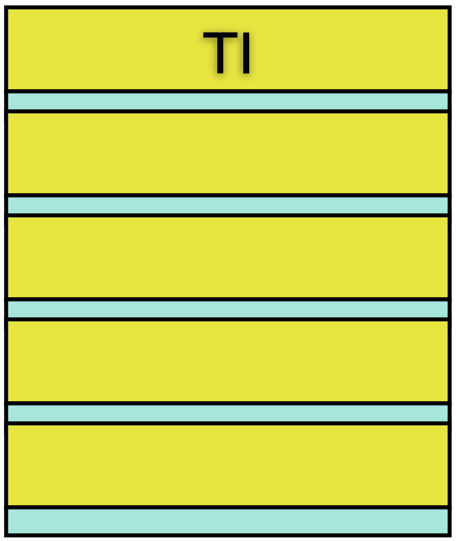




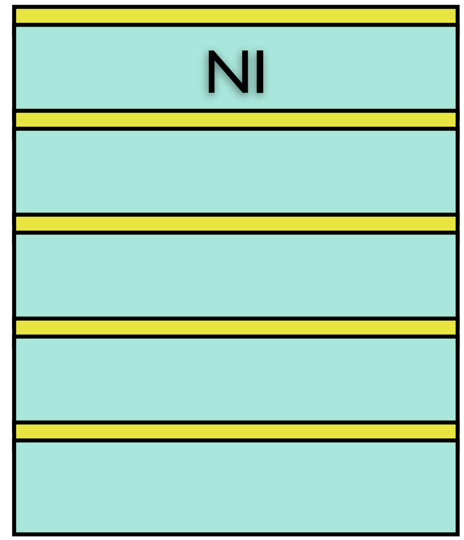
strong
tunneling
across the
NI “heals” TI

Tunneling
across TI
slabs kills the
3d TI

TI to NI transition



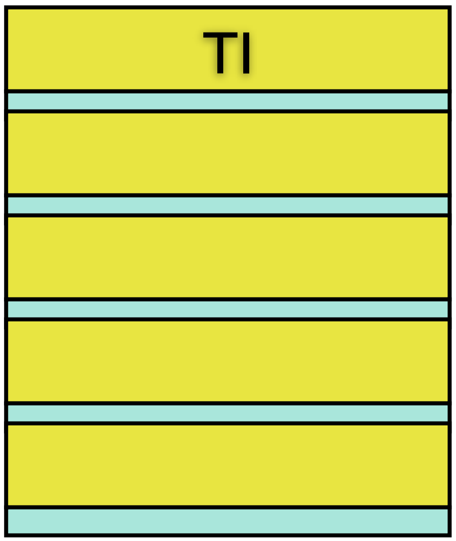
in between is a (quantum) phase transition



strong tunneling across the NI “heals” TI

Tunneling across TI slabs kills the 3d TI

TI to NI transition



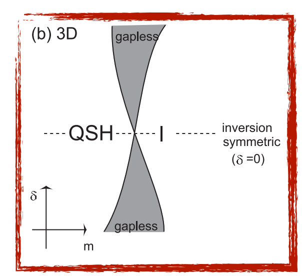
strong tunneling across the NI "heals" TI

in between is a (quantum) phase transition

We can turn this critical point into the Weyl semimetal by breaking I or TR

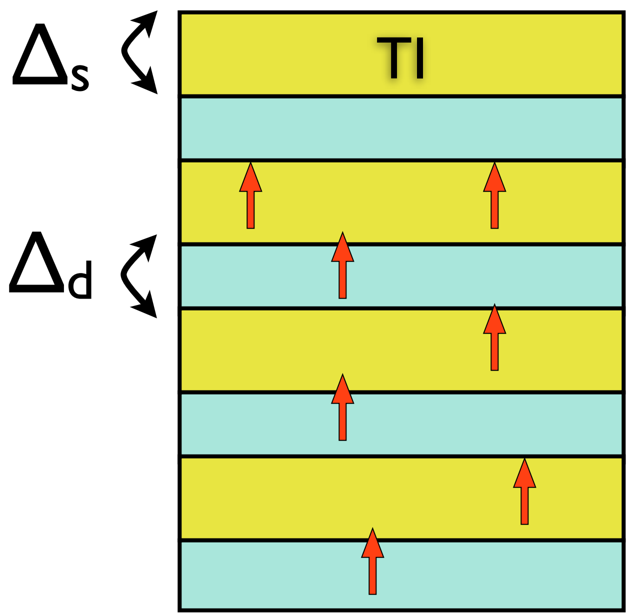
S. Murakami, 2007

Tunneling across TI slabs kills the 3d TI

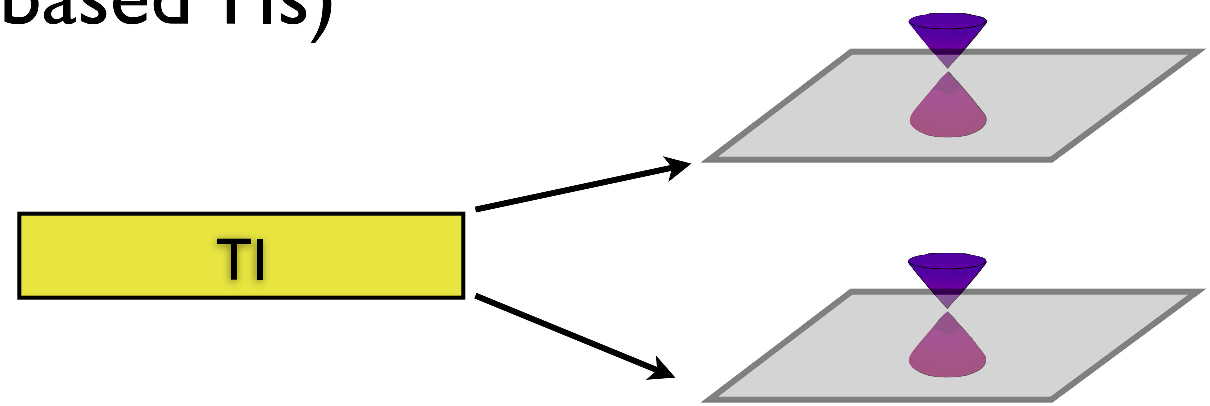


TR breaking

- Dope with magnetic impurities (already achieved in Bi-based TIs)



m = exchange energy



model just in terms of surface states

TR breaking

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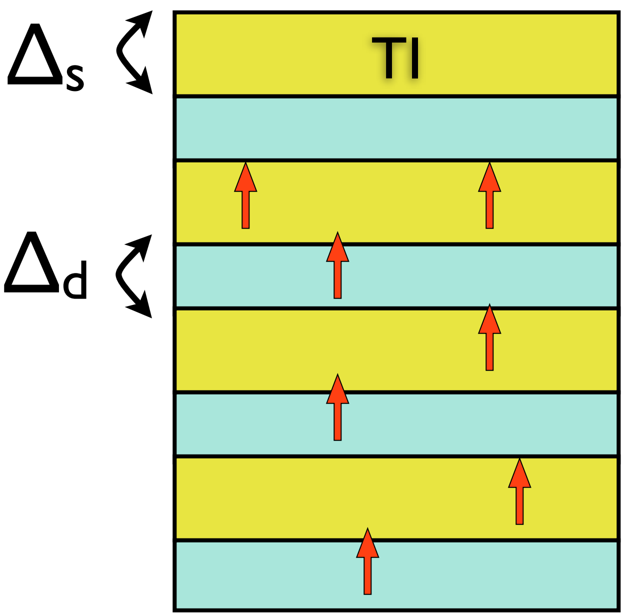

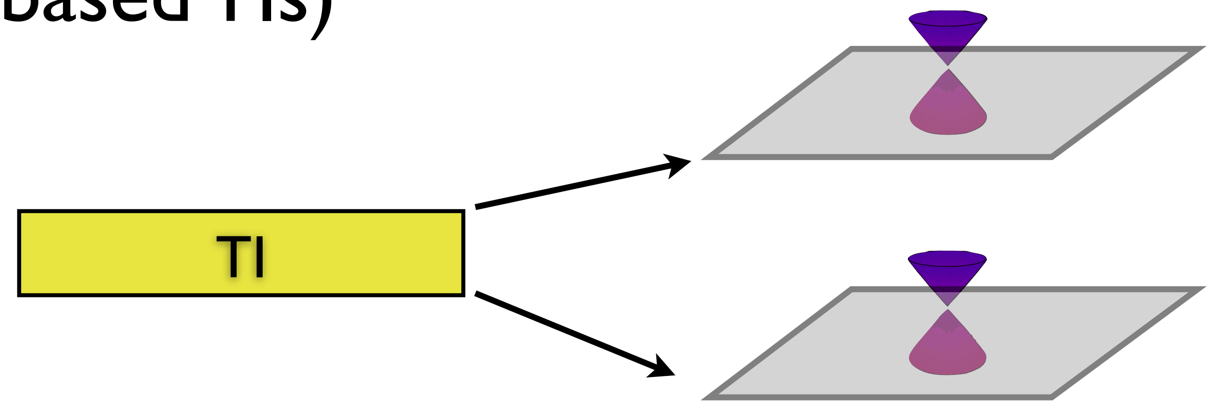

$$H = \sum_{\mathbf{k}_\perp, ij} \Big[v_F \tau^z (\hat{\mathbf{z}} \times \boldsymbol{\sigma}) \cdot \mathbf{k}_\perp \delta_{i,j} + m\sigma^z \delta_{i,j} + \Delta_S \tau^x \delta_{i,j} + \frac{1}{2}\Delta_d \tau^+ \delta_{j,i+1} + \frac{1}{2}\Delta_d \tau^- \delta_{j,i-1} \Big] c^\dagger_{\mathbf{k}_\perp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

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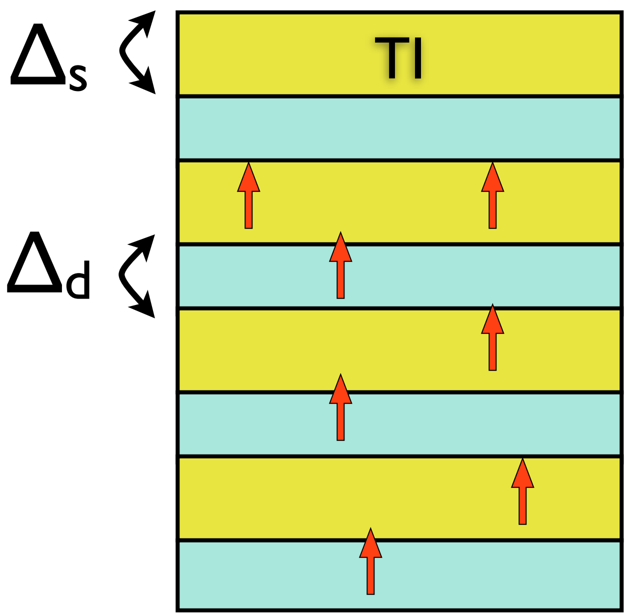

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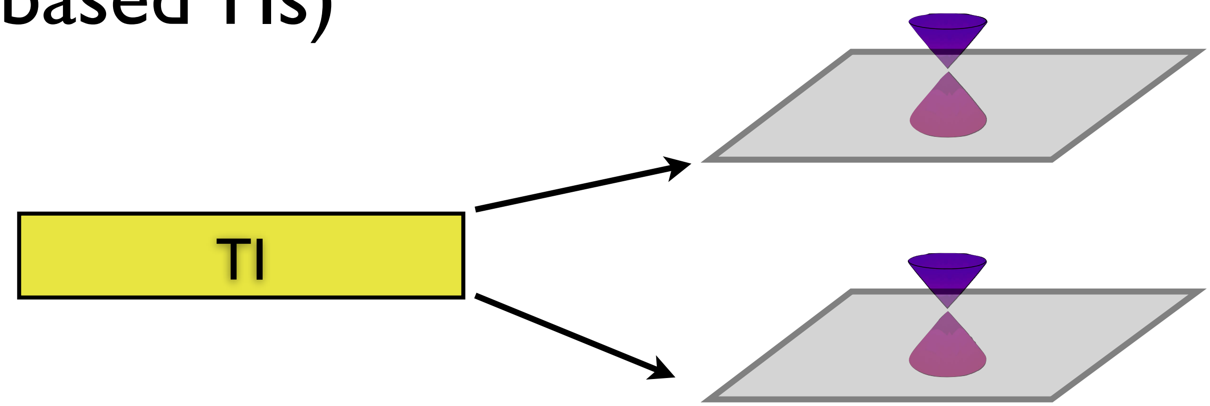

$$\epsilon^2_{k\pm} = v_F^2 k_\perp^2 + \left[m \pm \Delta(k_z)\right]^2$$

$$\Delta(k_z) = \sqrt{\Delta_s^2 + \Delta_d^2 + 2\Delta_s\Delta_d\cos(k_z d)}$$

TR breaking

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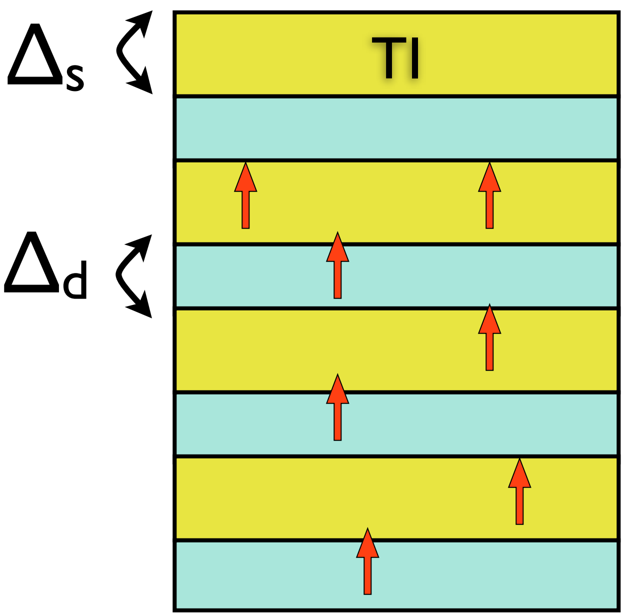

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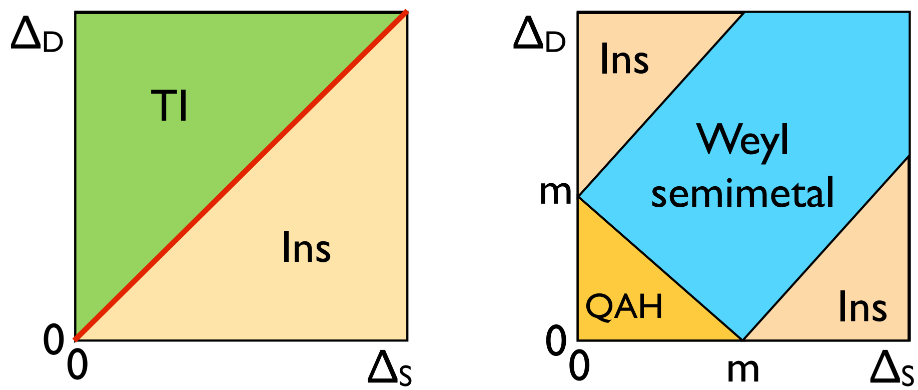

(a) m=0 (b) m≠0

TR breaking

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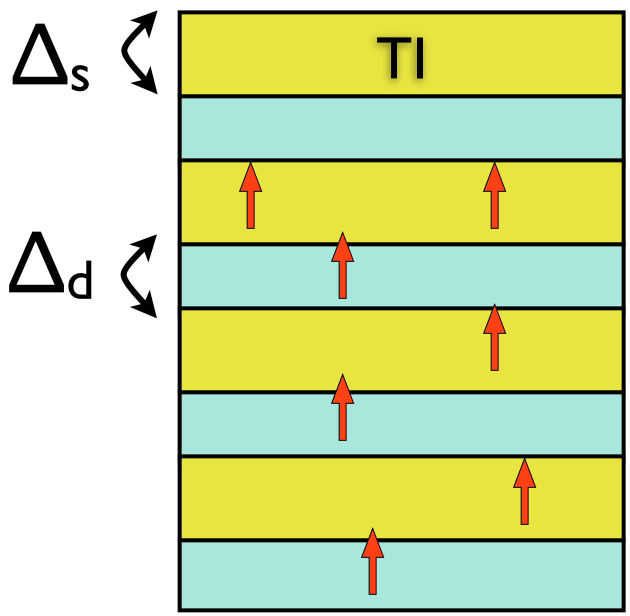

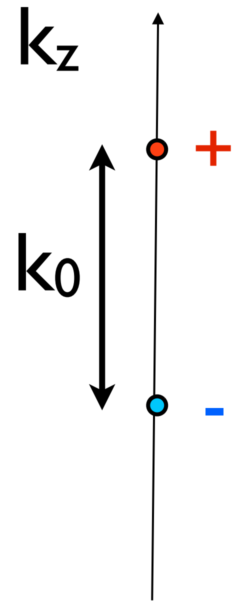

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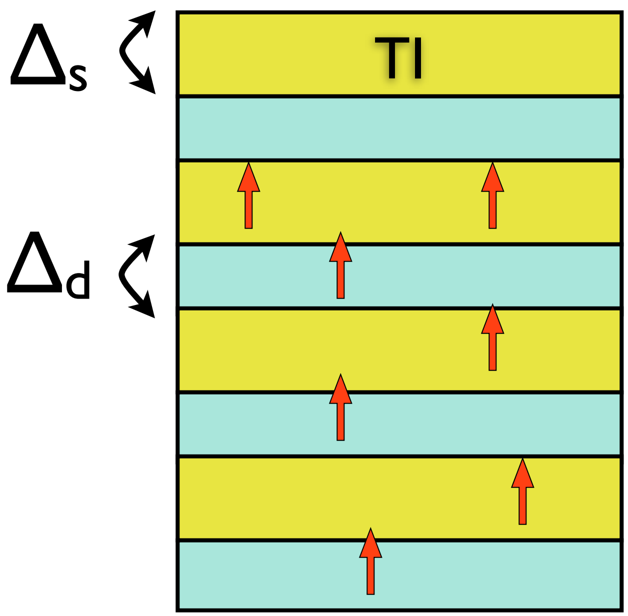

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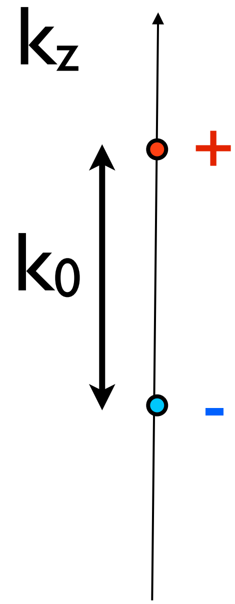


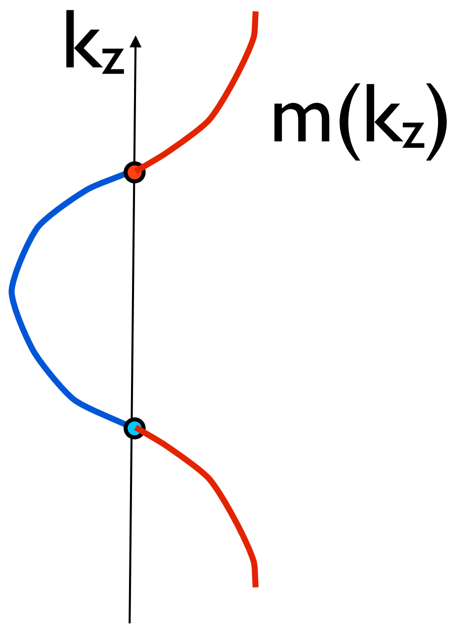
$$B_\mu(k) = \frac{1}{8\pi}\epsilon_{\mu\nu\lambda}\hat{\mathbf{d}}\cdot\partial_\nu\hat{\mathbf{d}}\times\partial_\lambda\hat{\mathbf{d}}$$

$$\partial_\mu B_\mu(k) = \sum_i q_i\delta(k-k_i)$$

“monopoles” of Berry curvature

Quantum Hall effect

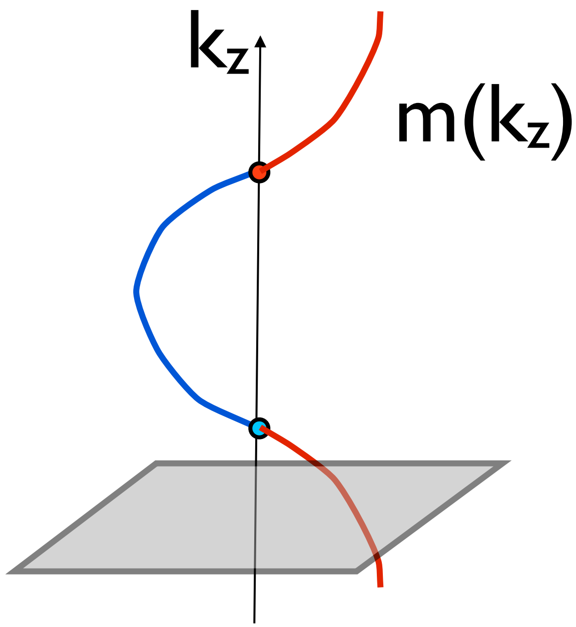
c.f. Haldane 1988



$$H = vk_x\sigma^x + vk_y\sigma^y + m(k_z)\sigma^z$$

Quantum Hall effect

c.f. Haldane 1988

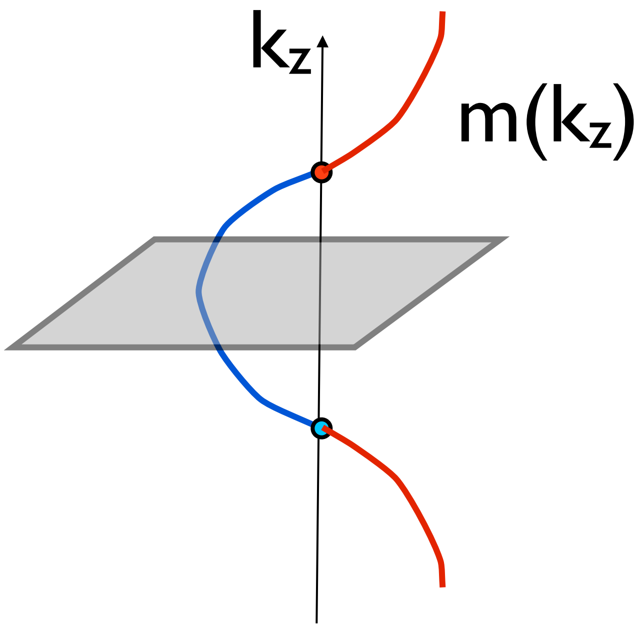


$$H = vk_x\sigma^x + vk_y\sigma^y + m(k_z)\sigma^z$$

$$\sigma_{xy} = 0$$

Quantum Hall effect

c.f. Haldane 1988



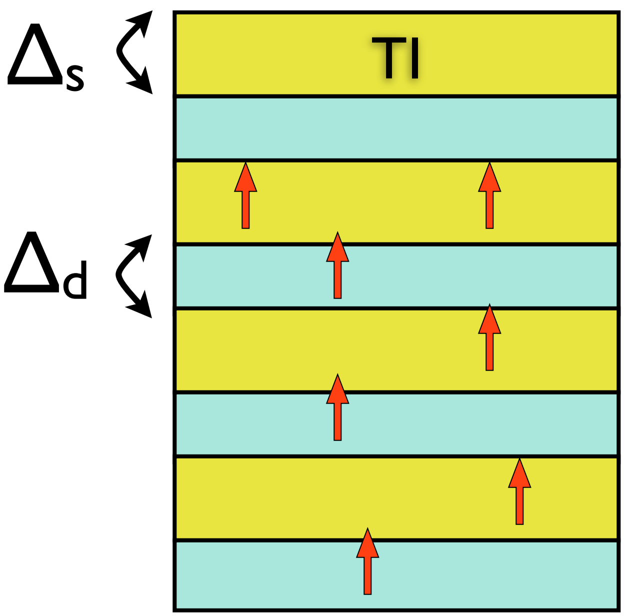
$$H = vk_x\sigma^x + vk_y\sigma^y + m(k_z)\sigma^z$$

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

TR breaking

- Dope with magnetic impurities (already achieved in Bi-based TIs)

c.f. Volovik, 2005



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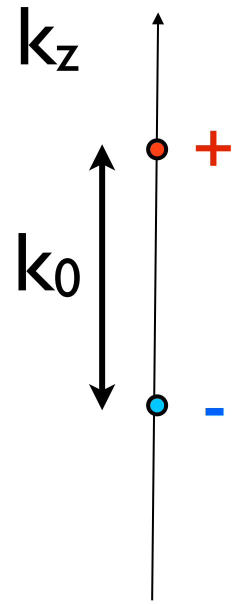

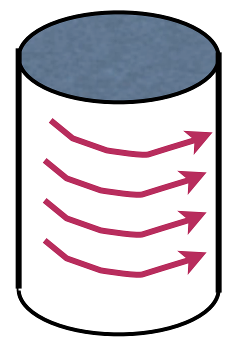

$$\sigma_{xy} = \frac{e^2}{h} \frac{k_0}{2\pi}$$

semi-quantum AHE

TR breaking

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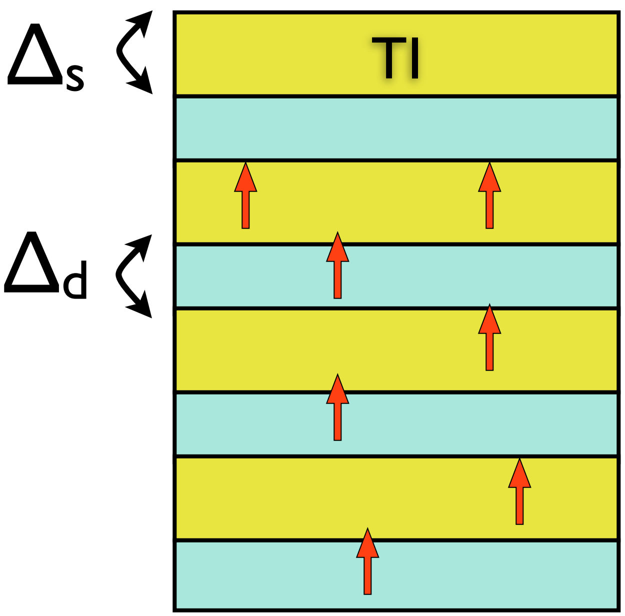

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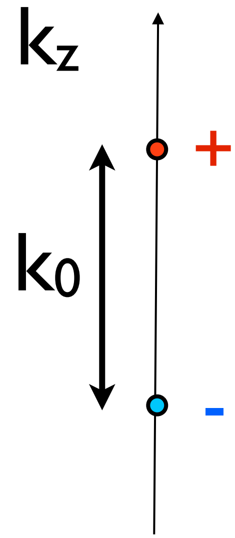
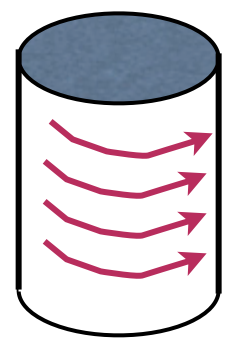




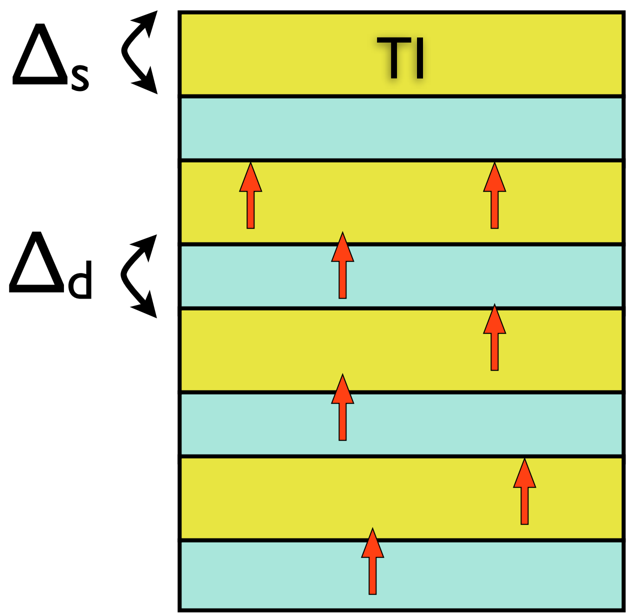
$$\sigma_{\mu\nu} = \frac{e^2}{2\pi h}\epsilon_{\mu\nu\lambda}Q_\lambda$$

in general

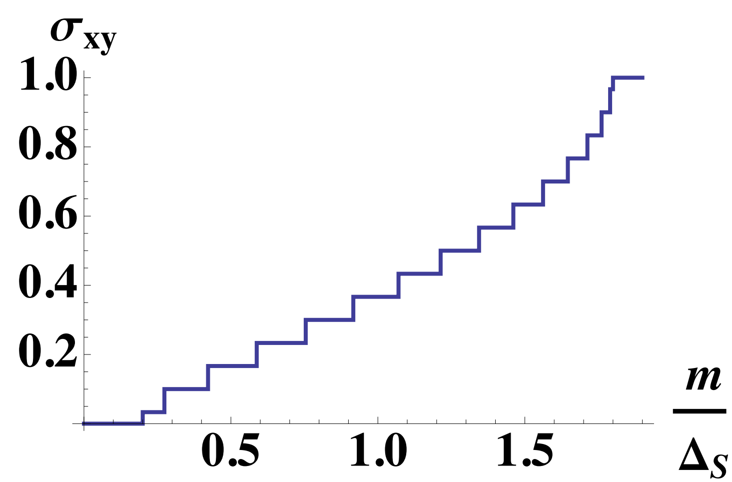
$$\vec{Q} = \sum_i \vec{k}_i q_i + \vec{Q}_{RLV}$$

TR breaking

- Dope with magnetic impurities (already achieved in Bi-based TIs)



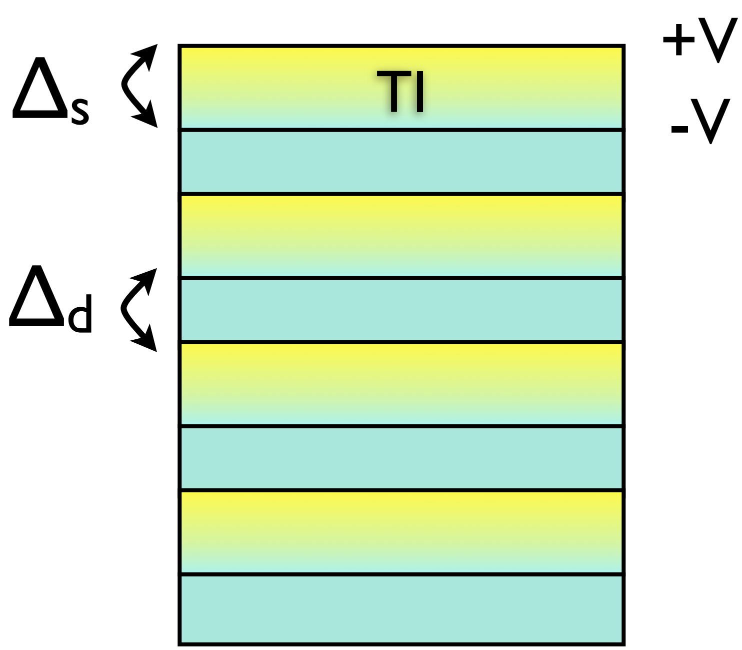
m = exchange energy



QAHE in finite multilayer

I breaking

- Asymmetric heterostructure, or intrinsic I breaking



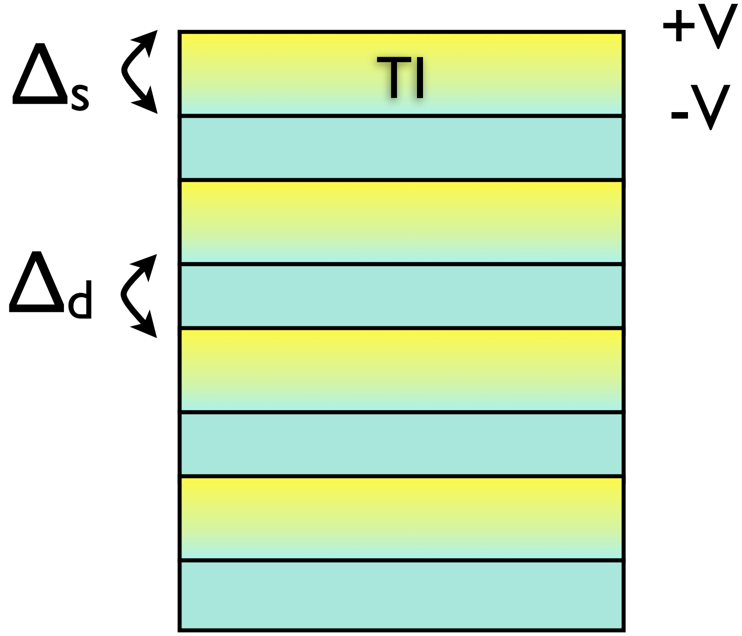
electrostatic potential asymmetry

$$\epsilon_{k\pm}^2 = v_F^2(|k_\perp| \pm V)^2 + |\Delta(k_z)|^2$$

m = exchange energy

I breaking

- Asymmetric heterostructure, or intrinsic I breaking



m = exchange energy

electrostatic potential asymmetry

$$\epsilon^2_{k\pm} = v_F^2(|k_\perp| \pm V)^2 + |\Delta(k_z)|^2$$

Naively gives nodal *ring* at critical point with Δ_s=Δ_d

I breaking

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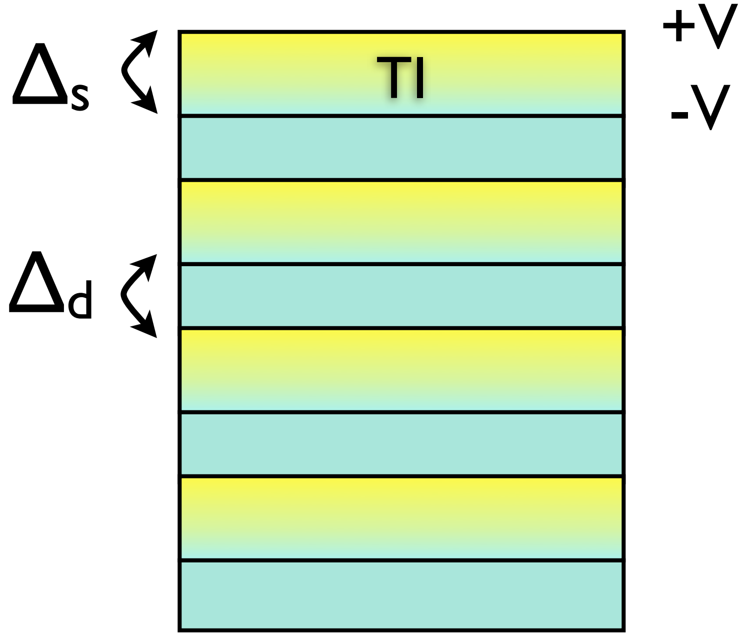

m = exchange energy

electrostatic potential asymmetry

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Need to include k-dependence of Δ_s,Δ_d

I breaking

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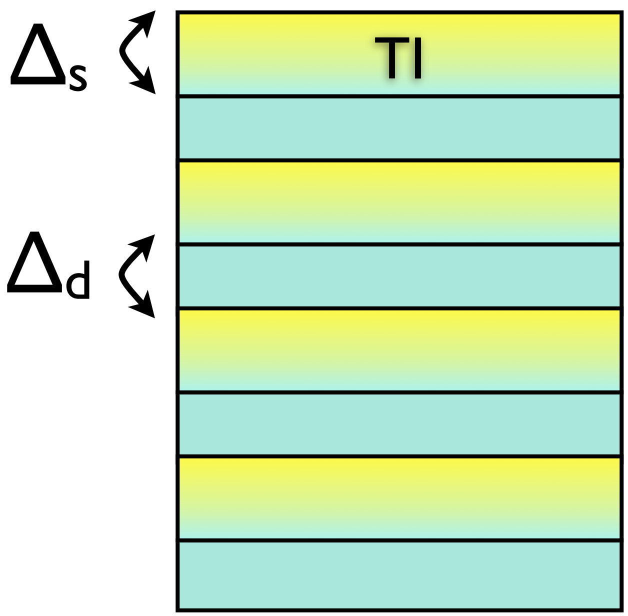

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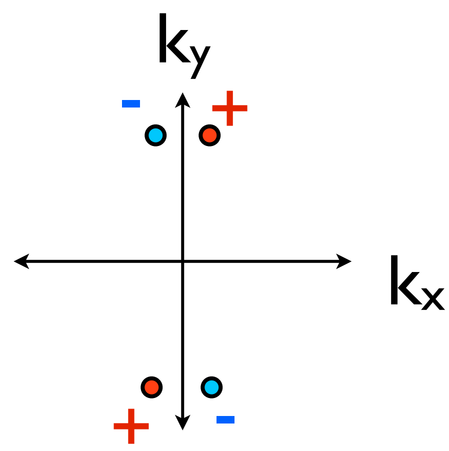
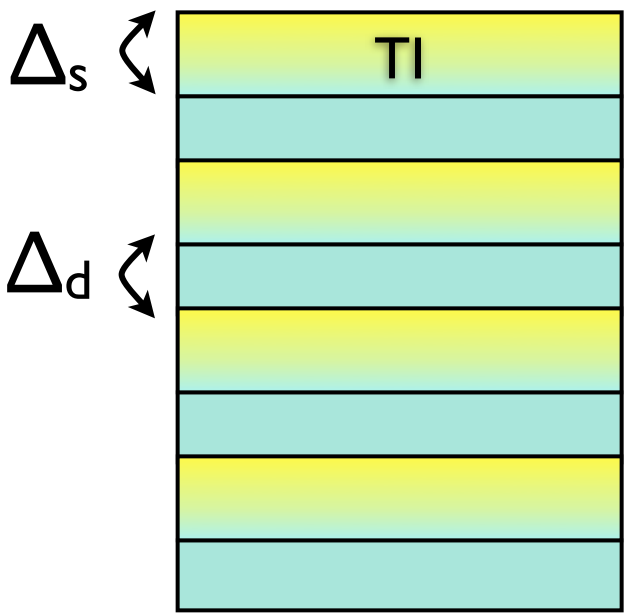


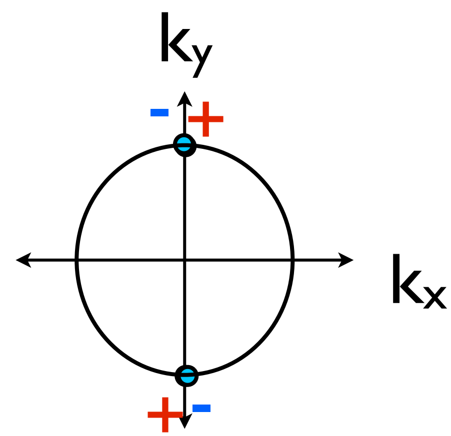
no AHE

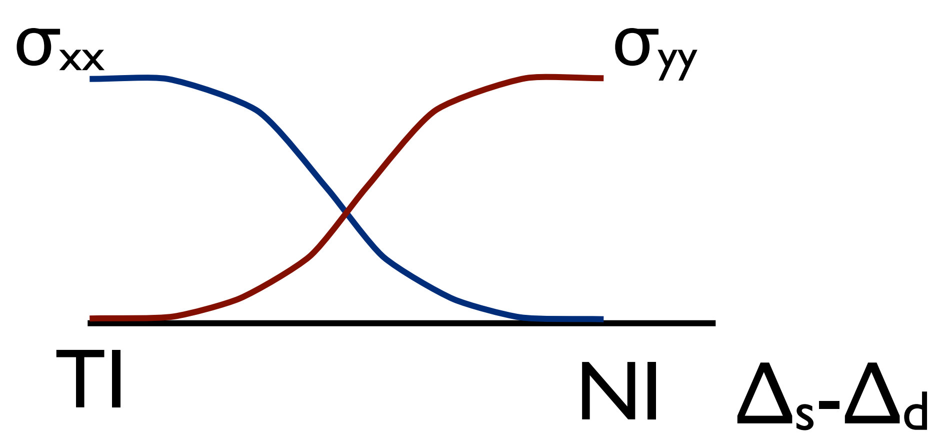
I breaking

- Asymmetric heterostructure, or intrinsic I breaking



m = exchange energy





$Hg_{1-x}Cd_xTe$ structures

- Checked this with semi-realistic 10-orbital tight binding model for (Hg,Cd)Te superlattices with asymmetry
- Advantage: can be grown with very high quality
- Disadvantage: strain must be controlled

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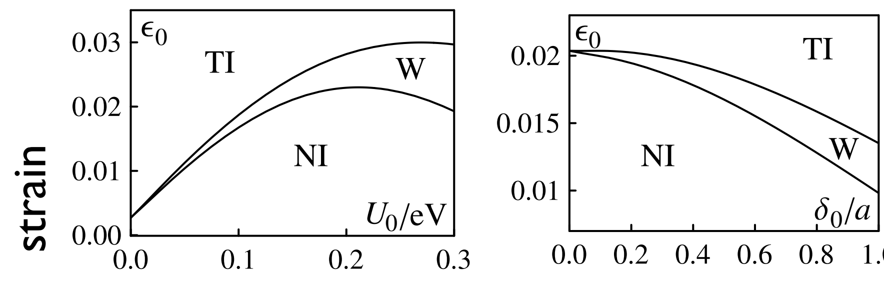
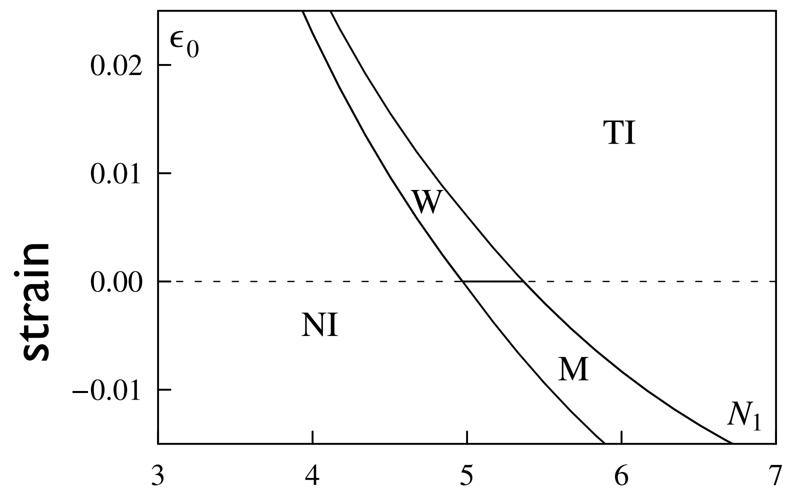


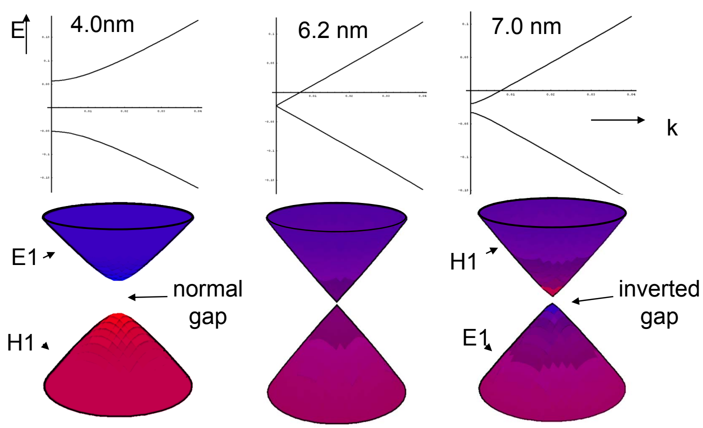
asymmetry

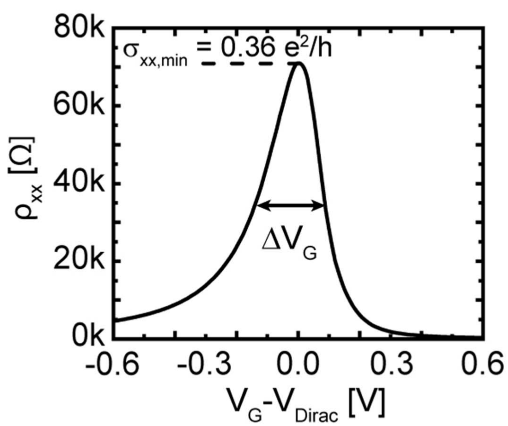


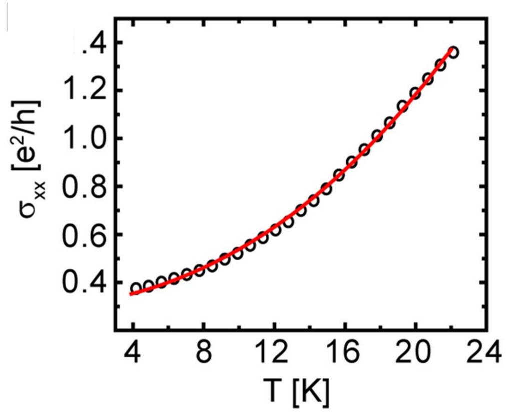
HgTe thickness

Graphene-like Physics

- 2d graphene physics can already be achieved in HgTe quantum wells







Peak width and mobilities comparable with/better than free standing graphene
Scattering mechanisms: probably mass fluctuations + Coulomb (fit is Kubo model)

L. Molenkamp: HgTe QWs are "better graphene"

“3d graphene”

- The transport behavior of 3d Dirac/Weyl fermions is subtle and interesting!
- Naive argument (no disorder or interactions):

$$\mathrm{Re}\,\sigma(\omega, T=0) \propto \omega$$

  - insulating?

With impurities

- Usually impurities induce elastic scattering that dominates at low T
  - Here, Born approximation is valid (disorder is *irrelevant* in RG sense)

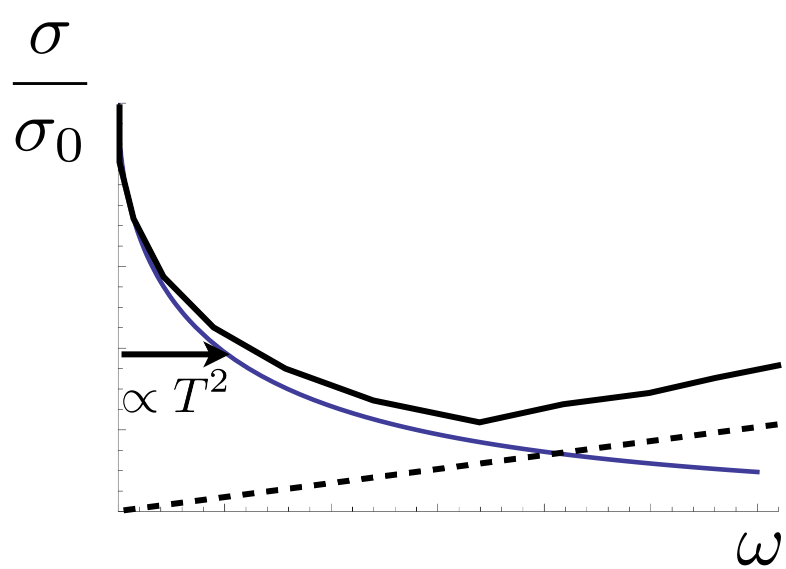
$$\Rightarrow \quad 1/\tau \sim u_{\mathrm{imp}}\omega^2$$

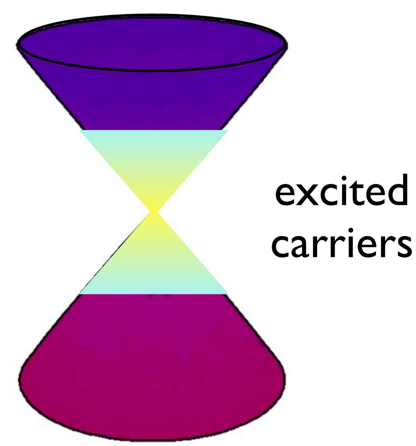
  - Contrast graphene: higher order corrections induce non-zero scattering rate at zero frequency (SCBA) $1/\tau \sim e^{-\frac{c}{u_{\mathrm{imp}}}}$

With impurities

- Neutral impurities w/o interactions leads to non-zero DC conductivity

$$\mathrm{Re}\,\sigma(\omega, T) \propto \sigma_0 f(\omega/T^2)$$





$$1/\tau \sim u_{\mathrm{imp}}\omega^2$$

With interactions

- Coulomb interactions are *marginal* - characterized by dimensionless fine structure constant $\alpha = e^2/\varepsilon v_F$
  - Leads to strong scattering

$$1/\tau \sim \alpha^2 \max(\omega, T) \gg u_{\mathrm{imp}} \omega^2$$

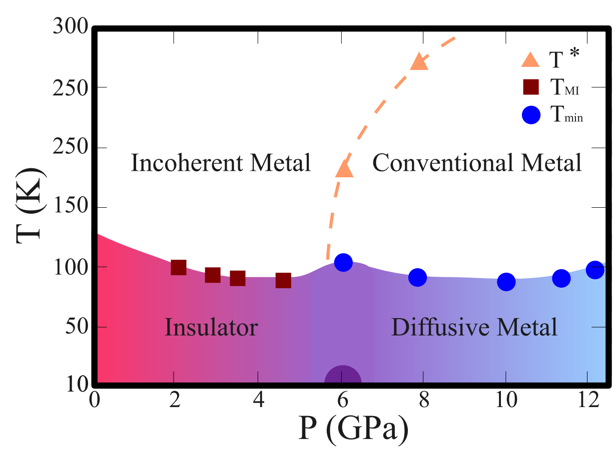
  - Then expect

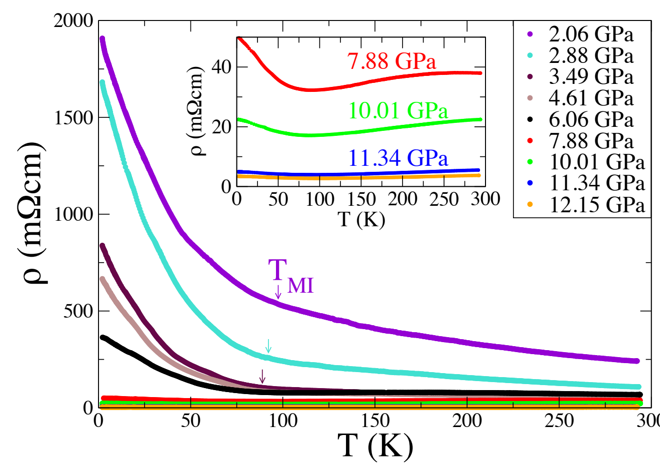
$$\sigma_{\mathrm{dc}} \sim e^2 \left(\frac{\epsilon^2}{v_F^3} \right) v_F^2 \tau \sim \frac{k_B T}{\alpha}$$

power law insulator

Experiment?

- Experiments on $Eu_2Ir_2O_7$ find "weak" insulator





Tafti *et al*, 2011 and private communications

Donors

- This is likely related to combined effect of small carrier density and Coulomb scattering from donors - O vacancies
- Follow ideas of calculation for graphene but for 3d

c.f. Nomura+MacDonald, 2007

Donors

- Screening

$$V(q) \sim \frac{e^2}{q^2 + \xi^{-2}} \qquad\qquad \xi^{-2} \sim \alpha k_F^2$$

- Scattering

$$\tau^{-1} \sim n \int d^3q\, \delta(\epsilon_q - \epsilon_F)|V(k+q)|^2 v(k \cdot q)$$
$$\sim e^2 k_F \alpha \int d\cos\theta \, \tfrac{1-\cos^2\theta}{[2(1+\cos\theta)+\alpha]^2}$$

c.f. Nomura+MacDonald, 2007

Donors

- Conductivity

$$\sigma \sim e^2 \left(\frac{k_F^2}{v_F} \right) v_F^2 \tau$$

$$\boxed{\sim f(\alpha) e^2 n^{1/3}} \qquad f(\alpha) \sim 1 + \frac{1}{\alpha^2 \ln \alpha}$$

- Mean free path

$$\sigma \sim e^2 k_F \cdot k_F \ell \qquad k_F \ell \sim f(\alpha)$$

c.f. Nomura+MacDonald, 2007

Conclusions

- Weyl semimetals occur in the same sorts of materials as topological insulators (and others!), if *inversion* or *time reversal* are broken
- They can be *designed* as intermediate states between certain TIs and NIs
- They have unique transport properties and surface states, and in some respects are 3d analogs of graphene, with interactions and defects playing crucial roles