Topological Physics in Band Insulators

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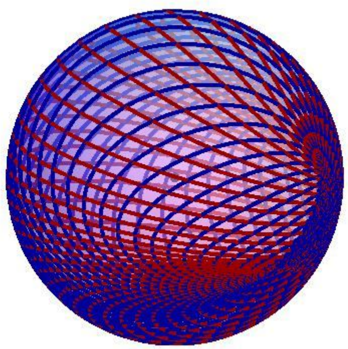


A Brief History of Topological Insulators

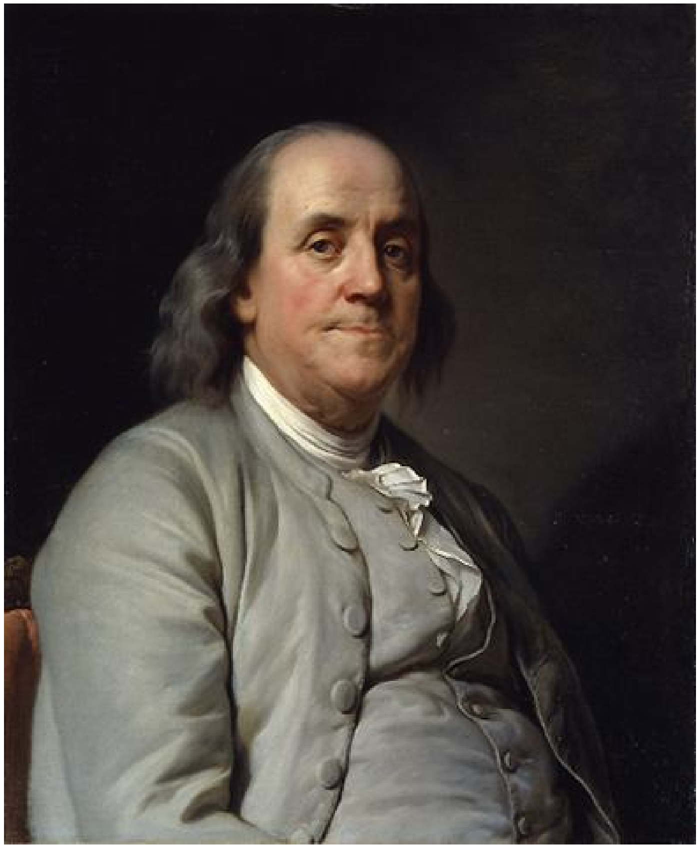
What they are

How they were discovered

Why they are important

Electronic States of Matter

Benjamin Franklin (University of Pennsylvania)



That the Electrical Fire freely removes from Place to Place in and thro' the Substance of a Non-Electric, but not so thro' the Substance of Glass. If you offer a Quantity to one End of a long rod of Metal, it receives it, and when it enters, every Particle that was before in the Rod pushes it's Neighbour and so on quite to the farther End where the Overplus is discharg'd… But Glass from the Smalness of it's Pores, or stronger Attraction of what it contains, refuses to admit so free a Motion. A Glass Rod will not conduct a Shock, nor will the thinnest Glass suffer any Particle entring one of it's Surfaces to pass thro' to the other.

Electronic States of Matter

Conductors & Insulators…

This taxonomy is incomplete…

…“Superconductors” (1911)

Electronic States of Matter

Conductors, Insulators & Superconductors

(Onnes 1911)

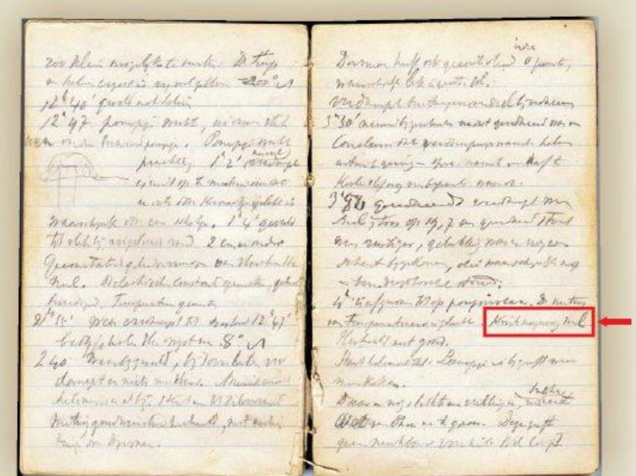


Figure 2. A terse entry for 8 April 1911 in Heike Kamerlingh Onnes's notebook 56 records the first observation of superconductivity. The highlighted Dutch sentence *Kwik nagenoeg nul* means "Mercury['s resistance] practically zero [at 3 K]." The very next sentence, *Herhaald met goud,* means "repeated with gold." (Courtesy of the Boerhaave Museum.)

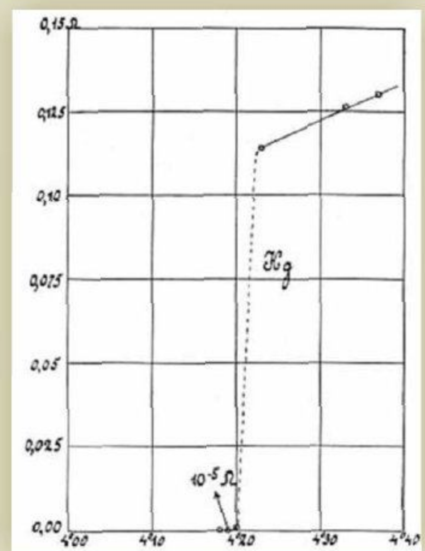
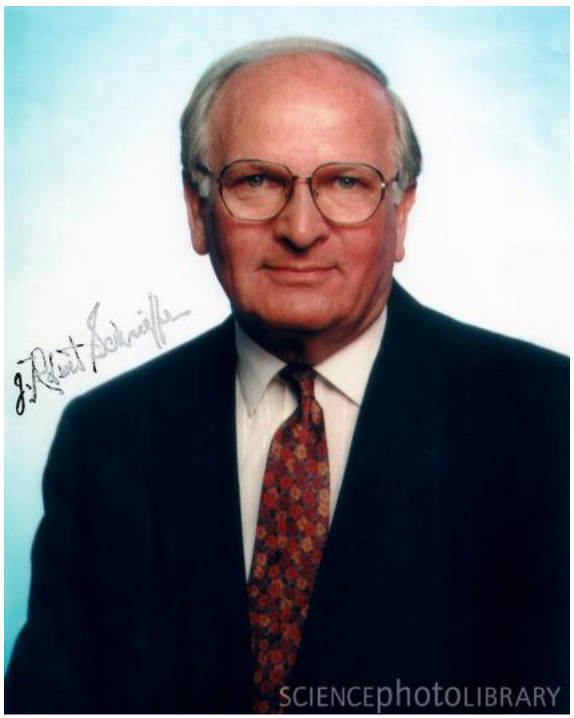


Figure 4. Historic plot of resistance (ohms) versus temperature (kelvin) for mercury from the 26 October 1911 experiment shows the superconducting transition at 4.20 K. Within 0.01 K, the resistance jumps from unmeasurably small (less than $10^{-5}\,\Omega$) to 0.1 Ω. (From ref. 9.)

from Physics Today, September 2010

Electronic States of Matter

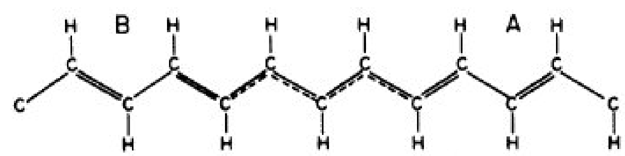
Conductors, Insulators & Superconductors



BCS mean field theory of the superconducting state (1957)

Soliton theory of doped polyacetylene (1978)

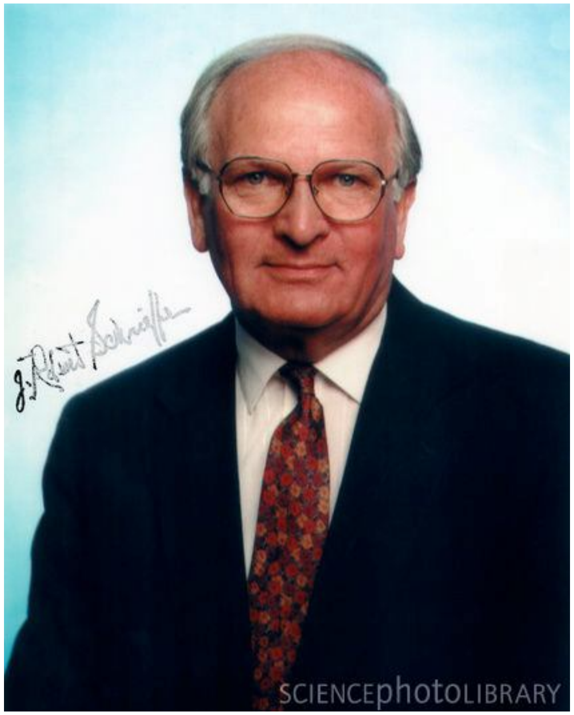
(a)



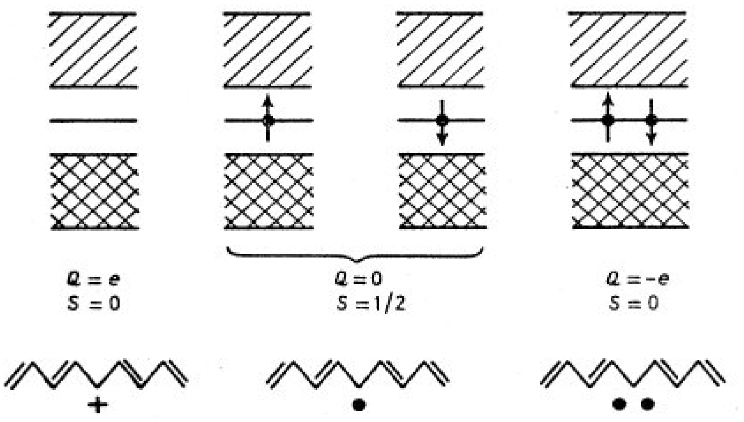
Univ. of Penn. (1962-1980)

Electronic States of Matter

Conductors, Insulators & Superconductors



Topological Defects in $(CH)_x$



W.P. Su, J.R. Schrieffer & A.J. Heeger (Penn);
GM & M.J. Rice (Penn/Xerox)

Electronic States of Matter

Conductors, Insulators & Superconductors…

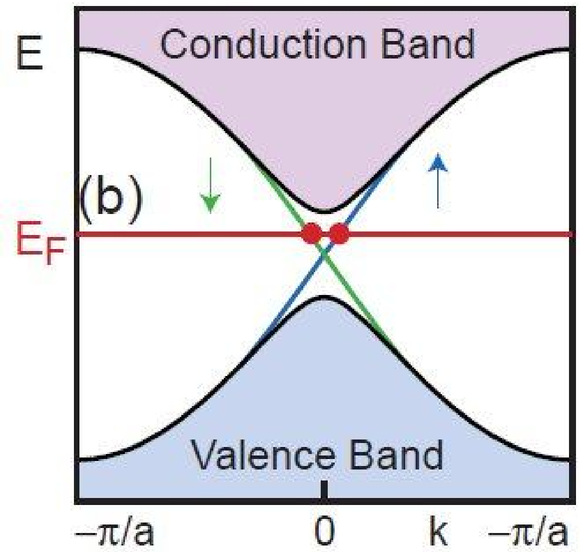
This taxonomy is still incomplete…

…"Topological Insulators" (2005)

Electronic States of Matter

Topological Insulators

This novel electronic state of matter is gapped in the bulk and supports the transport of spin and charge in gapless edge states that propagate at the sample boundaries. The edge states are … insensitive to disorder because their directionality is correlated with spin.



2005 Charlie Kane and GM
University of Pennsylvania

Electron spin admits a topologically distinct insulating state

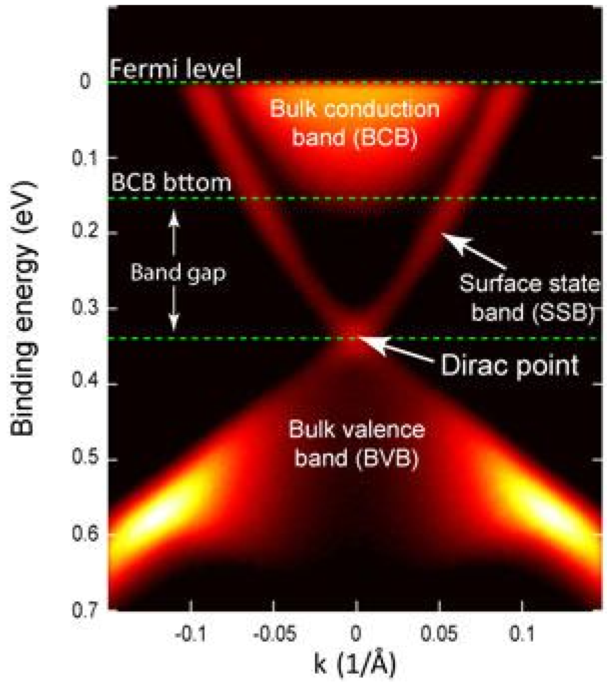
Electronic States of Matter

Topological Insulators

This state is realized in three dimensional materials where spin orbit coupling produces a bandgap "inversion."

It has boundary modes (surface states) with a 2D Dirac singularity protected by time reversal symmetry.

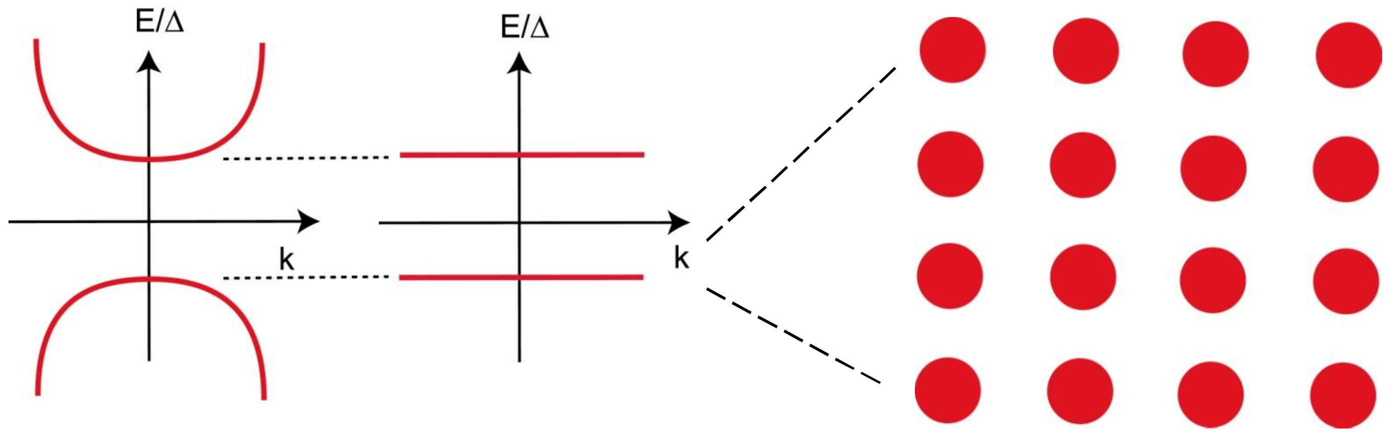
Bi_2Se_3 is the prototype.



Hasan/Cava (2009)

Modern view: Gapped (T-invariant) electronic states are equivalent

Kohn (1964): insulator is exponentially insensitive to boundary conditions



weak coupling strong coupling "nearsighted", local

Postmodern: Gapped electronic states are distinguished by topological invariants

Cell Doubling (Peierls, SSH)

$$H(k) = \begin{pmatrix} 0 & t_1 + t_2 e^{-2ika} \\ t_1 + t_2 e^{2ika} & 0 \end{pmatrix}$$

smooth gauge $$H\left(k + \frac{2\pi}{2a}\right) = H(k)$$

$$H(k) = \vec{h}(k) \cdot \vec{\sigma} \qquad \begin{cases} h_x = t_1 + t_2 \cos 2ka \\ h_y = t_2 \sin 2ka \\ h_z = 0 \end{cases}$$

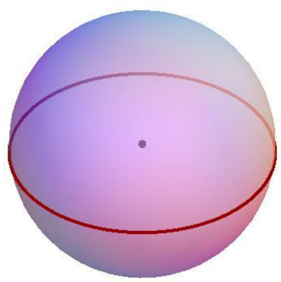
Su, Schrieffer, Heeger (1979)

Project onto Bloch Sphere

$$H = |h(k)|\,\vec{d}(k)\cdot\vec{\sigma}$$

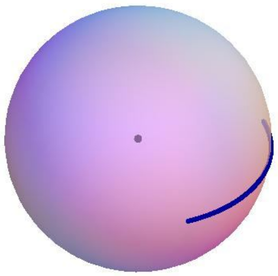
$$|h(k)| = \sqrt{t_1^2 + t_2^2 + 2t_1t_2\cos 2ka}$$

$$t_2 > t_1$$



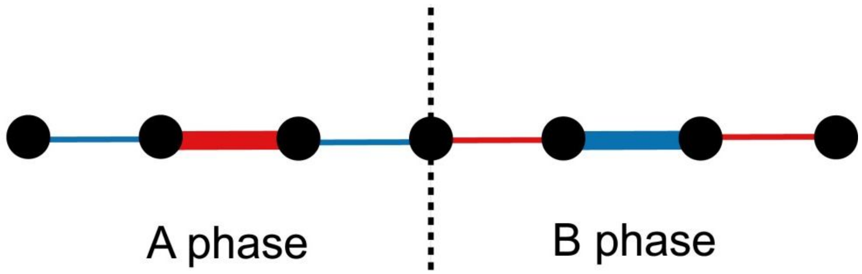
Closed loop

$$t_1 > t_2$$



Retraced path

Domain Walls

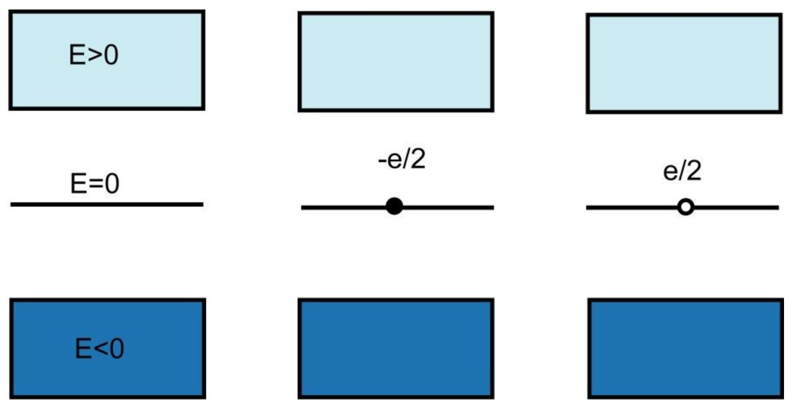


Particle-hole symmetry

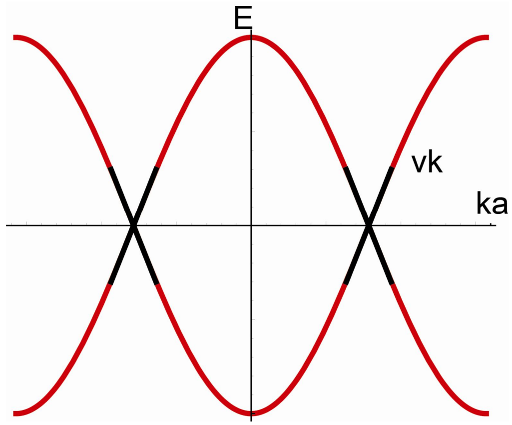
$$C\ H\ C^{-1} = -H; \quad C = \sum_n (-1)^n c_n^\dagger c_n$$

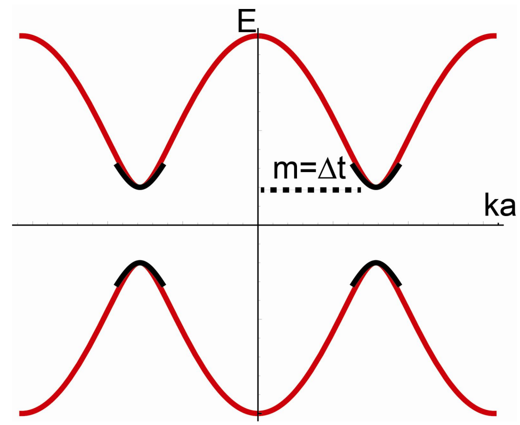
on an odd N chain

self conjugate state
on one sublattice



Continuum Model





$$\begin{pmatrix} e^{-\frac{i\pi}{4}} & 0 \\ 0 & e^{\frac{i\pi}{4}} \end{pmatrix} H\left(\frac{\pi}{2a}+q\right)\begin{pmatrix} e^{\frac{i\pi}{4}} & 0 \\ 0 & e^{-\frac{i\pi}{4}} \end{pmatrix} = -iv_F\hat{\sigma}_x\frac{\partial}{\partial x}+m\hat{\sigma}_y$$

$$E = \pm\sqrt{m^2+v^2q^2}$$

“relativistic bands” back-scattered by mass $m = t_1 - t_2$

Key Ideas from SSH Model

Topological classification of insulating state (winding number)

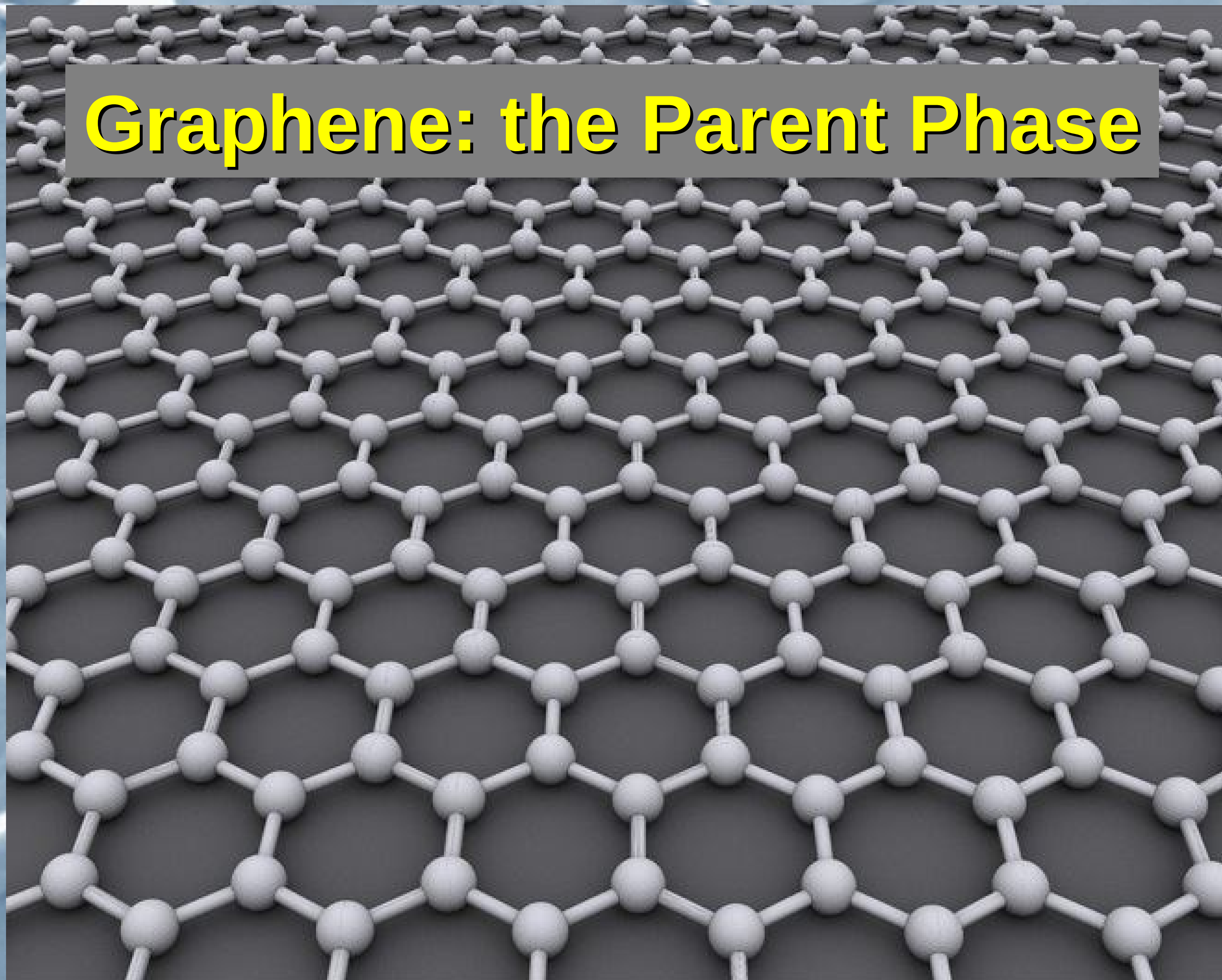
Change of topology at interface (the mass changes sign!)

Universal spectral signature from topology (self conjugate, spin-charge reversed etc.)

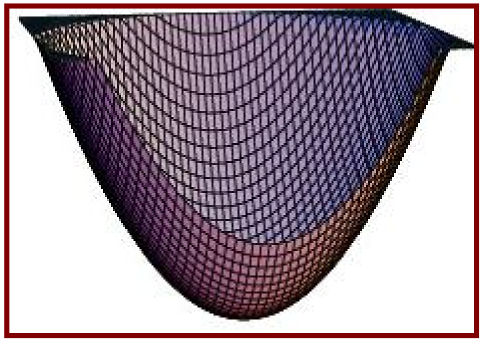
Kohn: "Insulating states are equivalent"

Postmodern: "Actually, <u>interfaces</u> between inequivalent insulating states are equivalent"

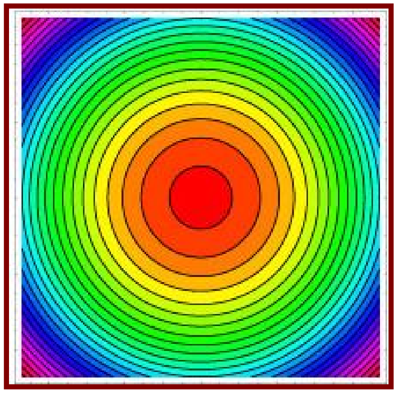
Graphene: the Parent Phase

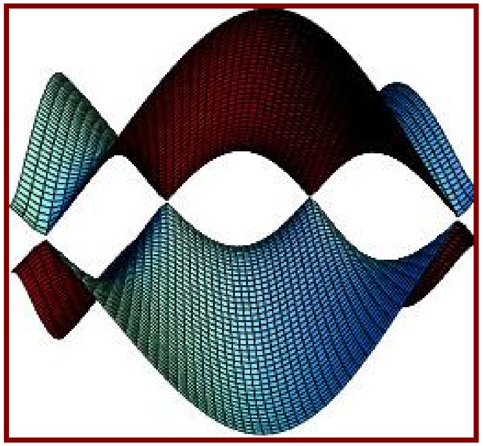


…. it has a critical electronic state

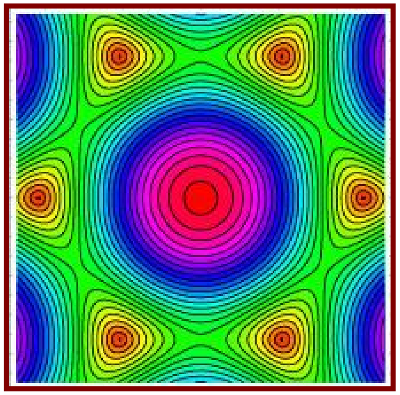


The dispersion of a free particle in 2D..





…is replaced by an unconventional E(k) relation on the graphene lattice



The low energy theory is described by an effective mass theory for <u>massless</u> electrons

$$\left(Bloch\ Wavefunction\right) = \left(Wavefunction\mathbf{(}s\mathbf{)}\ at\ K\right) \bullet \psi\mathbf{(}\vec{r}\,\mathbf{)}$$

$$\boxed{H_{eff}\psi(\vec{r}\,) = -iv_F\left(\vec{\sigma}\bullet\nabla\right)\psi(\vec{r}\,)}$$

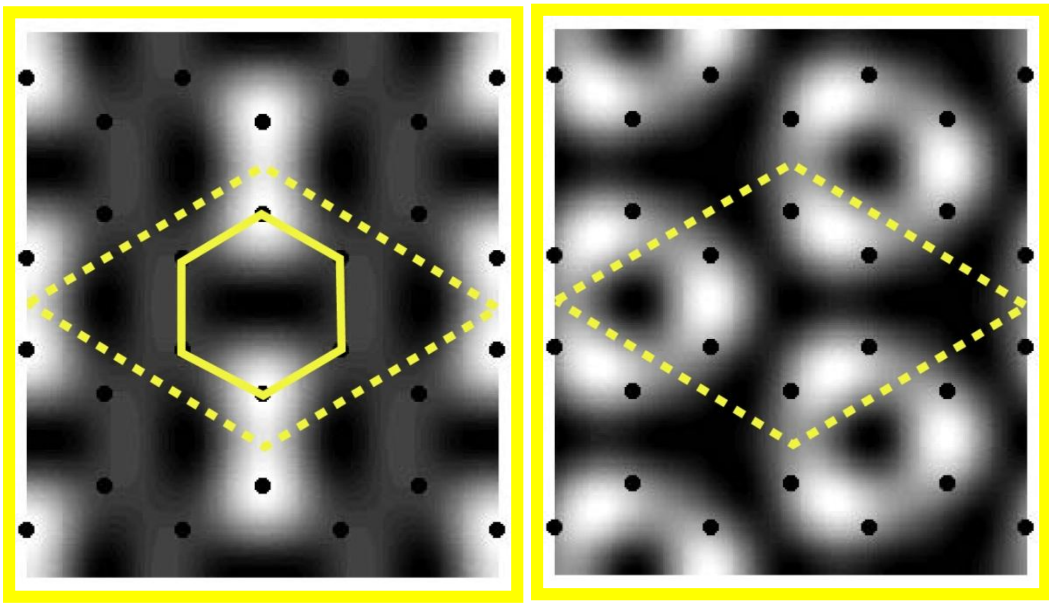
It is a massless Dirac Theory in 2+1 Dimensions

NOTE: Here the "spin" degree of freedom describes the sublattice polarization of the state, called <u>pseudospin</u>. In addition electrons carry a <u>physical</u> spin ½ and an <u>isospin</u> ½ describing the valley degeneracy.

D.P. DiVincenzo and GM (1984)

Gapping the Dirac Point

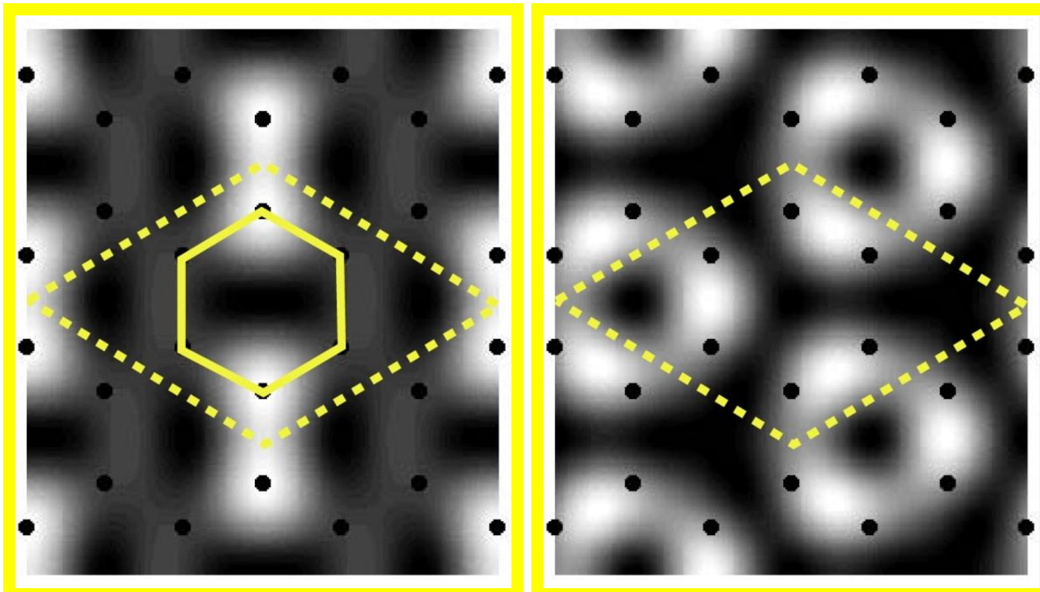
Valley mixing from broken translational symmetry



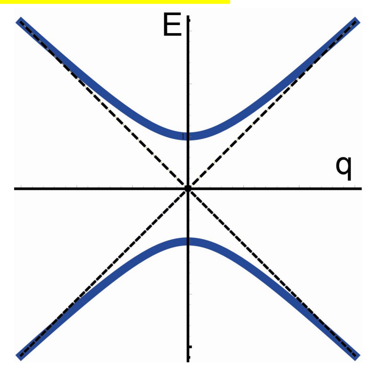
A continuum of structures all with $\sqrt{3} \times \sqrt{3}$ period hybridizes the two valleys

Gapping the Dirac Point

Valley mixing from broken translational symmetry

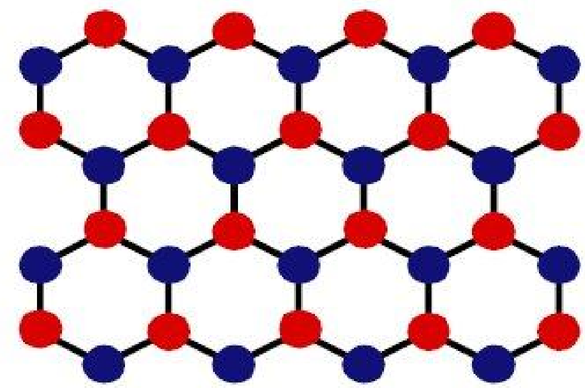


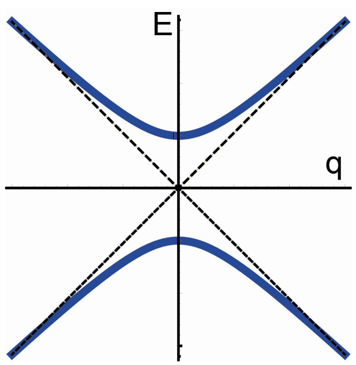
$$H' = \Delta_{\text{Kekule}} \begin{pmatrix} 0 & e^{i\vartheta}\sigma_x \\ e^{-i\vartheta}\sigma_x & 0 \end{pmatrix}_{\tau}$$



Gapping the Dirac Point

Charge transfer from broken inversion symmetry

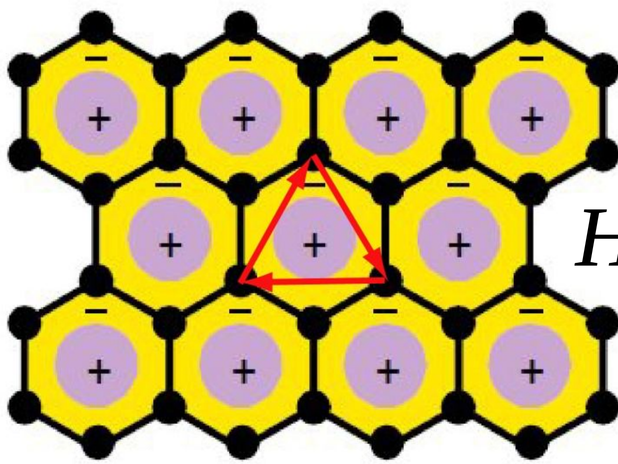




$$H' = \Delta_{\mathrm{BN}} \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}_{\tau}$$

Gapping the Dirac Point

Orbital currents from a modulated flux
(requires breaking T-symmetry)

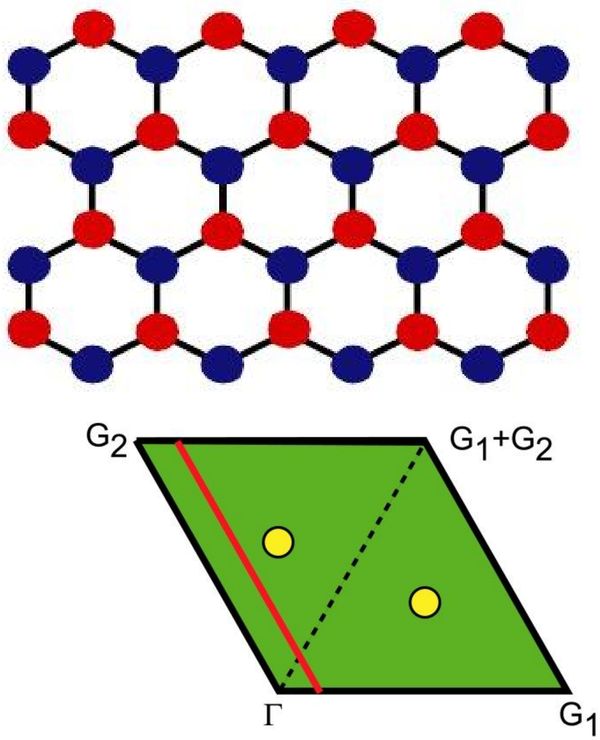


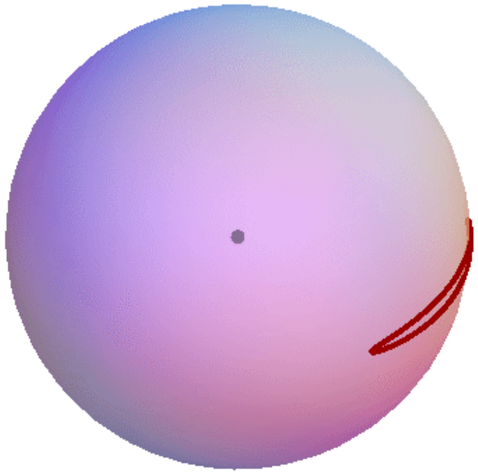
$$H' = \Delta_{\mathrm{FDMH}} \begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}_{\tau}$$

Gauged <u>second neighbor</u> hopping breaks T.
“Chern insulator” with Hall conductance e^2/h

FDM Haldane “Quantum Hall Effect without Landau Levels” (1988)

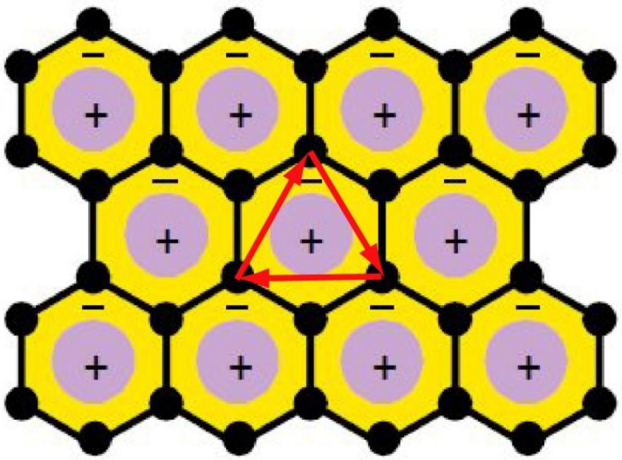
Topological Classification

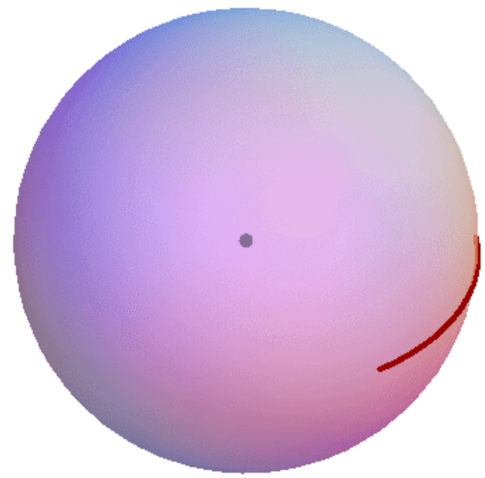




$$n = \frac{1}{4\pi}\int_S d^2k\ \left[\vec{d}(k_1,k_2)\cdot\left(\partial_{k_1}\vec{d}\times\partial_{k_2}\vec{d}\right)\right] = 0$$

Topological Classification





$$H' = \Delta_{\mathrm{FDMH}} \begin{pmatrix} \sigma_z & 0 \\ 0 & -\sigma_z \end{pmatrix}_\tau$$

$$n = \frac{1}{4\pi}\int_S d^2k\ \left[\vec{d}(k_1,k_2)\cdot\left(\partial_{k_1}\vec{d}\times\partial_{k_2}\vec{d}\right)\right] = 1$$

“Chern Insulator” with $\sigma_{xy} = \dfrac{e^2}{h}$ (has equal contributions from two valleys)

Mass Terms For Single Layer Graphene

$\sigma_x \tau_x, \sigma_x \tau_y$ Kekule: valley mixing

σ_z Heteropolar (breaks P)

$\sigma_z \tau_z$ Modulated flux (breaks T)

spinless

$\sigma_x \tau_z s_y - \sigma_y s_x$ Spin orbit (Rashba, broken z→-z)

$\boxed{\sigma_z \tau_z s_z}$ Spin orbit (parallel)*

with spin

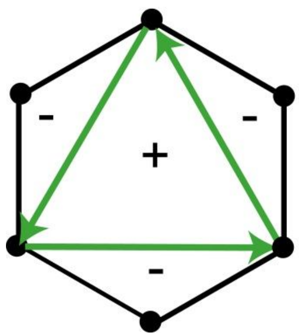
*This term respects all symmetries and it is therefore present, though possibly weak

For carbon it is **definitely** weak, but still important

Coupling orbital motion to the electron spin

Preserve mirror symmetry with a <u>parallel</u> spin orbit field

$$\varepsilon_{xy} \neq 0, \varepsilon_z = 0 \qquad H_{SO} = s_z \hat{n} \cdot \vec{\varepsilon} \times \vec{p} = \vec{p} \cdot (s_z \hat{n} \times \vec{\varepsilon}) = \vec{p} \cdot \vec{a}_{eff}$$



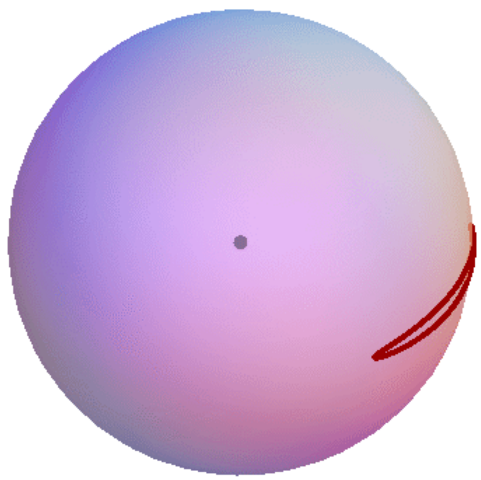
$$\left.\begin{array}{l} \oint_{\Omega} \vec{a}_{eff} \cdot d\vec{\ell} = 0 \\ \oint_{\Omega/2} \vec{a}_{eff} \cdot d\vec{\ell} \neq 0 \end{array}\right\} \quad \begin{array}{l} t_2 \left(e^{i\phi} c_n^\dagger c_m + e^{-i\phi} c_m^\dagger c_n \right) = \\ t_2 \left[\begin{array}{l} \cos\phi \left(c_n^\dagger c_m + c_m^\dagger c_n \right) \\ \quad + i \sin\phi \left(c_n^\dagger c_m - c_m^\dagger c_n \right) \end{array} \right] \end{array}$$

Generates a <u>spin-dependent</u> Haldane-type mass (which restores T)

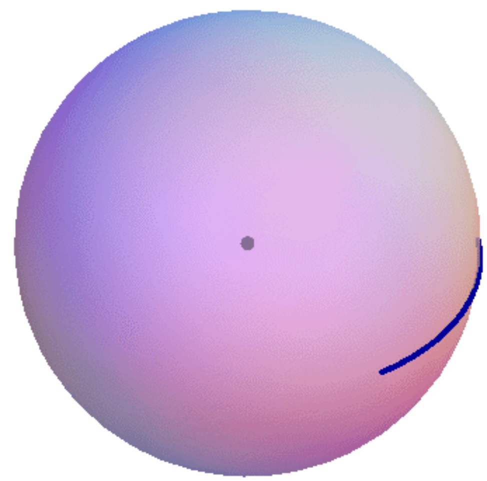
$$\Delta_{SO} = \lambda_{SO}\, \sigma_z \tau_z s_z$$

Topologically different states

Charge transfer insulator



Spin orbit coupled insulator



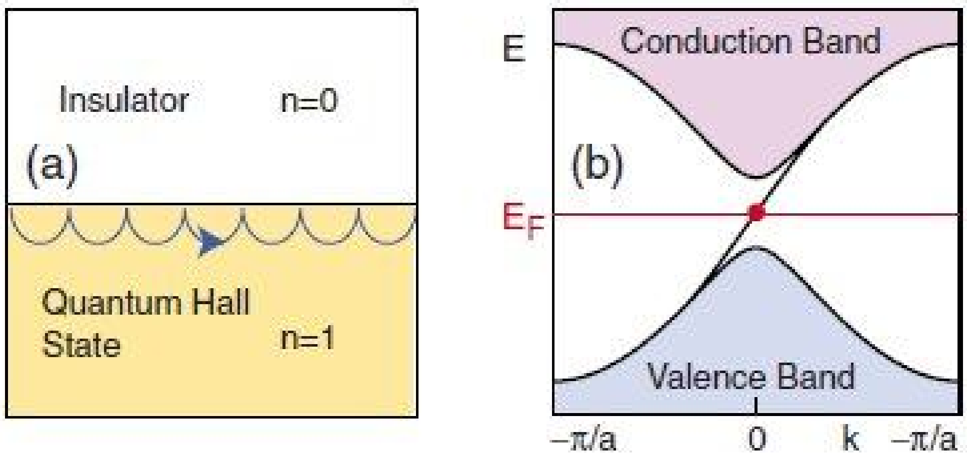
$$n = \frac{1}{4\pi}\int_S d^2k \left[\vec{d}(k_1,k_2)\cdot\left(\partial_{k_1}\vec{d}\times\partial_{k_2}\vec{d}\right)\right]$$

$$n = 0$$

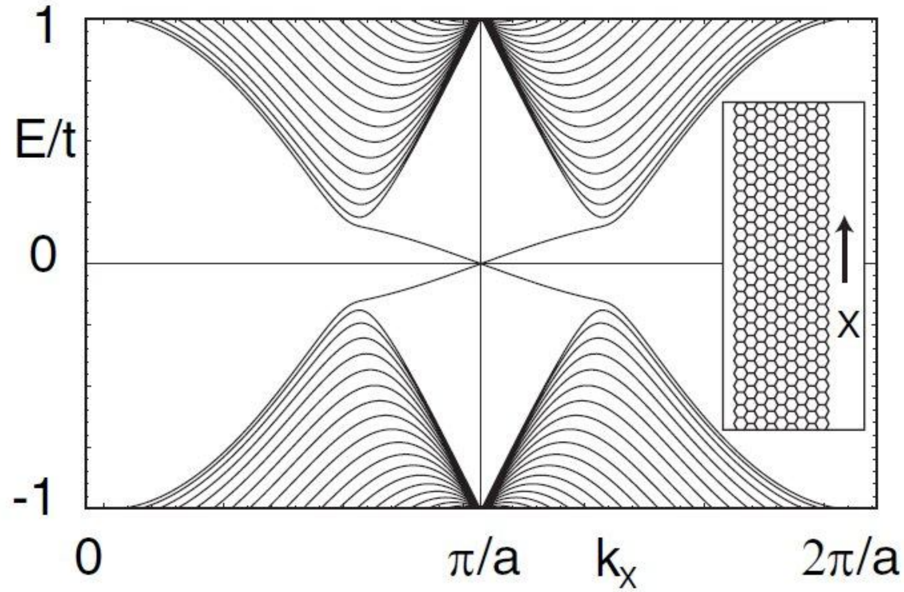
$$n = 1 + (-1) = 0$$

Topology of Chern insulator occurs in a time reversal invariant state

Topologically Protected Boundary Modes



Ballistic propagation through one-way edge state



Intrinsic SO-Graphene model on a ribbon

Symmetry Classification

Conductors: unbroken state[1]

Insulators: broken translational symmetry: bandgap from Bragg reflection[2]

Superconductor: broken gauge symmetry

Topological Insulator ?

[1]possibly with mass anisotropy

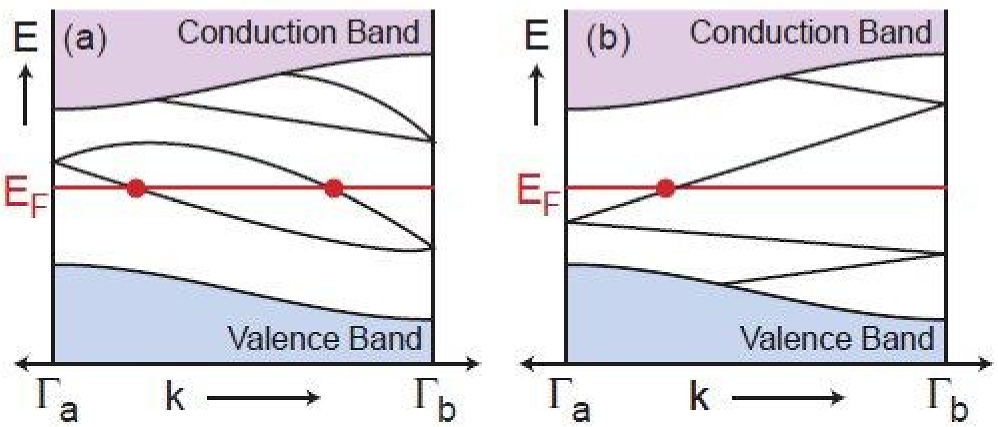
[2]band insulators

Symmetry Classification

Ordinary insulators and topological insulators are distinguished by a two-valued (even-odd) surface index.

Kramers Theorem: T-symmetry requires E(k,↑) =E(-k,↓)

But at special points k and -k are identified (TRIM)



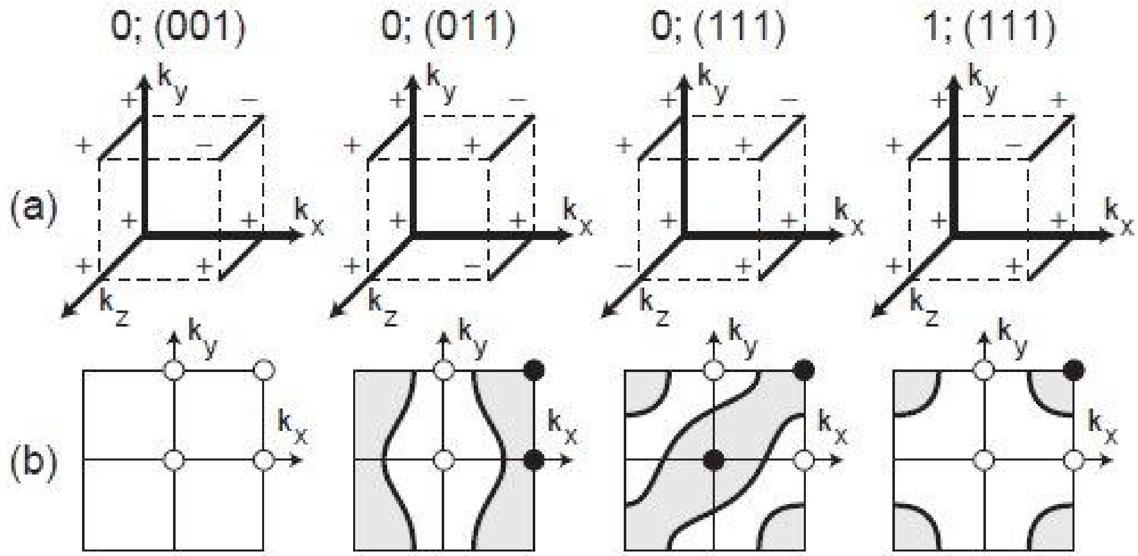
even: ordinary (trivial)   odd: topological

Kane and GM (2005)

With inversion symmetry

Ordinary insulators and topological insulators are distinguished by a two-valued (ν = 0,1) bulk index.

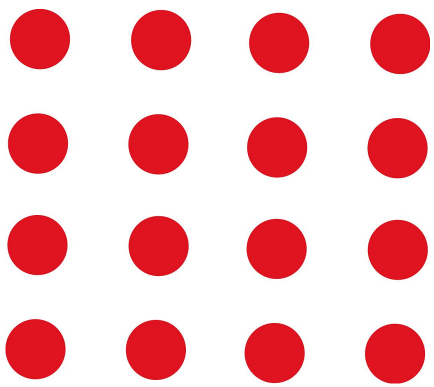
$$(-1)^{\nu} = \prod_{a=1}^{N} \delta_a \qquad \delta_a = \prod_m \xi_m$$ (parity eigenvalues, ±1)

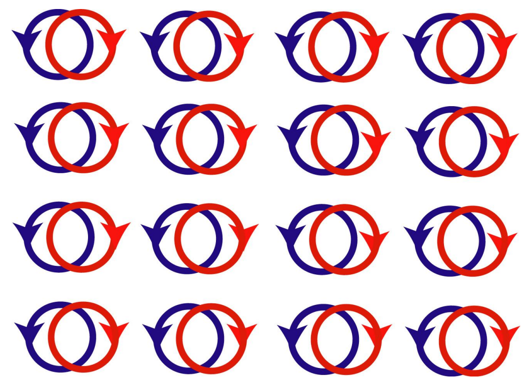


Fu, Kane and GM (2007)

Symmetry Classification

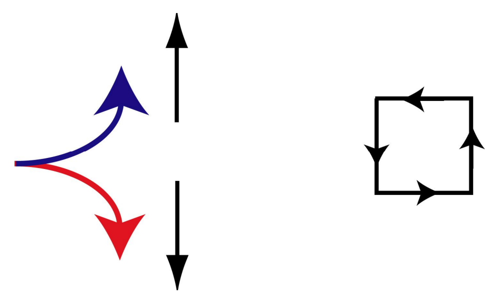
Ordinary insulators and topological insulators are distinguished by their strong coupling limits.





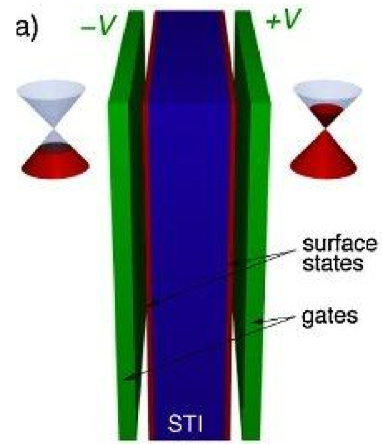
“nearsighted”, local

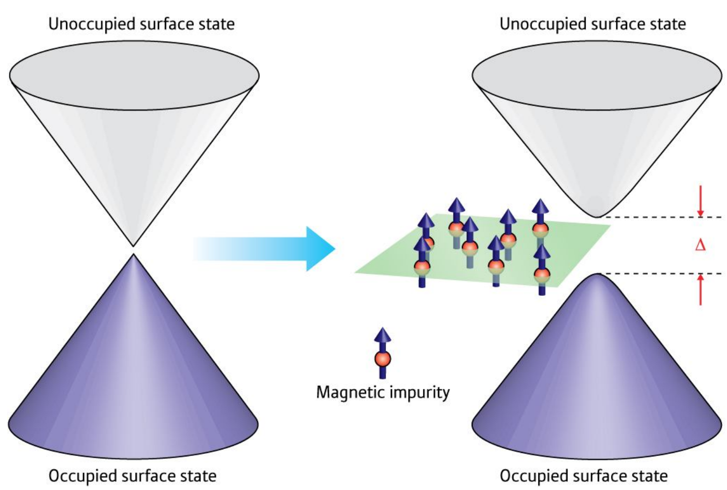
“nearsighted” topological



2D Surface of a (strong) 3D TI

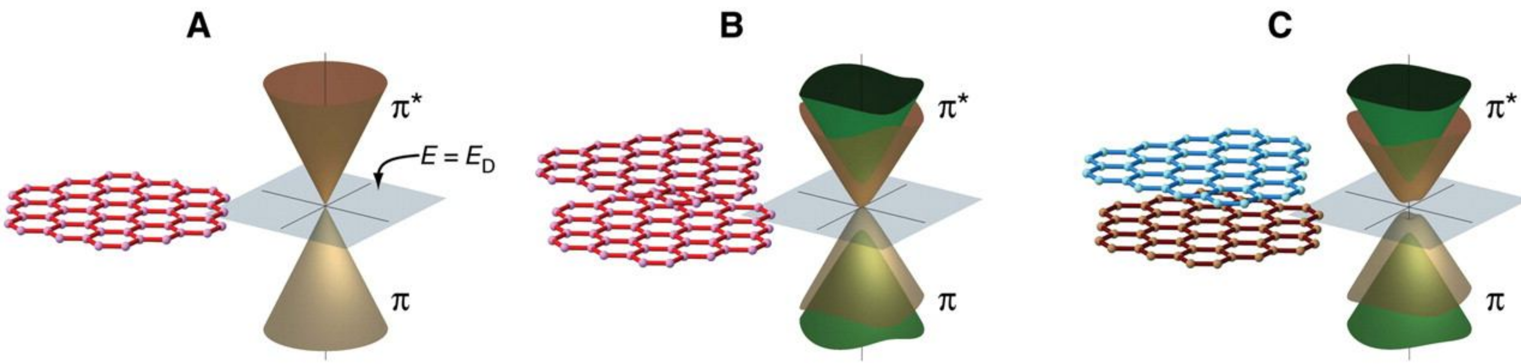
Discrete Kramers points:
Each surface has a single Dirac node, with a chiral partner on the opposite face.





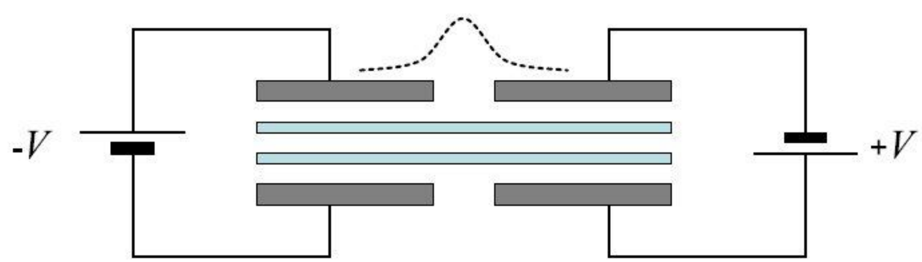
Gapped by an exchange field (breaks T) or by a pair field (via proximity effect)

Single Layer versus Bilayer Graphene

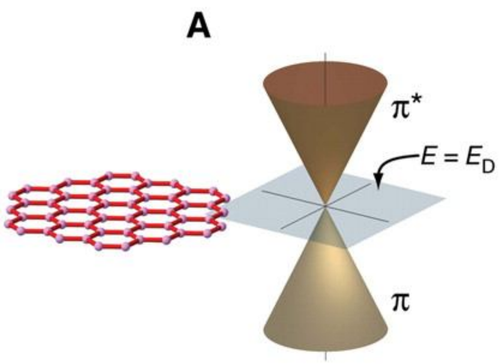


Single layer **Bilayer** **Asymmetric Bilayer**

Bias reversal produces a mass inversion

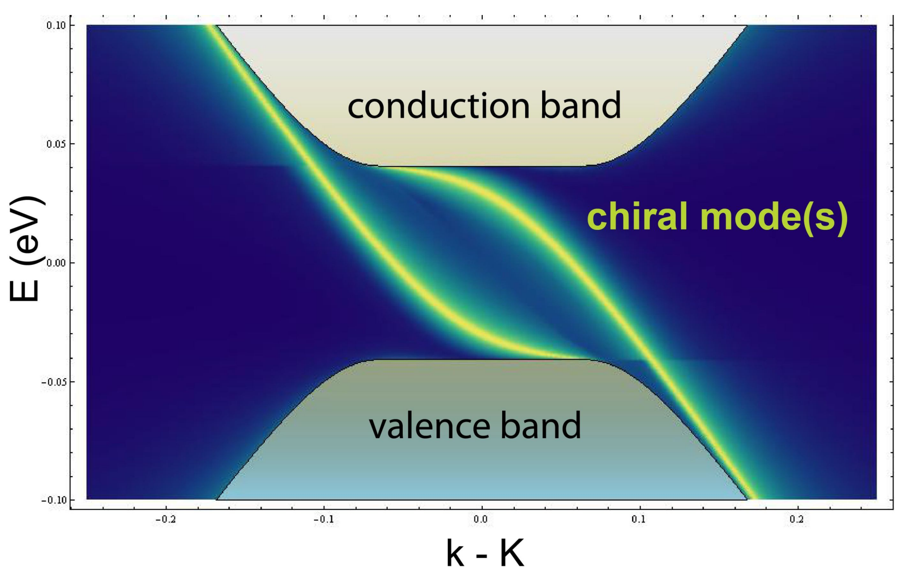


Single Layer versus Bilayer Graphene

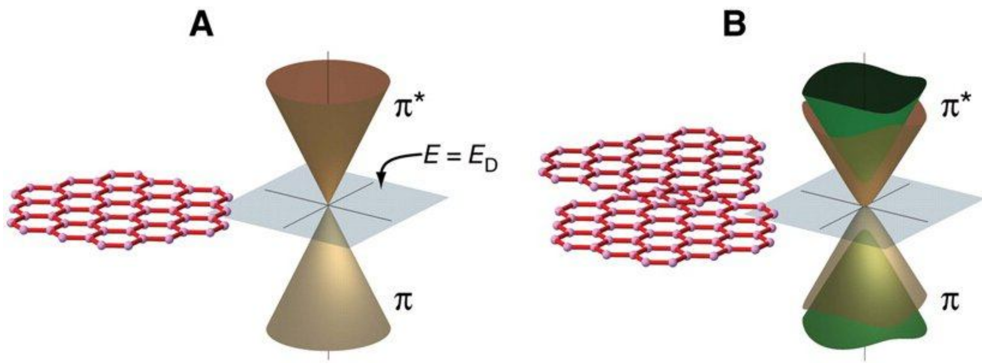


Single layer **Bilayer** **Asymmetric Bilayer**

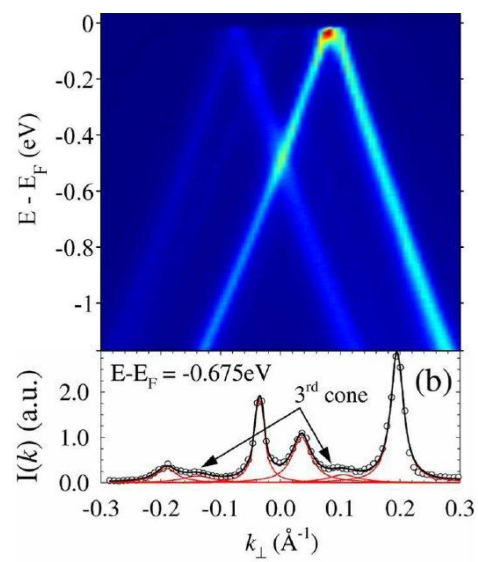
& valley polarized modes:
Martin et al, (2008);
F. Zhang and GM (2012)



The interlayer coherence scale for the Bernal stacked bilayer



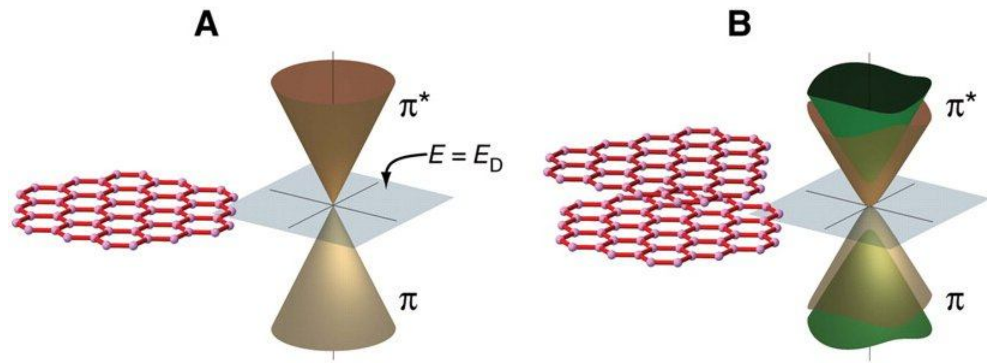
Single layer **Bernal Bilayer**



<u>collapses</u> in faulted multilayers (!)

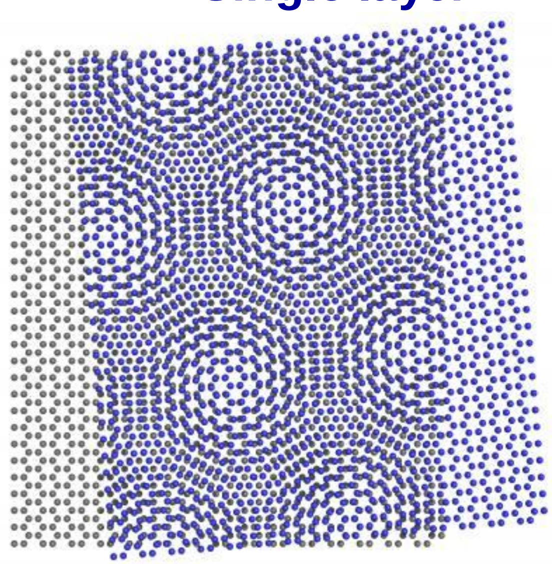
e.g. M. Sprinkle *et al.*
PRL <u>103</u>, 226803 (2009) (ARPES)

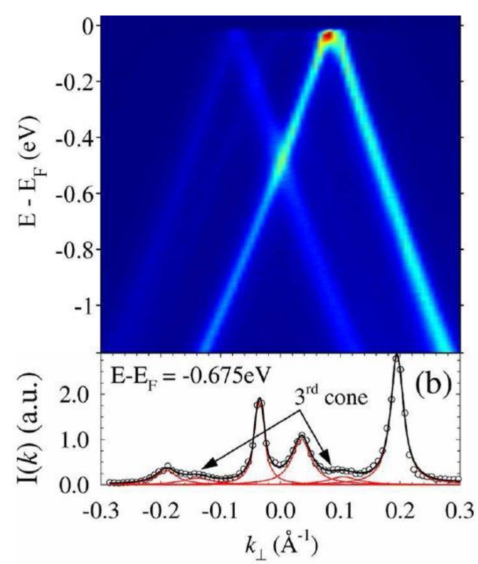
The interlayer coherence scale for the Bernal stacked bilayer



Single layer

Bernal Bilayer





Layer-polarized Dirac modes

This is a symmetry-protected band crossing.

It is controlled by the residual lattice registry in the moire-averaged interlayer coupling in its continuum (small angle) limit.

isotropic (canonical)

$$w\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

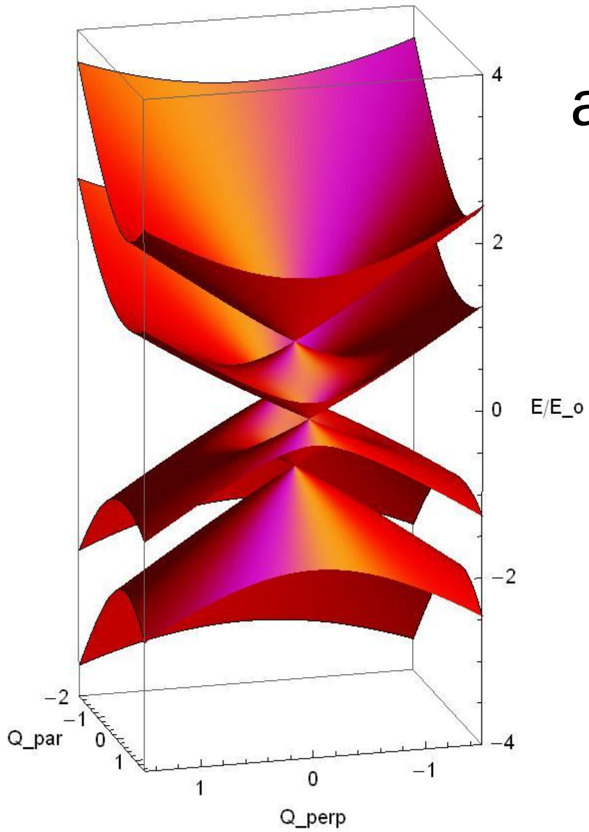
$$c_{ab}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

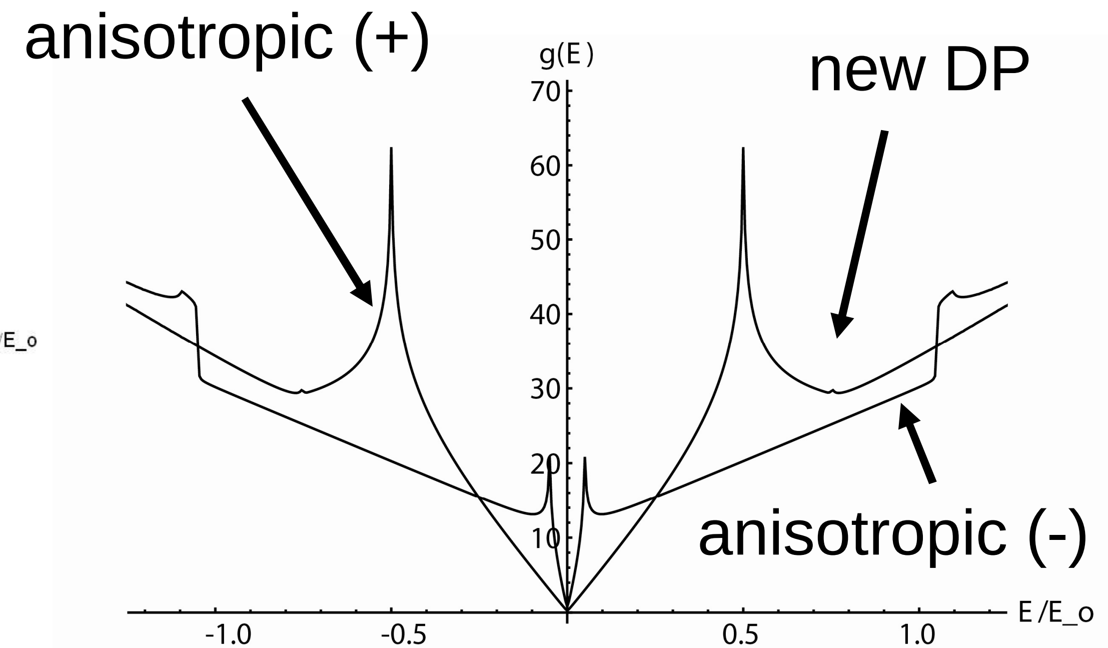
anisotropic (-)

$$c_{aa}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

anisotropic (+)

Symmetry-protected band crossing





Band insulators: a timeline

Study "all things practical and ornamental"

Late 1950's: The band theory of solids introduces novel quantum kinematics ("light" electrons, "holes" etc.) Blount, Luttinger, Kane, Dresselhaus, Bassani…

Mid 1980's: Identification of pseudo-relativistic physics at low energy (graphene and its variants)
DiVincenzo, Mele, Semenoff, Fradkin, Haldane…

Post 2000: Topological insulators and topological classification of gapped electronic states.
Kane, Mele, Zhang, Moore, Balents, Fu, Roy, Teo, Ryu, Ludwig, Schnyder..

Looking forward: Topological band theory as a new materials design principle.(developing)

Collaborators:

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David DiVincenzo
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Michael Rice
Saad Zaheer
Fan Zhang