Novel phenomena in topological insulators

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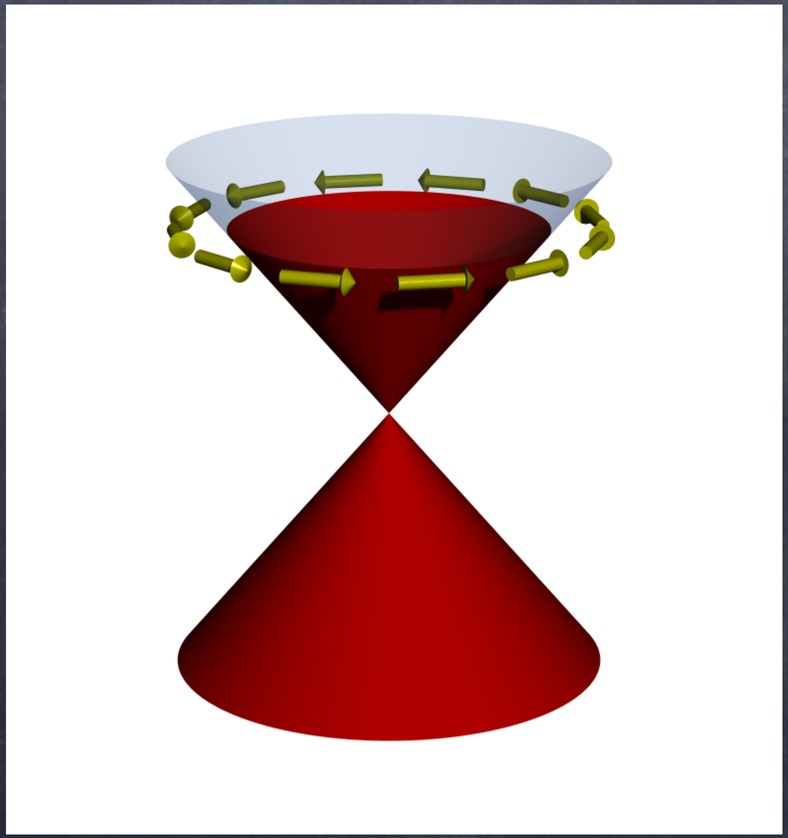

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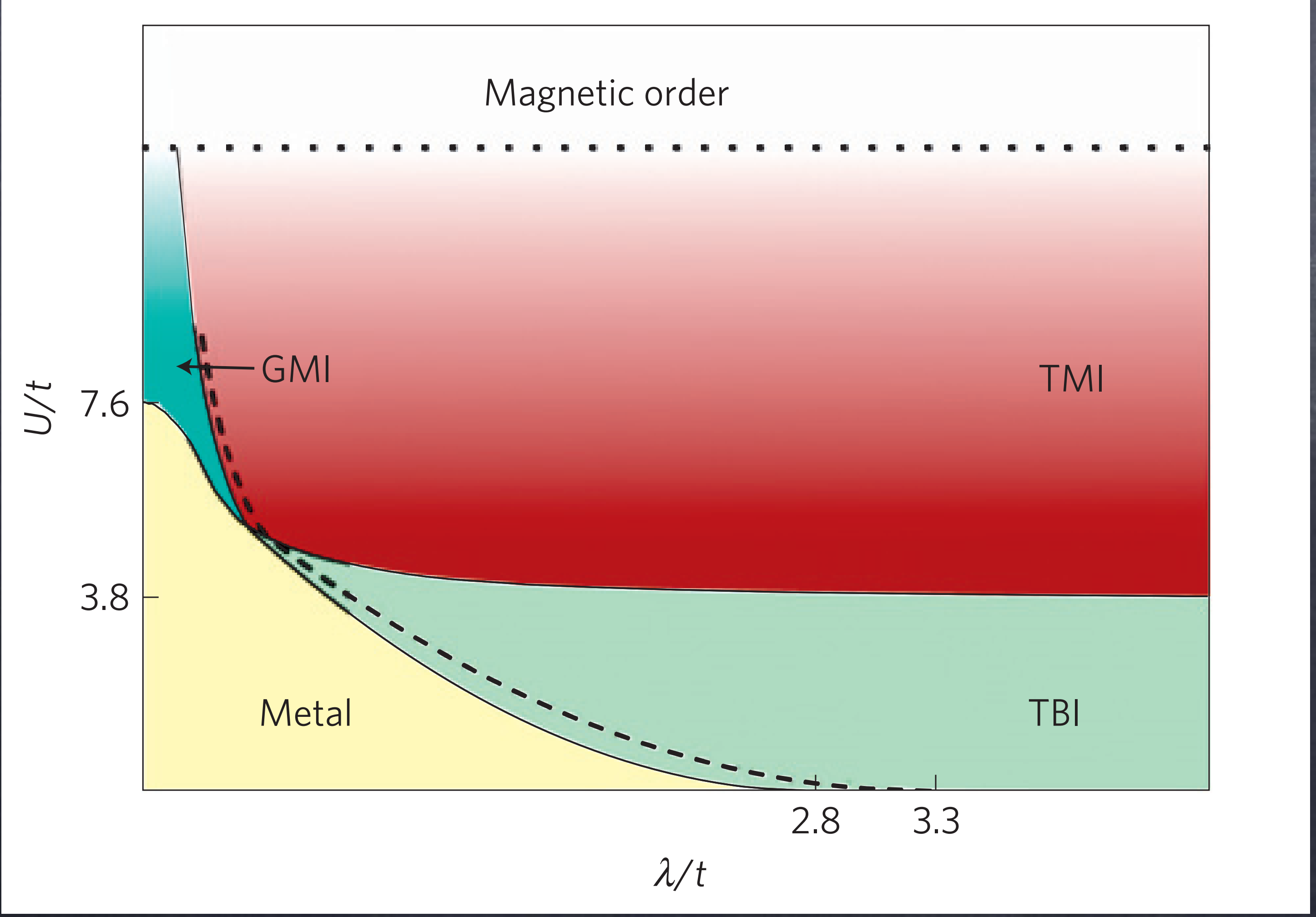
Mott physics and band topology in materials with strong spin–orbit interaction

Dmytro Pesin[1,2★†] and Leon Balents[2]

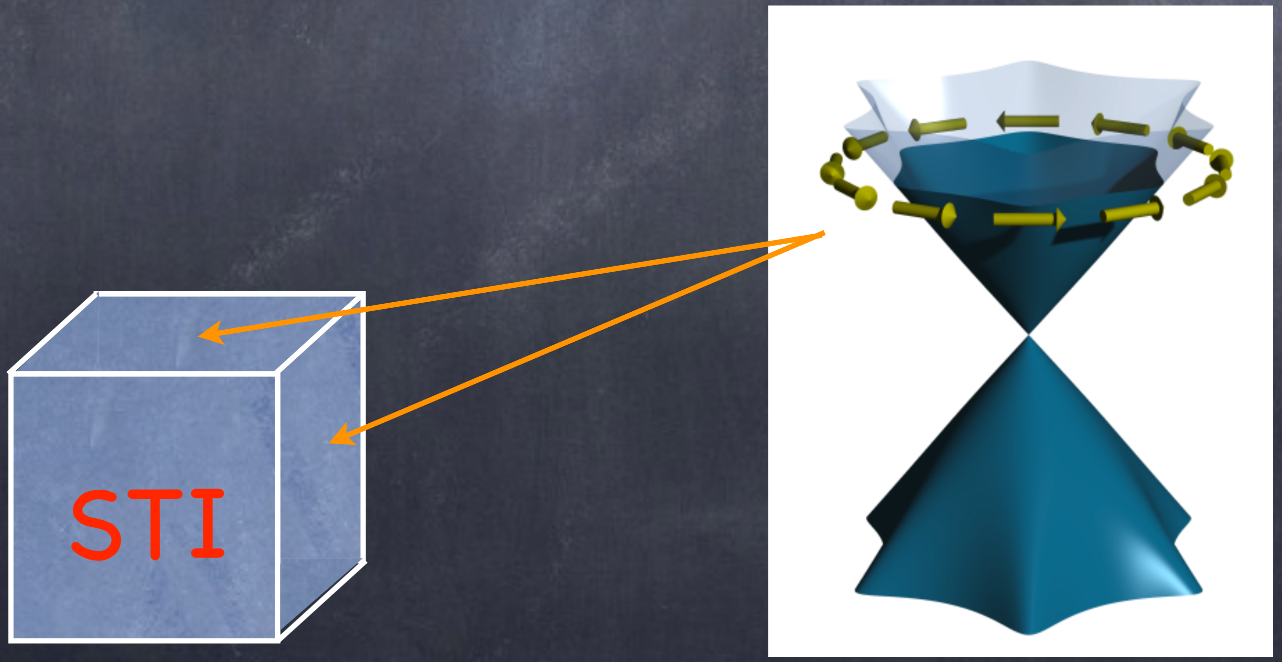
Recent theory and experiment have revealed that strong spin–orbit coupling can have marked qualitative effects on the band structure of weakly interacting solids, leading to a distinct phase of matter, the topological band insulator. We show that spin–orbit interaction also has quantitative and qualitative effects on the correlation-driven Mott insulator transition. Taking Ir-based pyrochlores as a specific example, we predict that for weak electron–electron interaction Ir electrons are in metallic and topological band insulator phases at weak and strong spin–orbit interaction, respectively. We show that by increasing the electron–electron interaction strength, the effects of spin–orbit coupling are enhanced. With increasing interactions, the topological band insulator is transformed into a 'topological Mott insulator' phase having gapless surface spin-only excitations. The proposed phase diagram also includes a region of gapless Mott insulator with a spinon Fermi surface, and a magnetically ordered state at still larger electron–electron interaction.

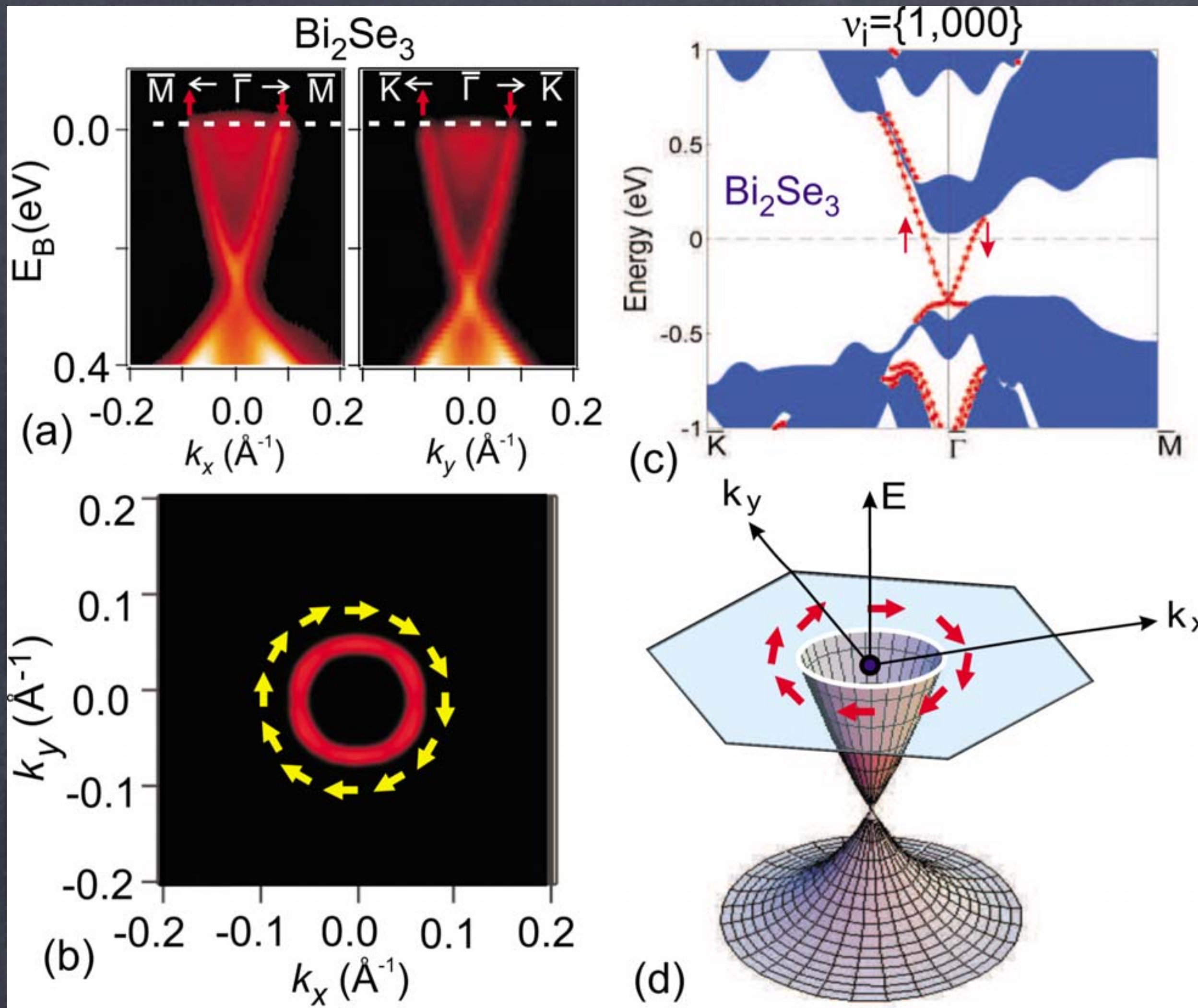


I. Surface states of 3D Topological Insulators

- Topological classification of 3D band insulators contains a surprise: in addition to the expected 3 `layered' invariants there exists a 4th, uniquely 3-dimensional `strong invariant' [Moore & Balents (2007); Fu, Kane & Mele (2007)

- Prediction: "Strong topological insulator (STI)": bulk insulator with gapless Dirac surface states.

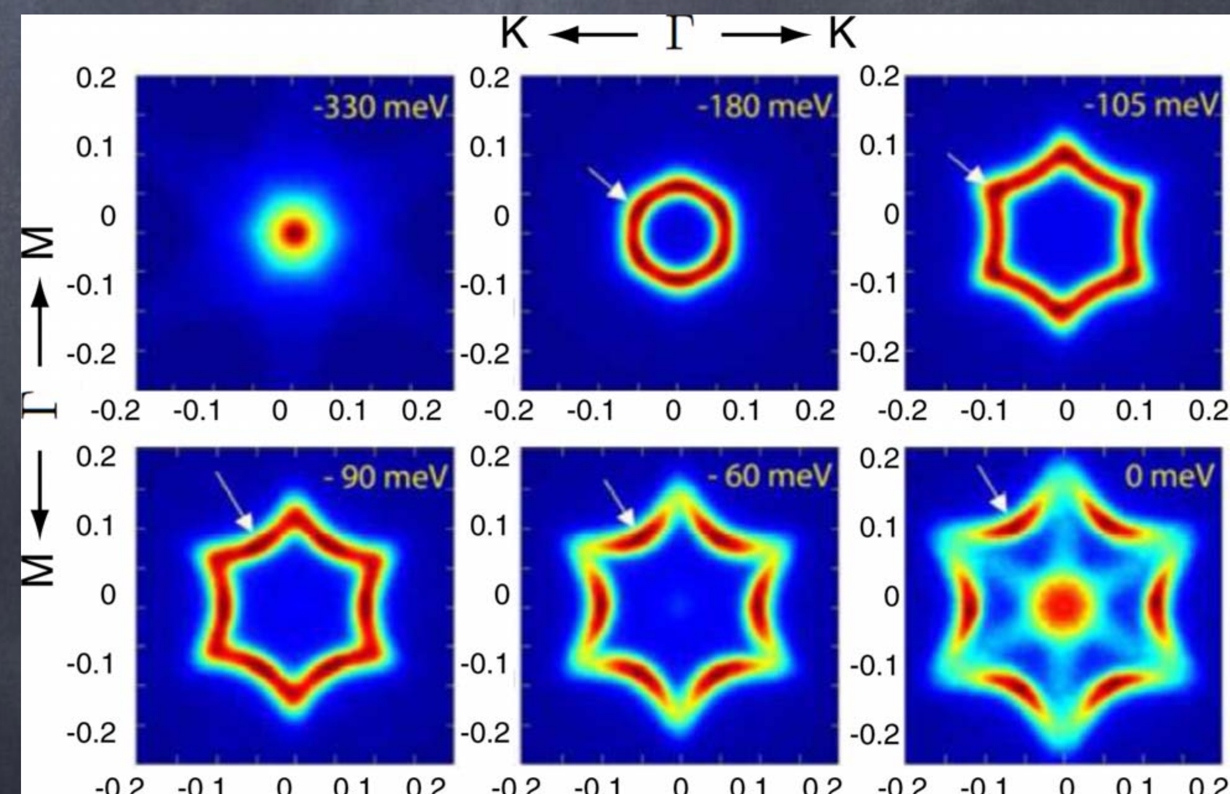




Xia et al, Nature Phys. 2009
Hsieh et al, Nature 2009
Zhang et al, Nature Phys. 2009, (prediction)

Surface Dirac cone seen by ARPES in Bi_2Se_3 crystals

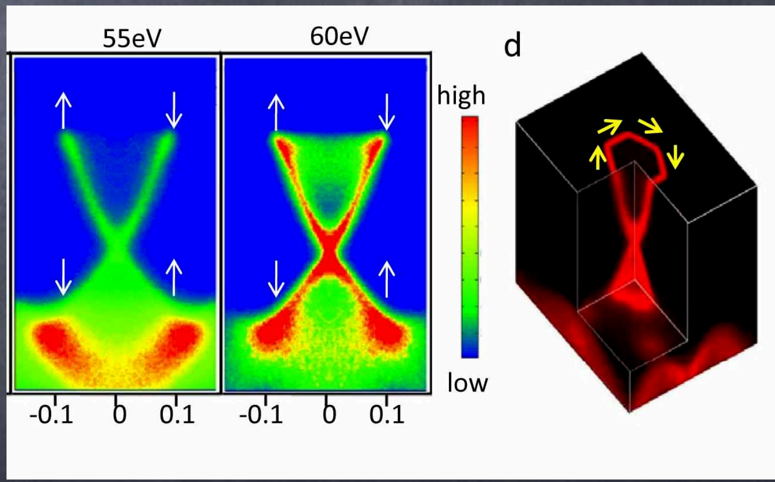
… and by STM in Bi_2Te_3 crystals



Alpichshev et al, PRL 2010

Families of 3D topological insulators:

- $Bi_{1-x}Sb_x$ alloys
- Bi_2Se_3, Bi_2Te_3, Sb_2Te_3 crystals
- ternary $Bi_2Te_2Se_2$, $GeBi_2Te_3$
- Heusler compounds (Li_2AgSb, NdPtBi, SmPtBi, ...)
- chalcogenides ($TlBiTe_2$, $TlBiSe_2$)
- pyrochlores ($Pr_2Ir_2O_7$, $Cd_2Os_2O_7$)
- perovskites & antiperovskites (Sr_3NBi, Sr_3NBi)



... more to come?

Why is all this interesting?

Existence of a single Dirac fermion on a 2D surface appears to violate the 1981 Nielsen-Ninomiya `no-go' theorem

Absence of neutrinos on a lattice : (I). Proof by homotopy theory

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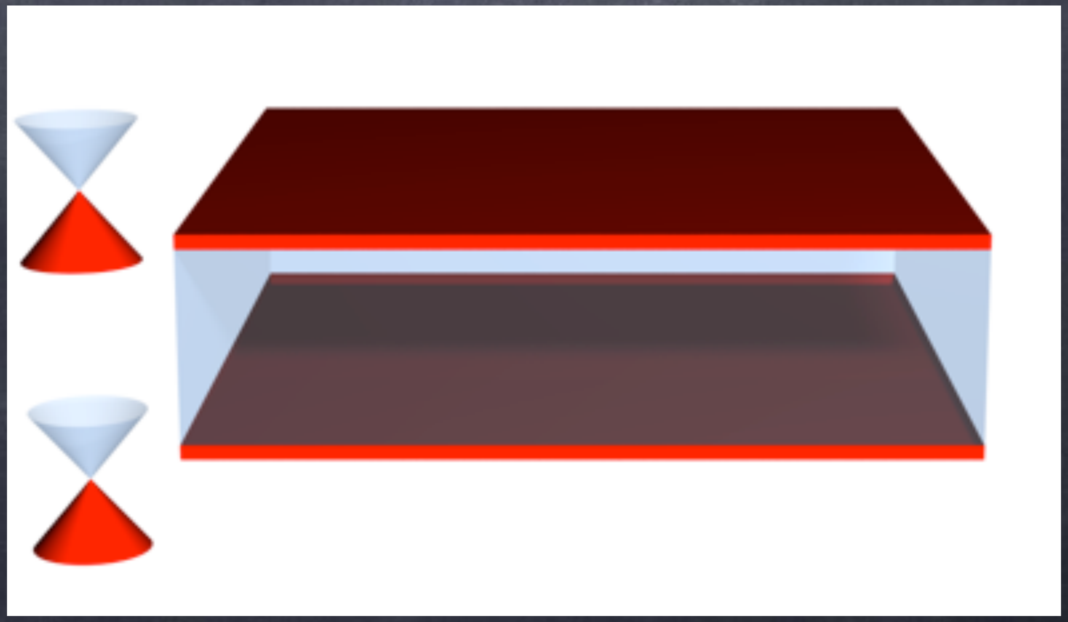
Abstract

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 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.

Two Dirac fermions located on opposite surfaces



Protected by time reversal symmetry

T is Implemented by an untiunitary operator

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

For Bloch Hamiltonians time reversal symmetry implies

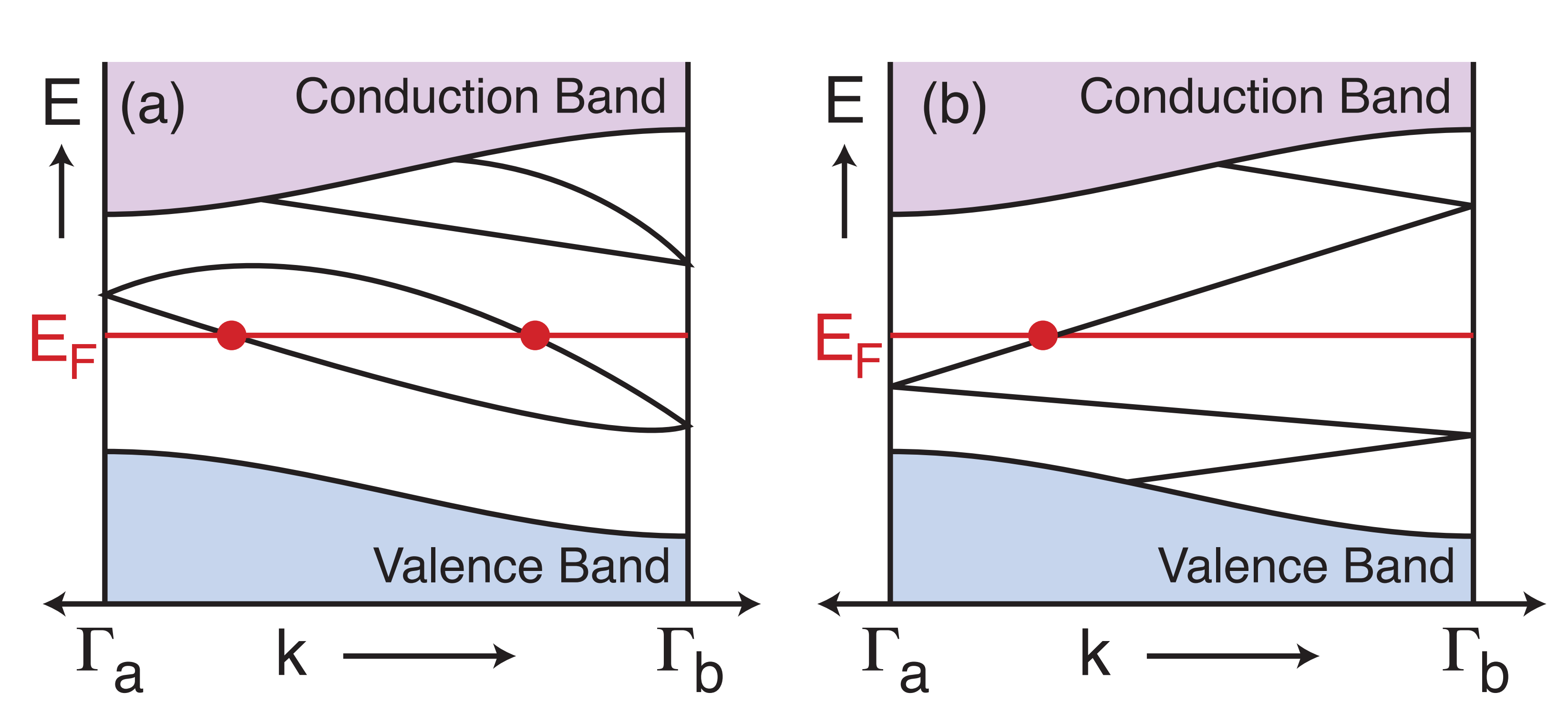
$$[\mathcal{H}, \Theta] = 0 \quad \Longrightarrow \quad \Theta\mathcal{H}(\mathbf{k})\Theta^{-1} = \mathcal{H}(-\mathbf{k})$$

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

$$\Theta\mathcal{H}(\Gamma_j)\Theta^{-1} = \mathcal{H}(\Gamma_j - \mathbf{G}) = \mathcal{H}(\Gamma_j)$$

All states at TRIM are doubly degenerate

The key observation (by Kane and Mele):



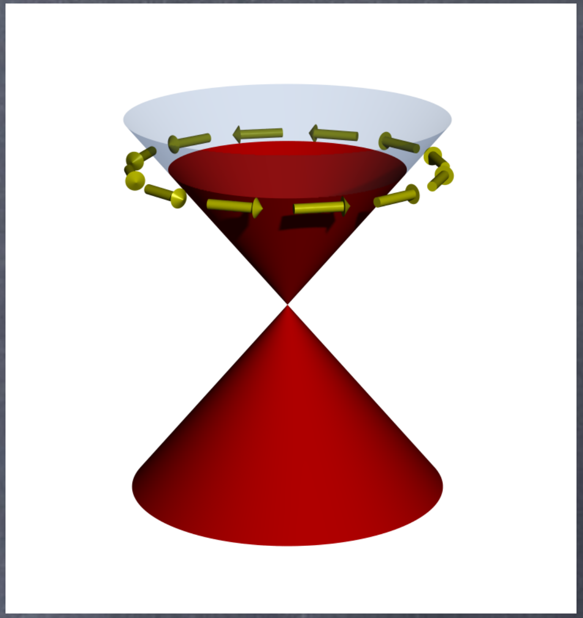
Trivial surface states

Topological surface states

Z_2 topological classification

Topological protection

Surface states are topologically protected: they cannot be destroyed by any $\mathcal{T}$-invariant perturbation.



Massless Dirac Hamiltonian

$$\mathcal{H} = v[\sigma_y p_x - \sigma_x p_y],$$

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:

$$(i\sigma_y K)[\sigma_y k_x - \sigma_x k_y](-i\sigma_y K) = -[\sigma_y k_x - \sigma_x k_y] = \mathcal{H}(-\mathbf{k})$$

- Spectrum: $\mathcal{H}\Psi = E\Psi, \qquad \Psi(\mathbf{r}) = \begin{pmatrix} \psi_\uparrow(\mathbf{r}) \\ \psi_\downarrow(\mathbf{r}) \end{pmatrix}$

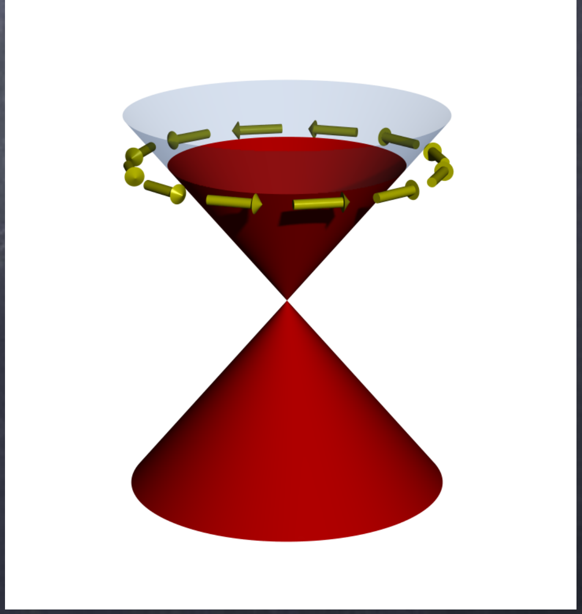
Assuming translational invariance take $\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} \psi_{\uparrow\mathbf{k}} \\ \psi_{\downarrow\mathbf{k}} \end{pmatrix}$

$$\longrightarrow \quad \mathcal{H}_{\mathbf{k}} = v[\sigma_y k_x - \sigma_x k_y],$$

To find the spectrum easy way square the Hamiltonian

$$\mathcal{H}_{\mathbf{k}}^2 = v^2[k_x^2 + k_y^2 - (\sigma_y\sigma_x + \sigma_x\sigma_y)k_x k_y]$$

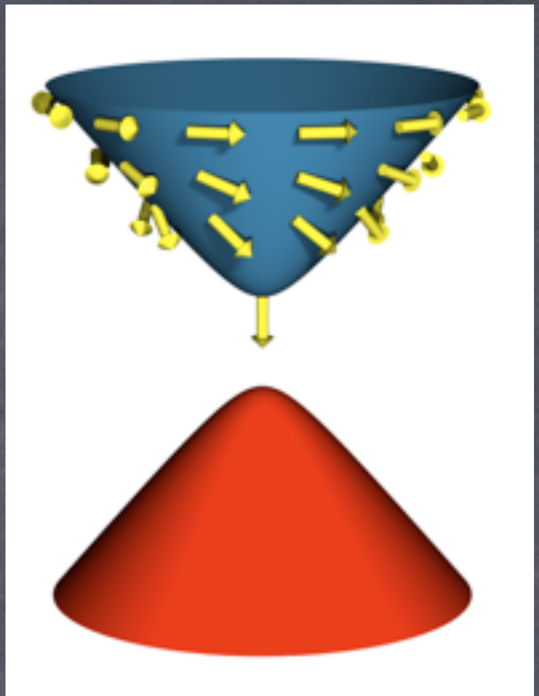
$$E_{\mathbf{k}} = \pm v\sqrt{k_x^2 + k_y^2}$$



$$\Psi_{\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \frac{k_y \pm i k_x}{k} \end{pmatrix}$$

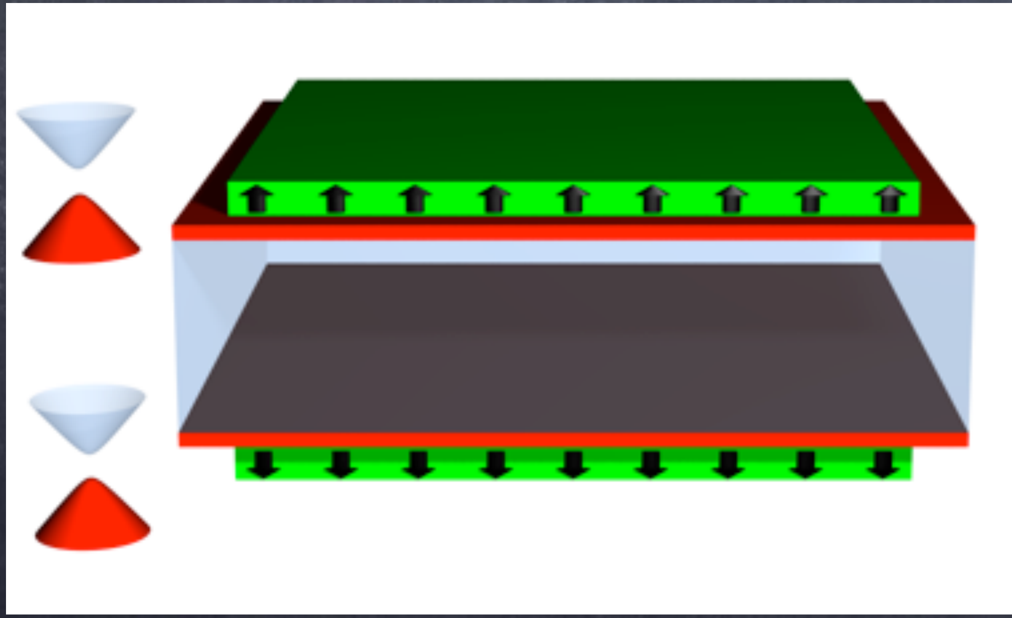
To open a gap one needs to add a term

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



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

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



Corresponds to depositing a ferromagnet on the surface of a TI

Gapless surface states are protected by $\mathcal{T}$

Massive Dirac Fermion on the Surface of a Magnetically Doped Topological Insulator

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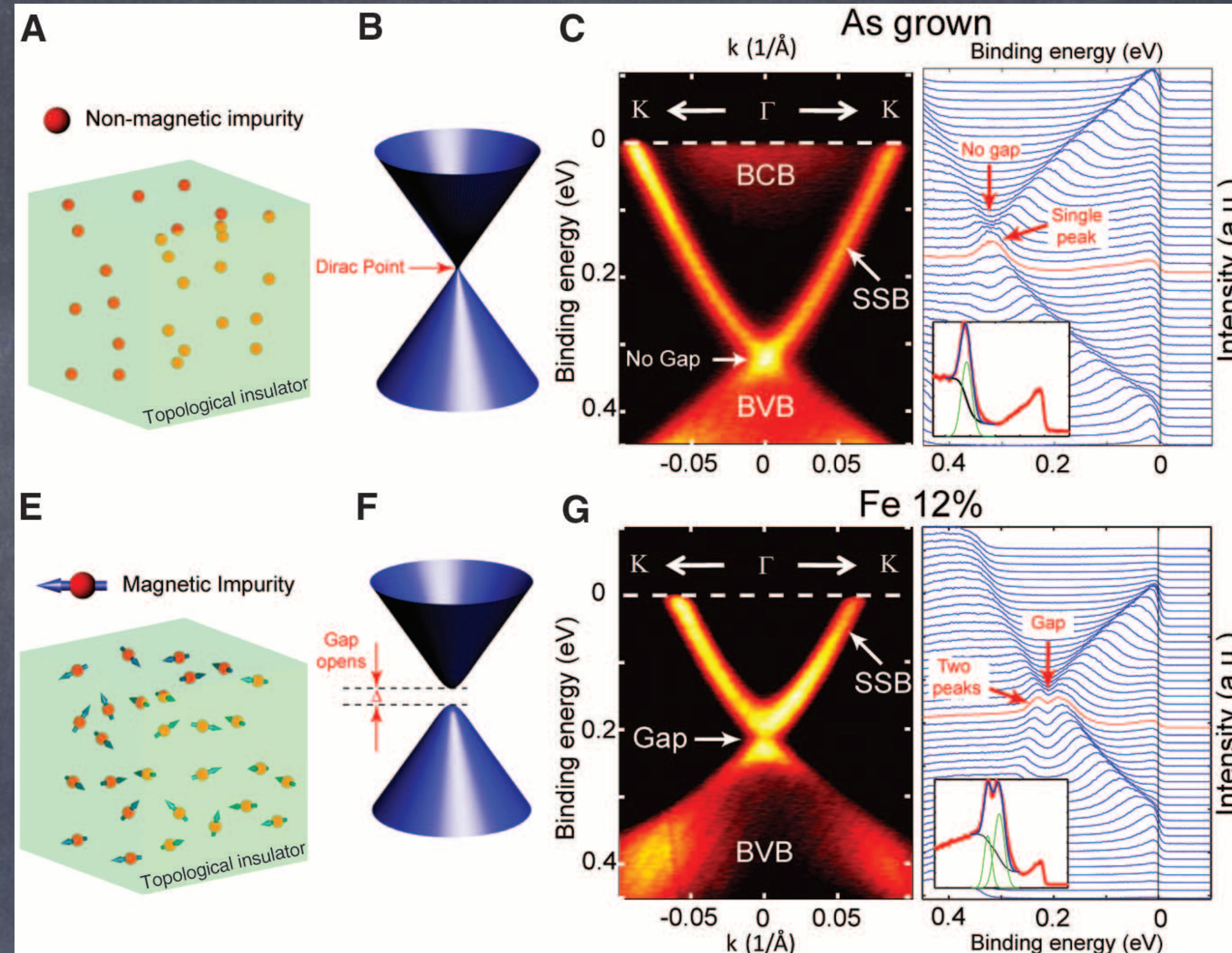
In addition to a bulk energy gap, topological insulators accommodate a conducting, linearly dispersed Dirac surface state. This state is predicted to become massive if time reversal symmetry is broken, and to become insulating if the Fermi energy is positioned inside both the surface and bulk gaps. We introduced magnetic dopants into the three-dimensional topological insulator dibismuth triselenide (Bi_2Se_3) 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



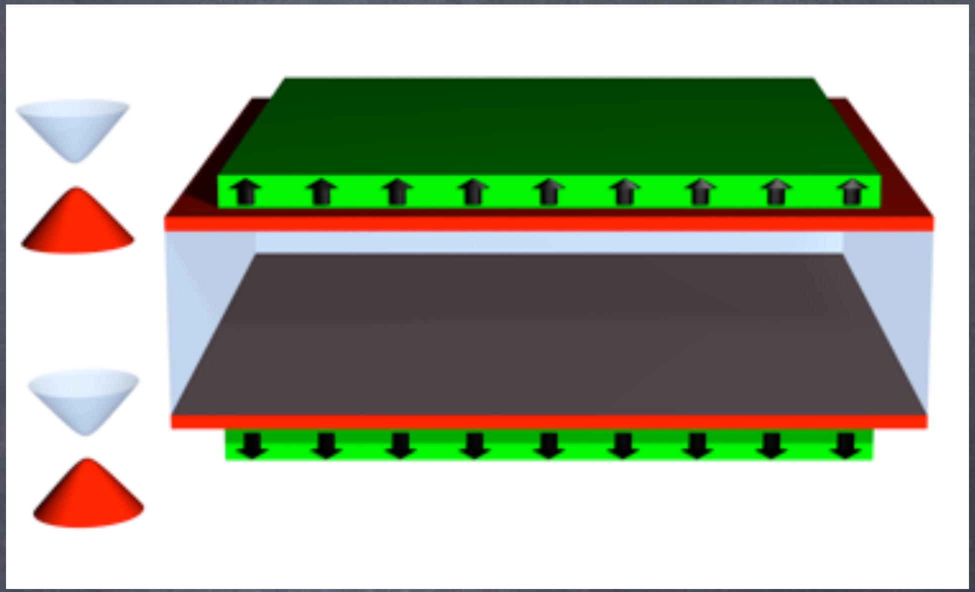
- Gap opens without bulk magnetic ordering.
- Could there be surface ordering?
- Could disordered magnetic moments open a gap?

II. Exact quantization in solids

Magnetized surface of a TI turns out to be a quantum Hall insulator with

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

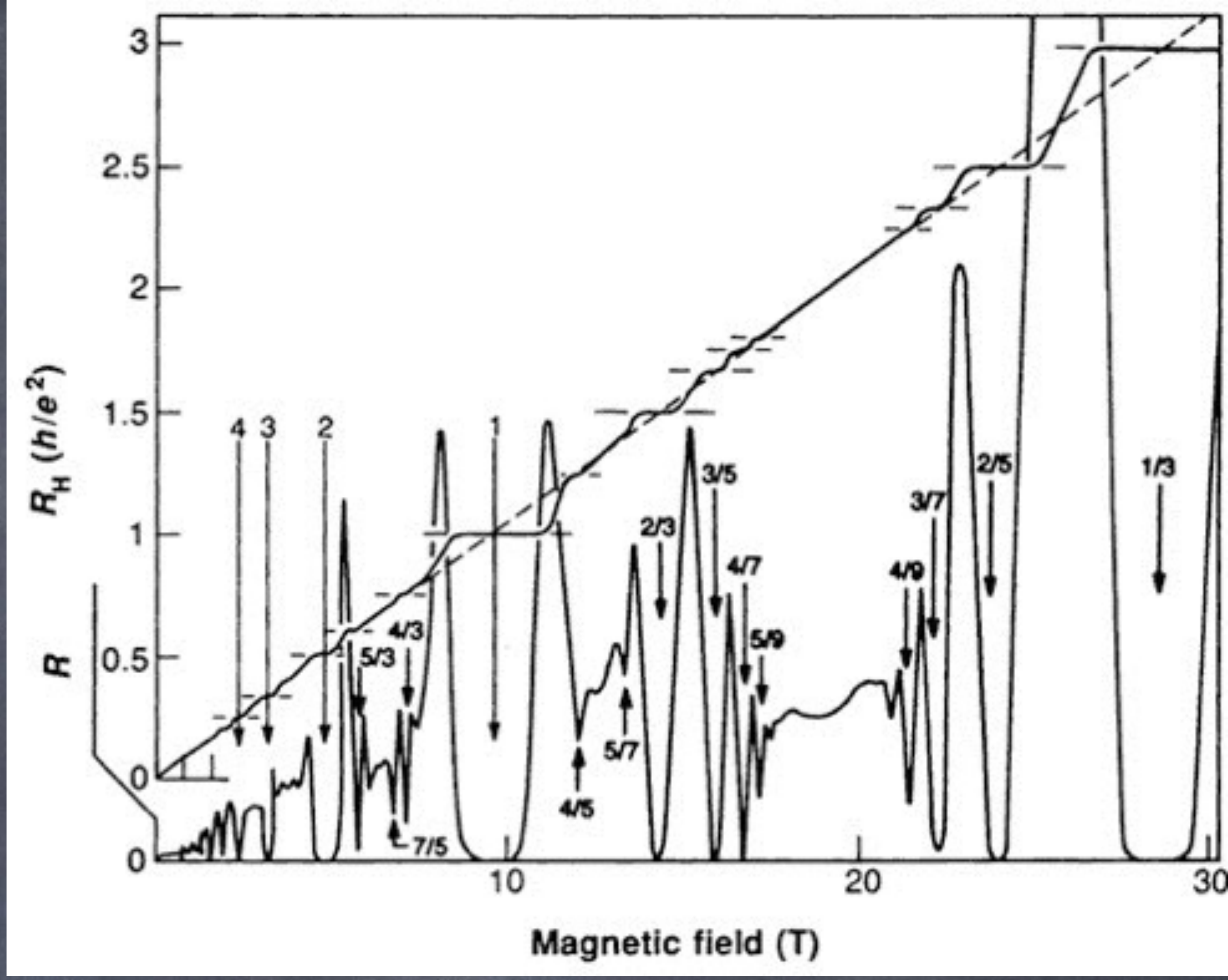
(experimentally untested)

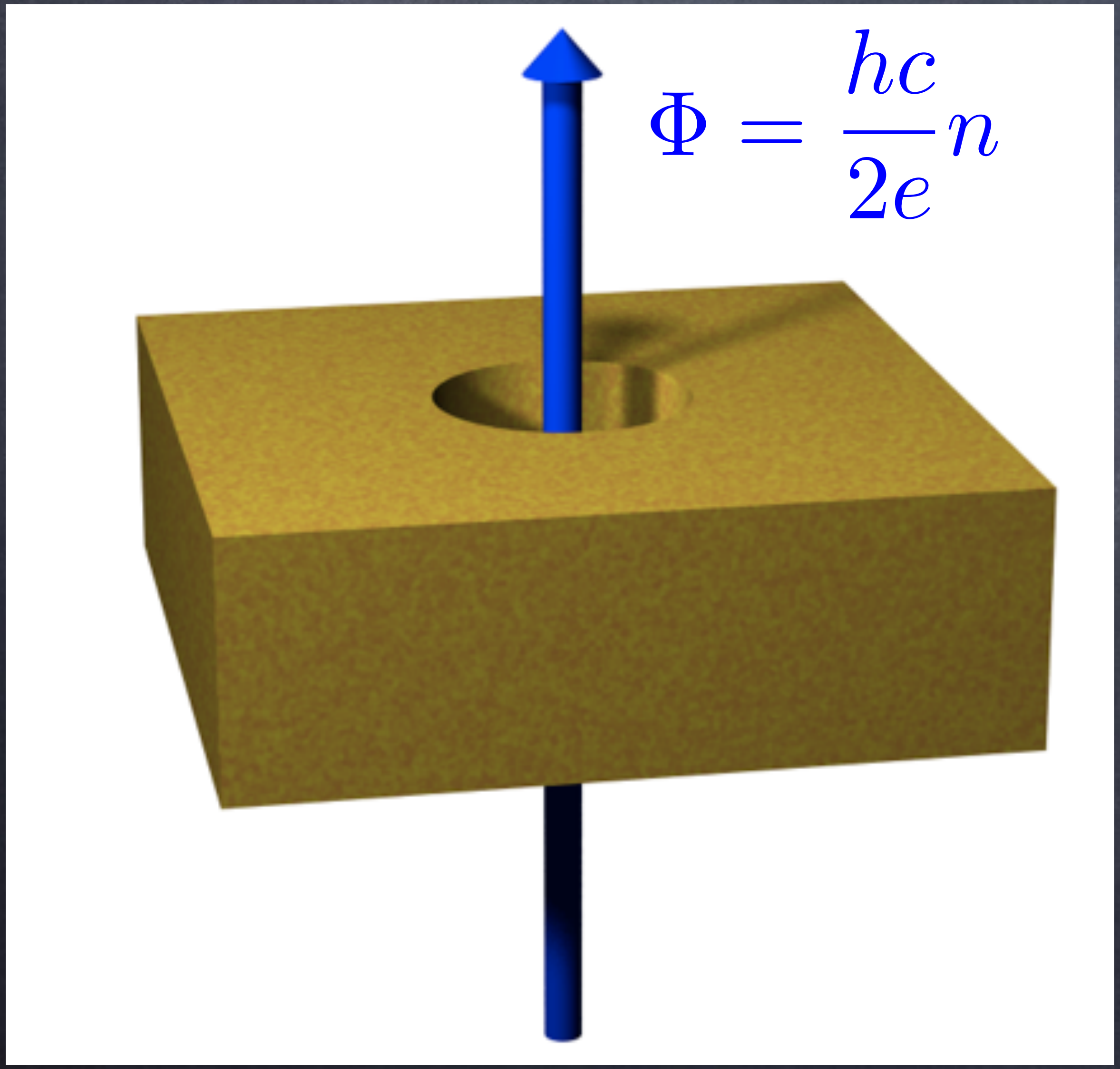


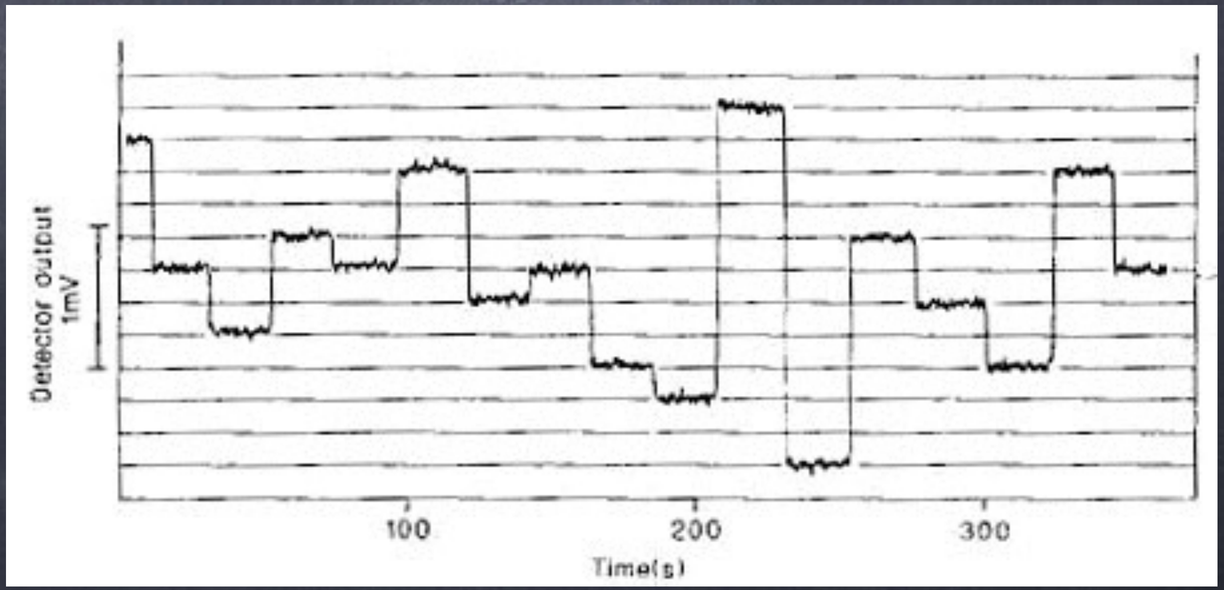
- Fractional quantum Hall effect in *non-interacting* system!

Exact quantization in solids

- quantum Hall effect
- superconductivity







REVIEWS OF MODERN PHYSICS, VOLUME 77, JANUARY 2005

CODATA recommended values of the fundamental physical constants: 2002*

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National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8401, USA

(Published 18 March 2005)

This paper gives the 2002 self-consistent set of values of the basic constants and conversion factors of physics and chemistry recommended by the Committee on Data for Science and Technology (CODATA) for international use. Further, it describes in detail the adjustment of the values of the subset of constants on which the complete 2002 set of recommended values is based. Two noteworthy additions in the 2002 adjustment are recommended values for the bound-state rms charge radii of the proton and deuteron and tests of the exactness of the Josephson and quantum-Hall-effect relations $K_J = 2e/h$ and $R_K = h/e^2$, where K_J and R_K are the Josephson and von Klitzing constants, respectively, e is the elementary charge, and h is the Planck constant. The 2002 set replaces the previously recommended 1998 CODATA set. The 2002 adjustment takes into account the data considered in the 1998 adjustment as well as the data that became available between 31 December 1998, the closing date

[For other recent comparisons, see Reymann *et al.* (1999); Reymann *et al.* (2001); Behr *et al.* (2003); Lo-Hive *et al.* (2003).] In summary, all of the results obtained during the last four years continue to support the view that K_J is a constant of nature and equal to $2e/h$.

E. Quantum Hall effect and von Klitzing constant R_K

For a fixed current I through a quantum Hall effect device of the usual Hall-bar geometry—either a heterostructure or metal oxide semiconductor field-effect transistor (MOSFET)—there are regions in the curve of Hall

sons of quantum Hall effect resistance standards are reported by Delahaye *et al.* (2000), Satrapinski *et al.* (2001), and Nakanishi *et al.* (2002). Intriguing work to create large arrays of quantum Hall effect devices in parallel to provide highly accurate quantized resistances that are large submultiples of R_K, for example, $R_K/100$ and $R_K/200$, has been carried out by Poirier *et al.* (2002). As for the Josephson constant $K_J = 2e/h$, all of the results obtained during the last four years continue to support the view that R_K is a constant of nature and equal to h/e^2.

Chern number or TKNN invariant

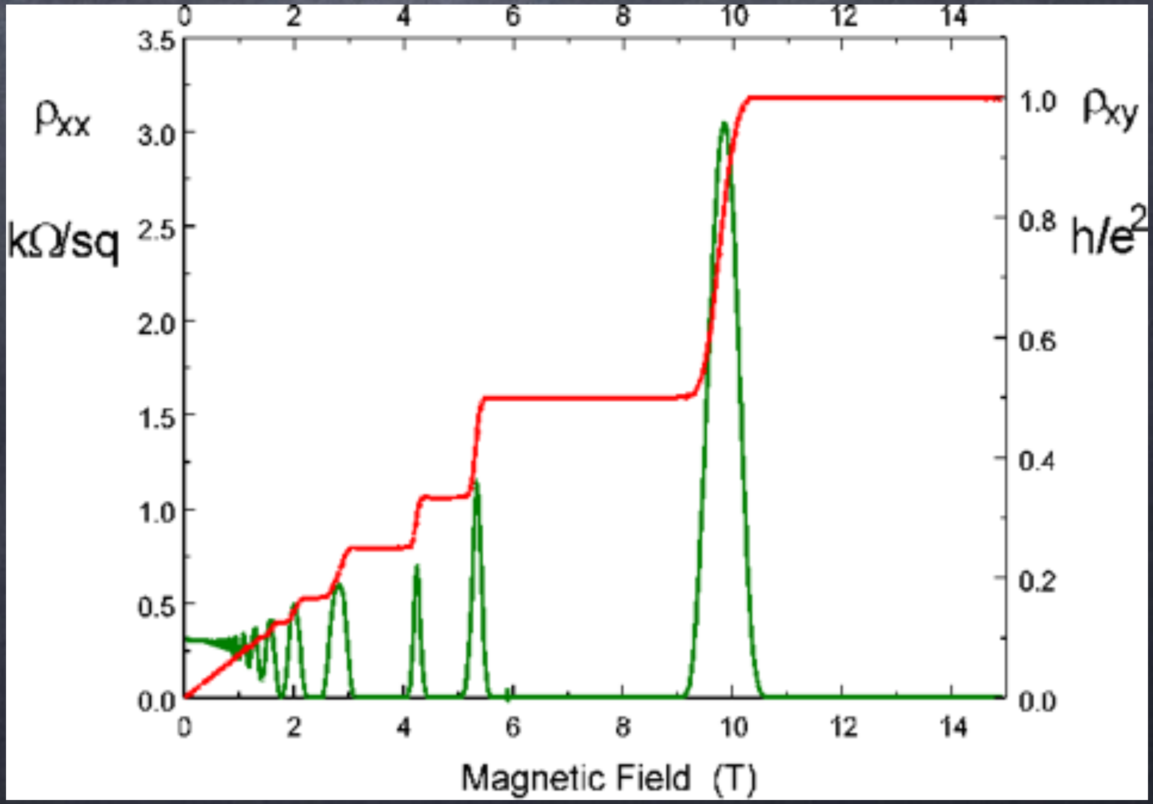
(Thouless-Kosterlitz-Nightingale-den Nijs, 1982)

S.S.Chern

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

$$n = \sum_{\text{bands}} \frac{1}{2\pi} \int_{\text{BZ}} d^2k (\nabla_{\mathbf{k}} \times \mathcal{A}_{\mathbf{k}})_z, \qquad \mathcal{A}_{\mathbf{k}} = -i \langle u_{\mathbf{k}} | \nabla_{\mathbf{k}} u_{\mathbf{k}} \rangle$$

"First Chern number" - integer topological invariant for filled energy bands. Can change only when bands touch.



Chern number of a Dirac Hamiltonian

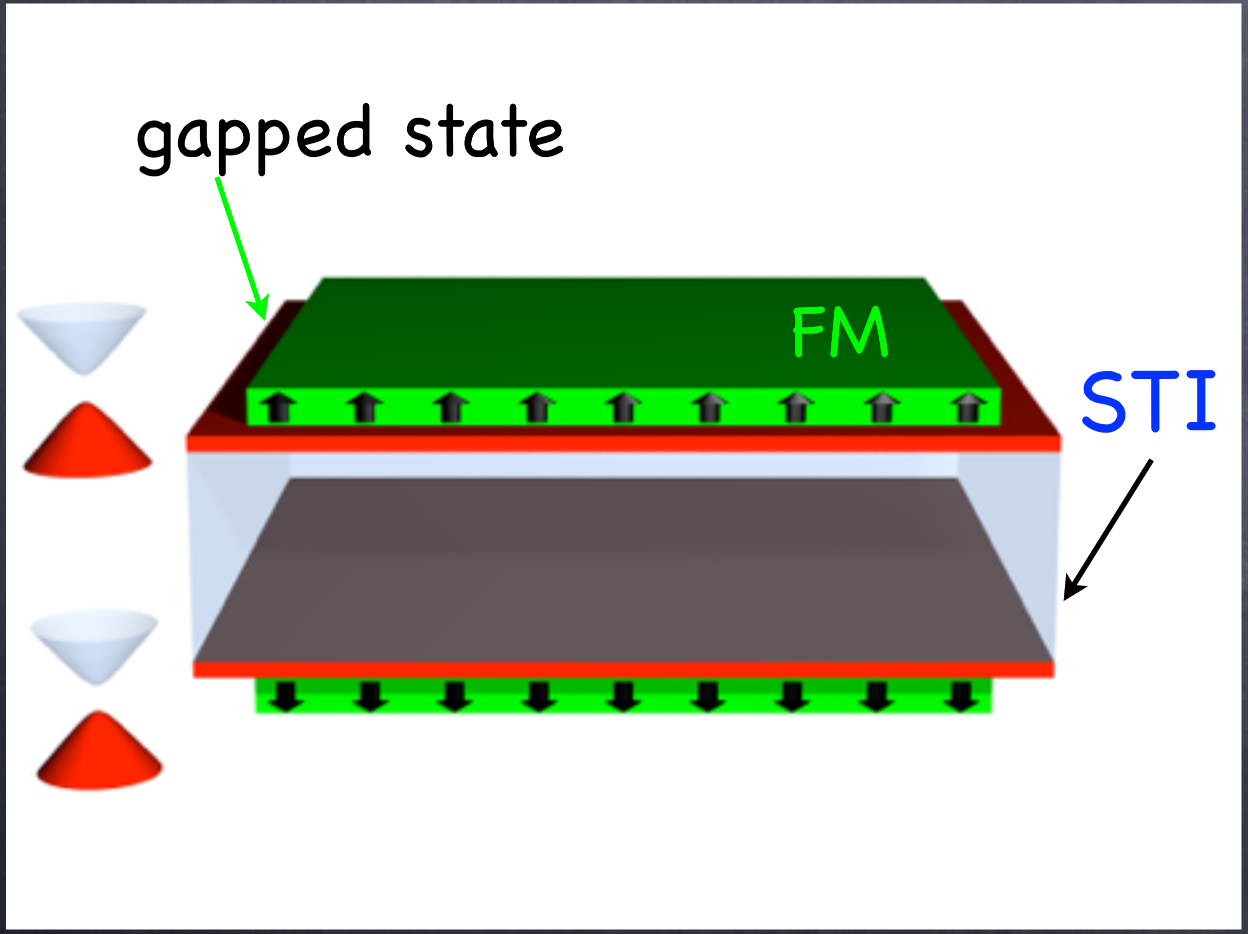
$$u_{\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\phi_{\mathbf{k}} \sqrt{1 - m/E_{\mathbf{k}}} \\ \sqrt{1 + m/E_{\mathbf{k}}} \end{pmatrix}, \qquad \phi_{\mathbf{k}} = (k_y - ik_x)/k$$

$$\mathcal{A}_{\mathbf{k}} = -i\langle u_{\mathbf{k}} | \nabla_{\mathbf{k}} u_{\mathbf{k}} \rangle = \frac{1}{2} \frac{\hat{z} \times \mathbf{k}}{E_{\mathbf{k}}(m + E_{\mathbf{k}})}$$

$$\begin{aligned} n &= \frac{1}{2\pi} \int_{\mathrm{BZ}} d^2\mathbf{k} \, (\nabla_{\mathbf{k}} \times \mathcal{A}_{\mathbf{k}}) \cdot \hat{z} \\ &= \frac{1}{2\pi} \int_{\mathrm{BZ}} d^2\mathbf{k} \, \frac{m}{2E_{\mathbf{k}}^3} = \frac{1}{2}\mathrm{sgn}(m) \end{aligned}$$

Chern number is half-integral!

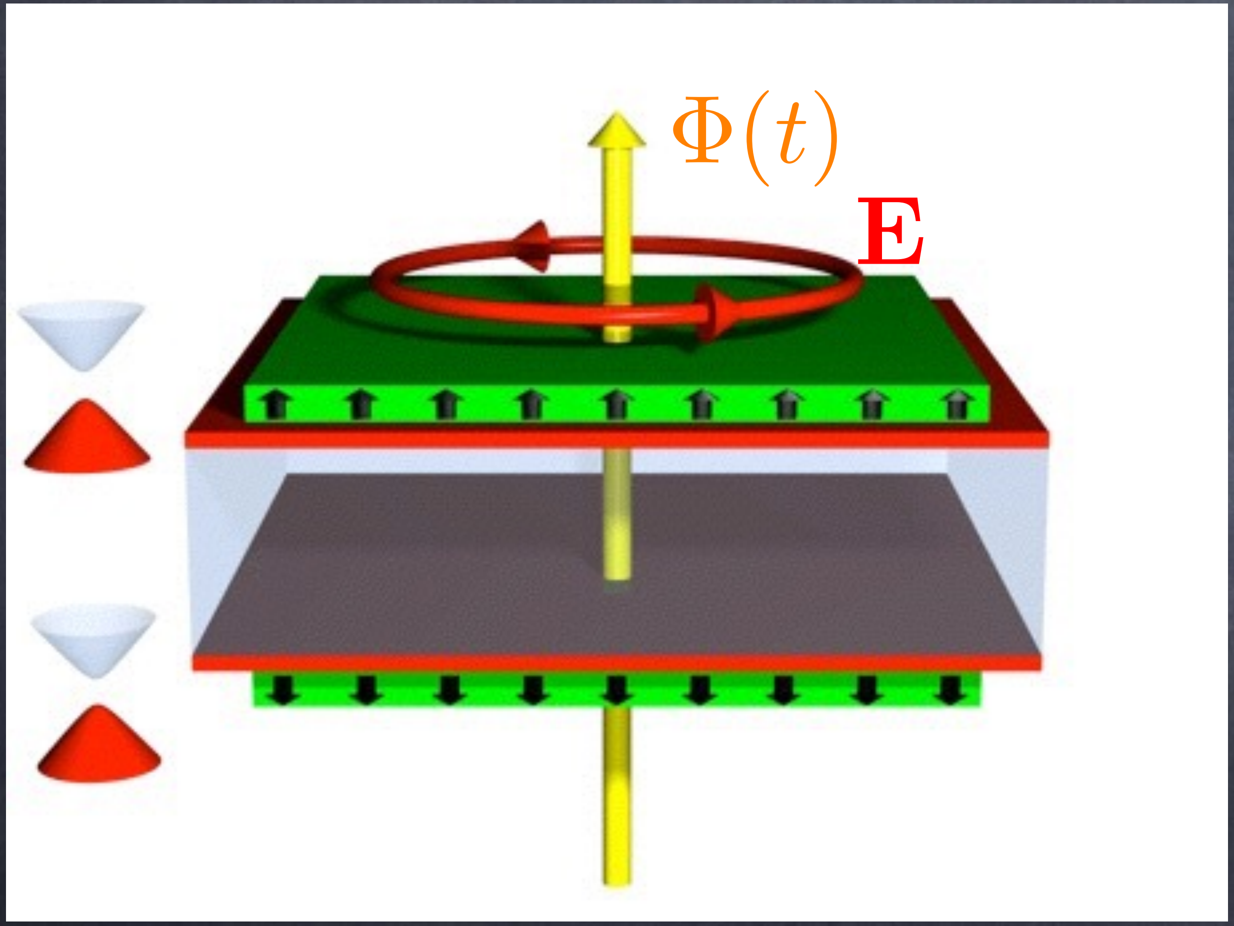
III. Bulk-surface correspondence



The gapped surface state has quantized Hall conductivity

$$\sigma_{xy} = \frac{e^2}{h}\left(n + \frac{1}{2}\right)$$

Laughlin's flux-insertion argument for the magnetized surface states



Flux insertion produces Faraday electric field

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}$$

...which in turn causes Hall current

$$\mathbf{j} = \sigma_{xy}(\mathbf{E} \times \hat{z})$$

- Integrating the current we find accumulated charge

$$\frac{dQ}{dt} = -\oint_C dl\ \mathbf{n}\cdot\mathbf{j} = -\sigma_{xy}\oint_C d\mathbf{l}\cdot\mathbf{E}$$

- Using Stoke's theorem and Faraday's law, $\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}$

$$\delta Q = \sigma_{xy}\frac{\delta\Phi}{c}$$

- For full flux quantum this becomes

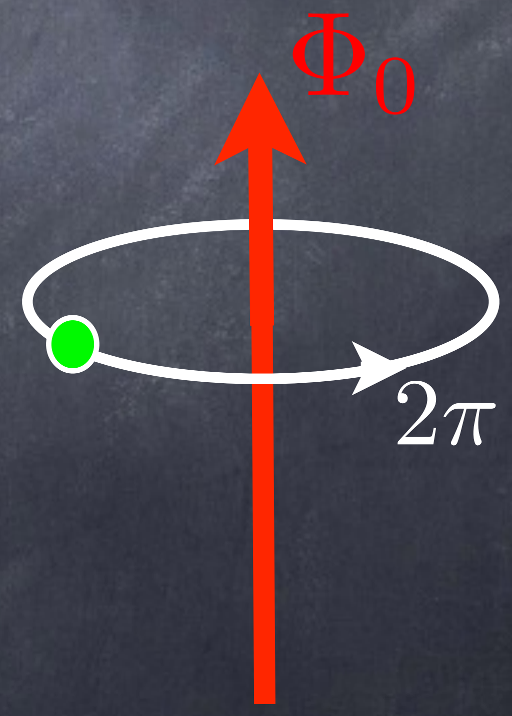
$$\delta Q = \sigma_{xy}\frac{\Phi_0}{c} = \left(n+\frac{1}{2}\right)e$$

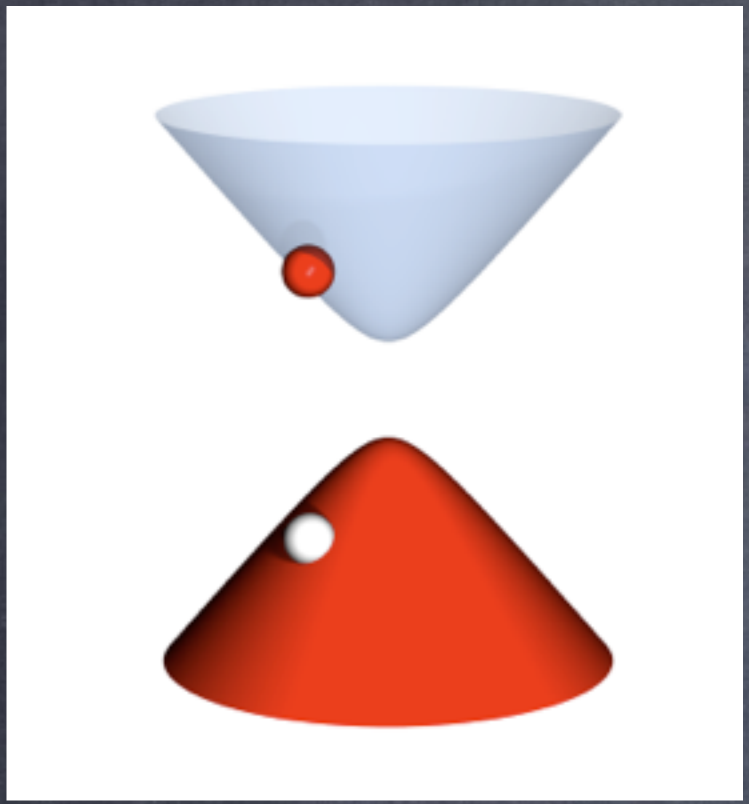
A solenoid carrying the full flux quantum can be removed by a gauge transformation:

↓

FRACTIONALLY CHARGED EXCITATIONS!

This is the essence of Laughlin's argument:
Physically, electron encircling such flux tube acquires Aharonov-Bohm phase 2π which is invisible to it.





Excitations of a massive Dirac Hamiltonian are electron-hole pairs which are charge neutral.

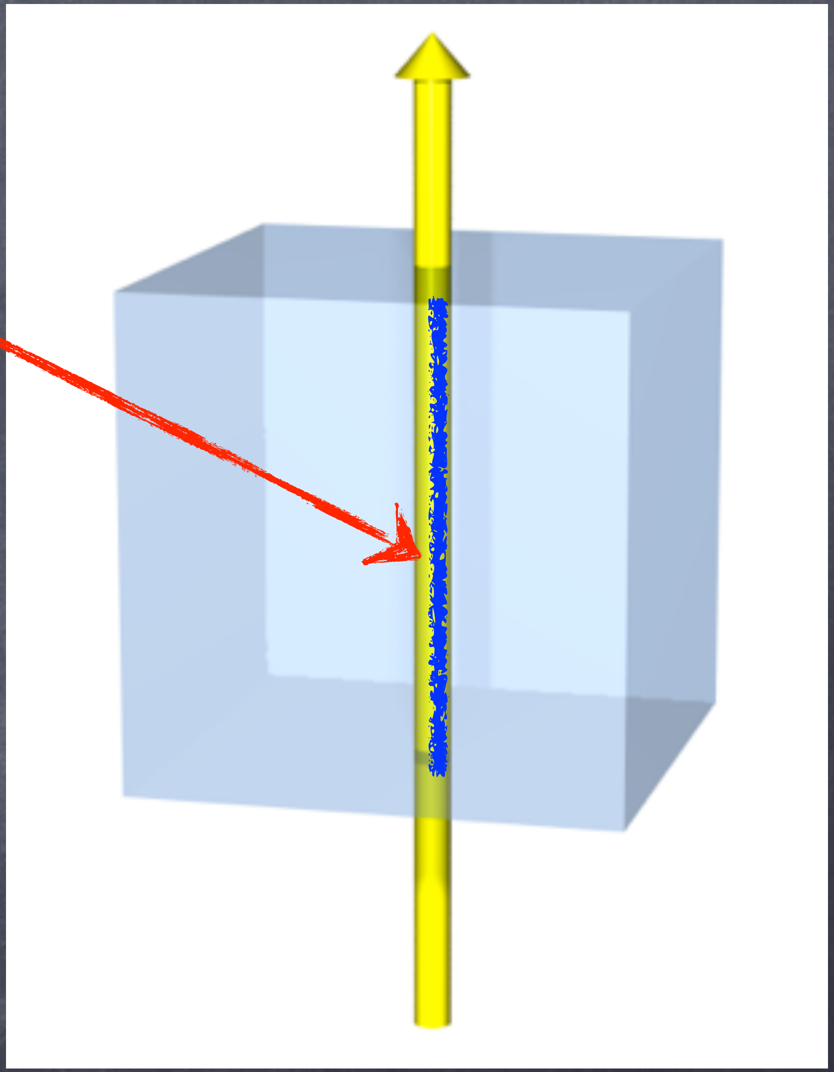
There should be no fractionally charged quasiparticles in this weakly interacting system!

What gives?

The Wormhole effect:

Flux tube inserted in a STI carries topologically protected gapless fermionic modes when

$$\Phi = \frac{hc}{2e} = \frac{1}{2}\Phi_0$$

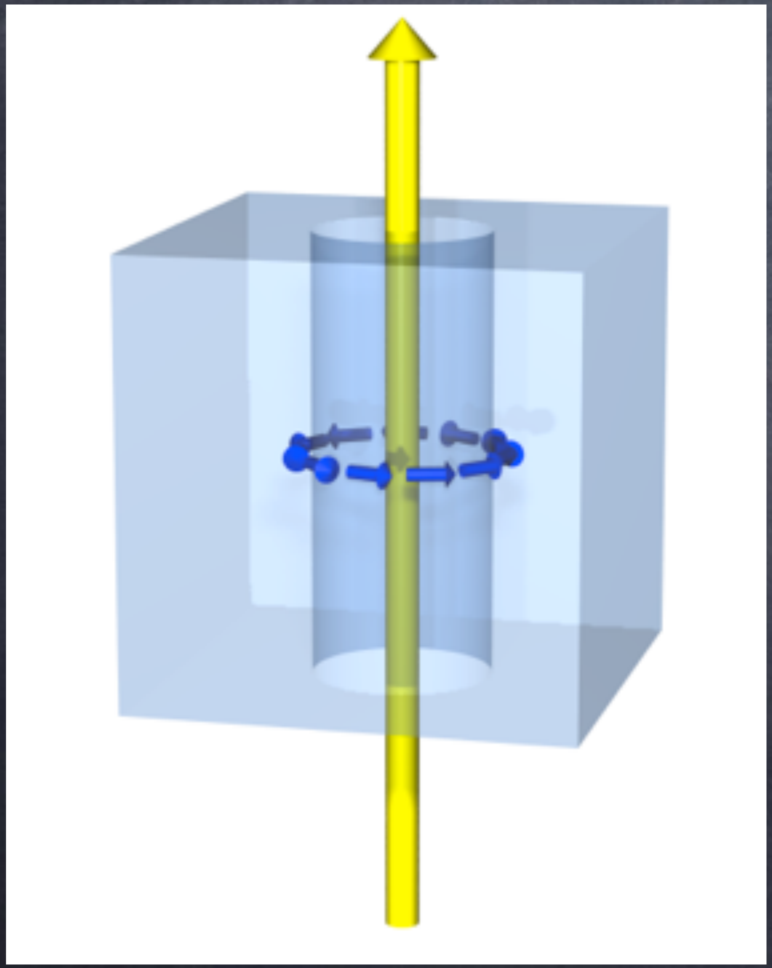


The surface charge implied by the Laughlin argument can escape through the bulk along the wormhole thus avoiding the fractional charge paradox.

Solve Dirac equation for the surface states along a hole threaded by flux

$$\mathcal{H} = \frac{1}{2} v \left[\hbar \nabla \cdot \mathbf{n} + \mathbf{n} \cdot (\mathbf{p} \times \sigma) + (\mathbf{p} \times \sigma) \cdot \mathbf{n} \right]$$

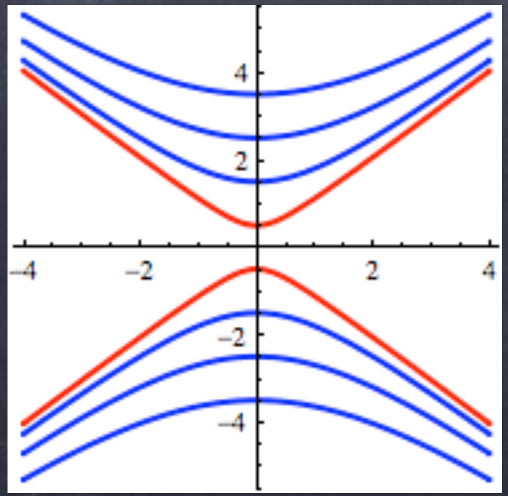
[see arXiv:0910.1338]



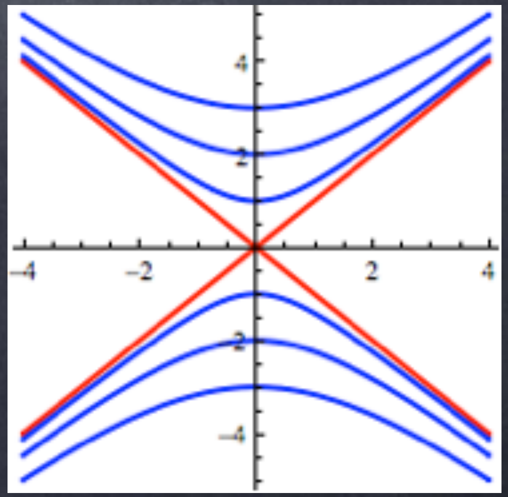
The spectrum is

$$E_{kl} = \pm v \hbar \sqrt{k^2 + \frac{(l + \frac{1}{2} - \eta)^2}{R^2}}; \quad \eta = \frac{\Phi}{\Phi_0}$$

$\eta \neq \frac{1}{2}$

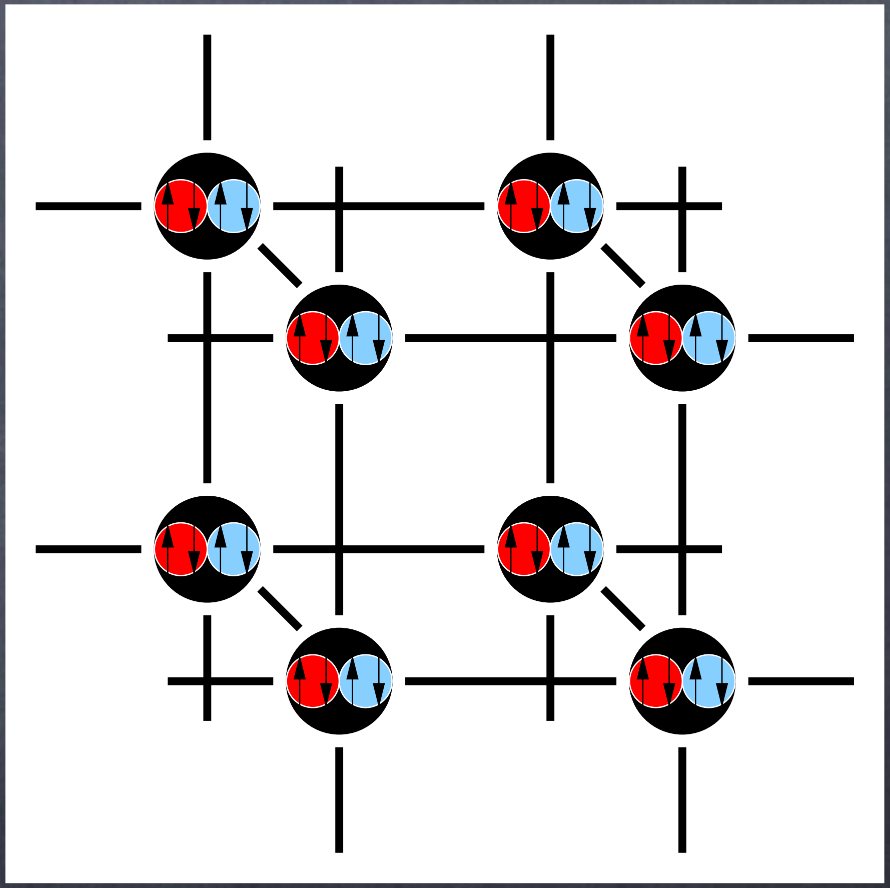


$\eta = \frac{1}{2}$



Lattice model for a topological insulator

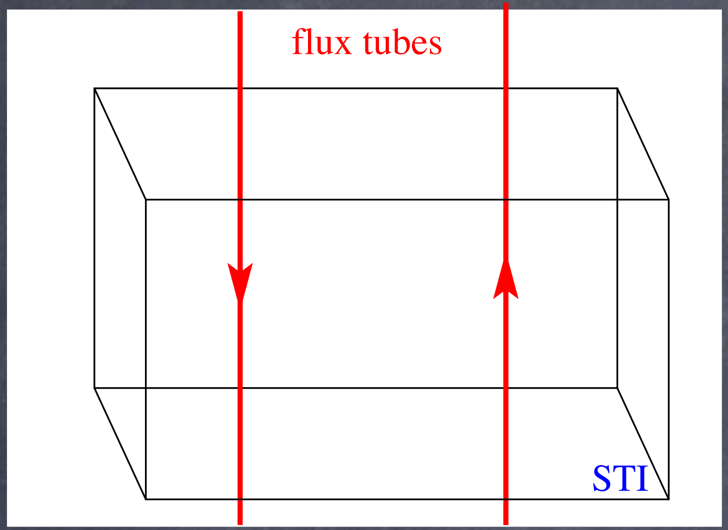
We consider a simple toy model for a topological insulator on the 3D cubic lattice. A minimal model will have 2 orbitals per lattice site

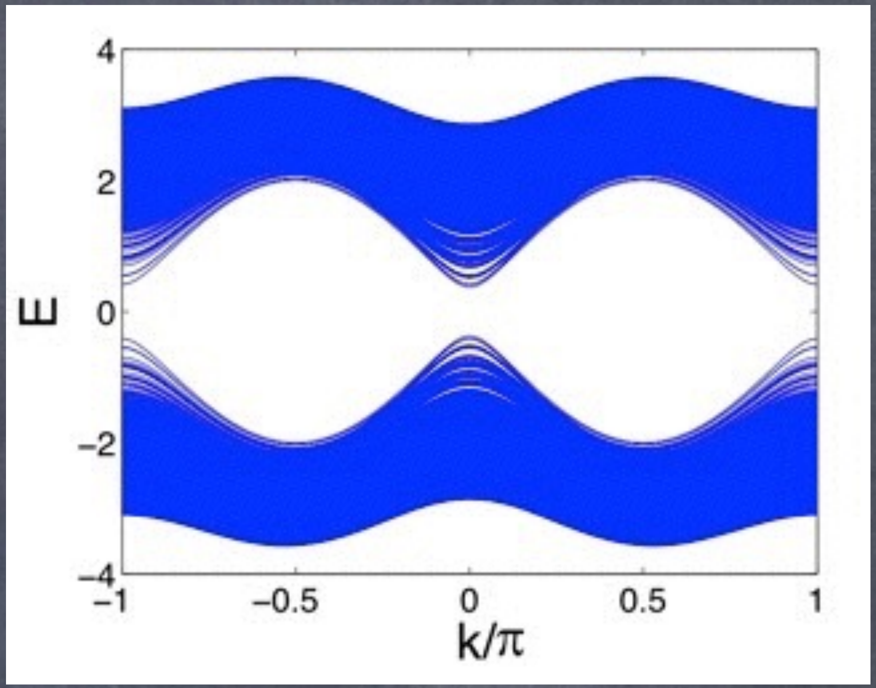


$$H_{\rm SO} = i\lambda \sum_{j,\mu} \Psi_j^\dagger \tau_z \sigma_\mu \Psi_{j+\mu} + \text{h.c.},$$

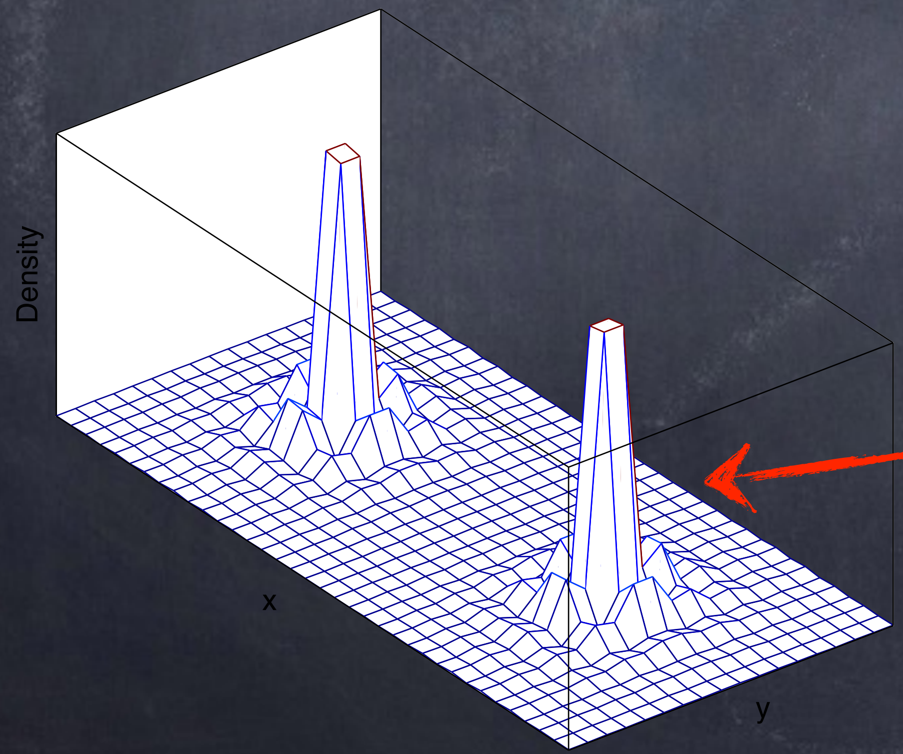
$$H_{cd} = \epsilon \sum_j \Psi_j^\dagger \tau_x \Psi_j - t \sum_{\langle ij \rangle} \Psi_i^\dagger \tau_x \Psi_j + \text{h.c.}$$

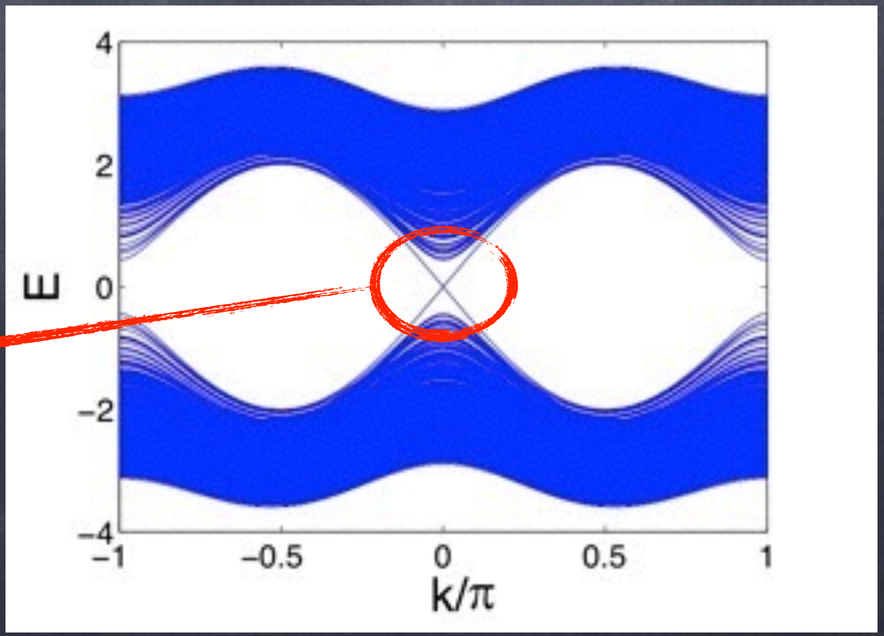
The Wormhole effect





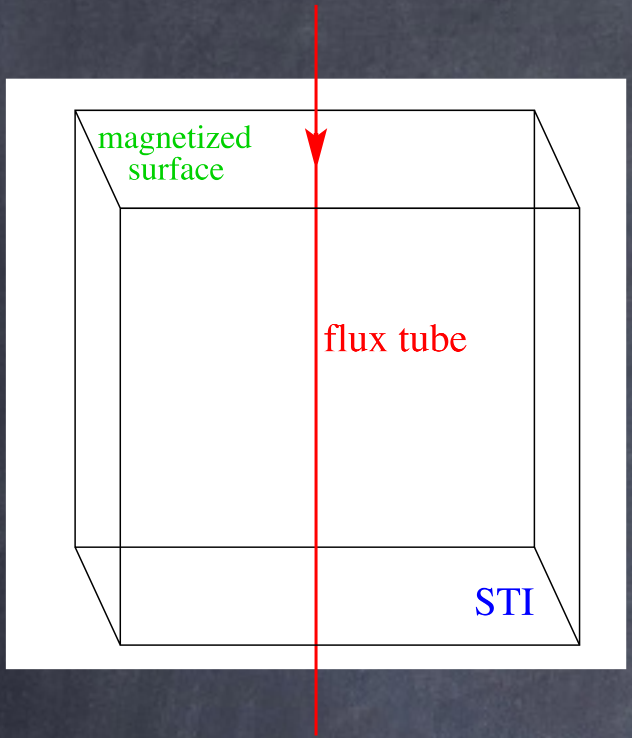
$$\Phi = \frac{\Phi_0}{4}$$



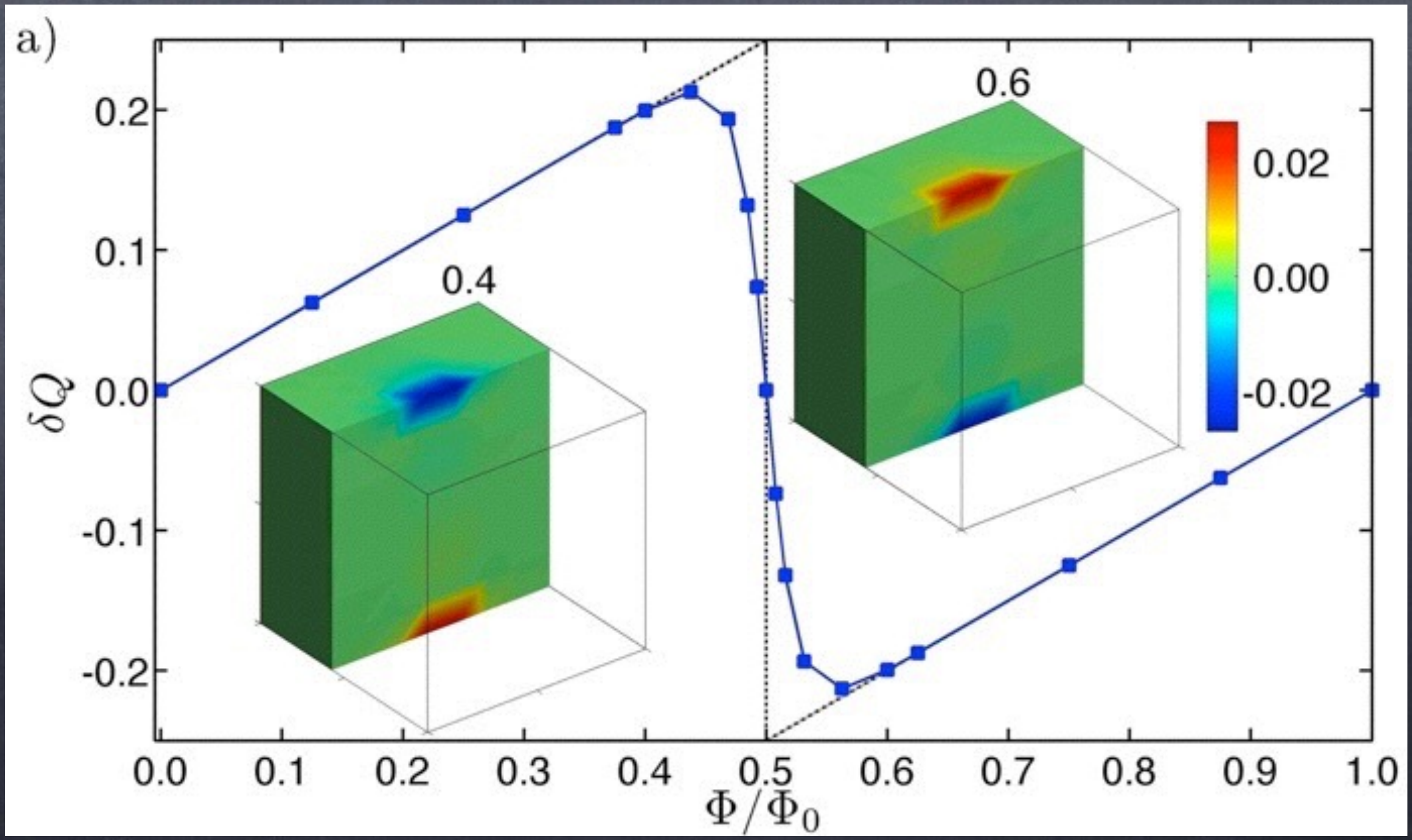


$$\Phi = \frac{\Phi_0}{2}$$

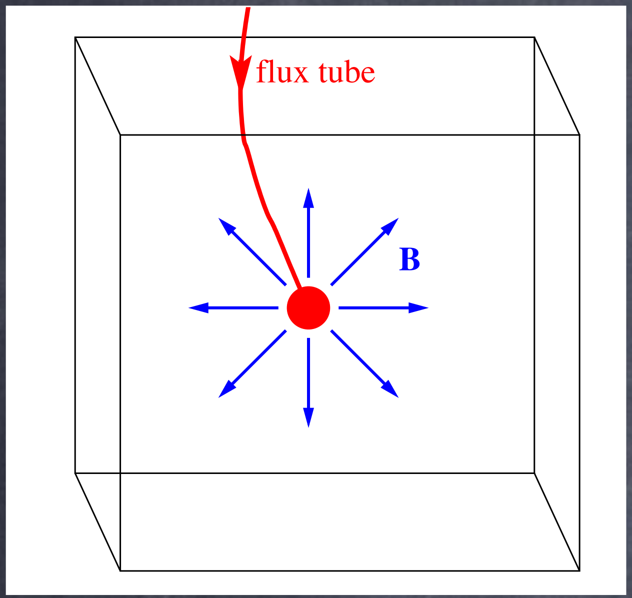
Cube with a magnetized surface



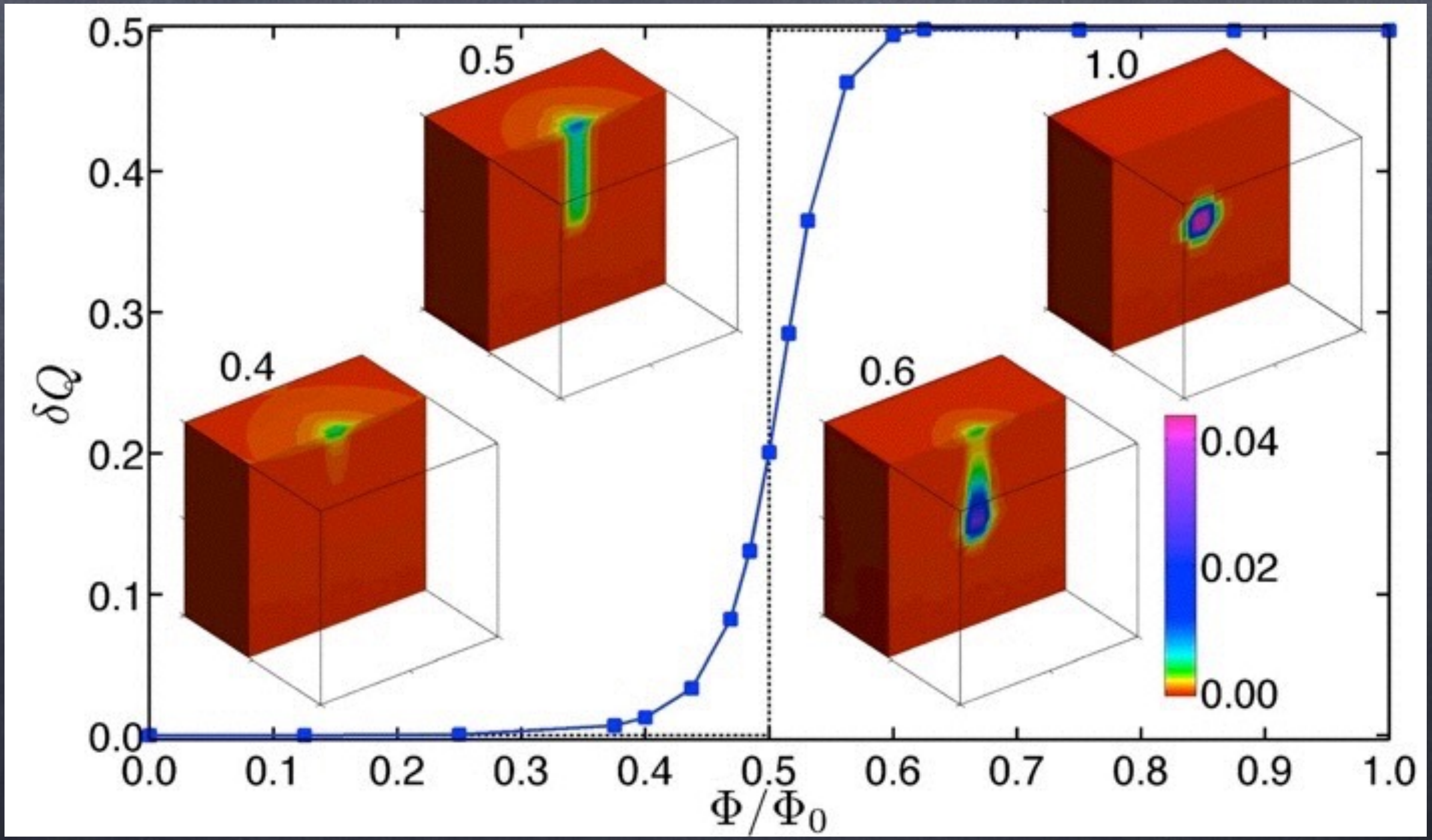
$$H_S = -\Omega_S \sum_{j \in \mathrm{surf}} \hat{\mathbf{r}}_j \cdot \left(\Psi_j^\dagger \sigma \Psi_j \right)$$



Different configuration: flux tube terminated by a magnetic monopole



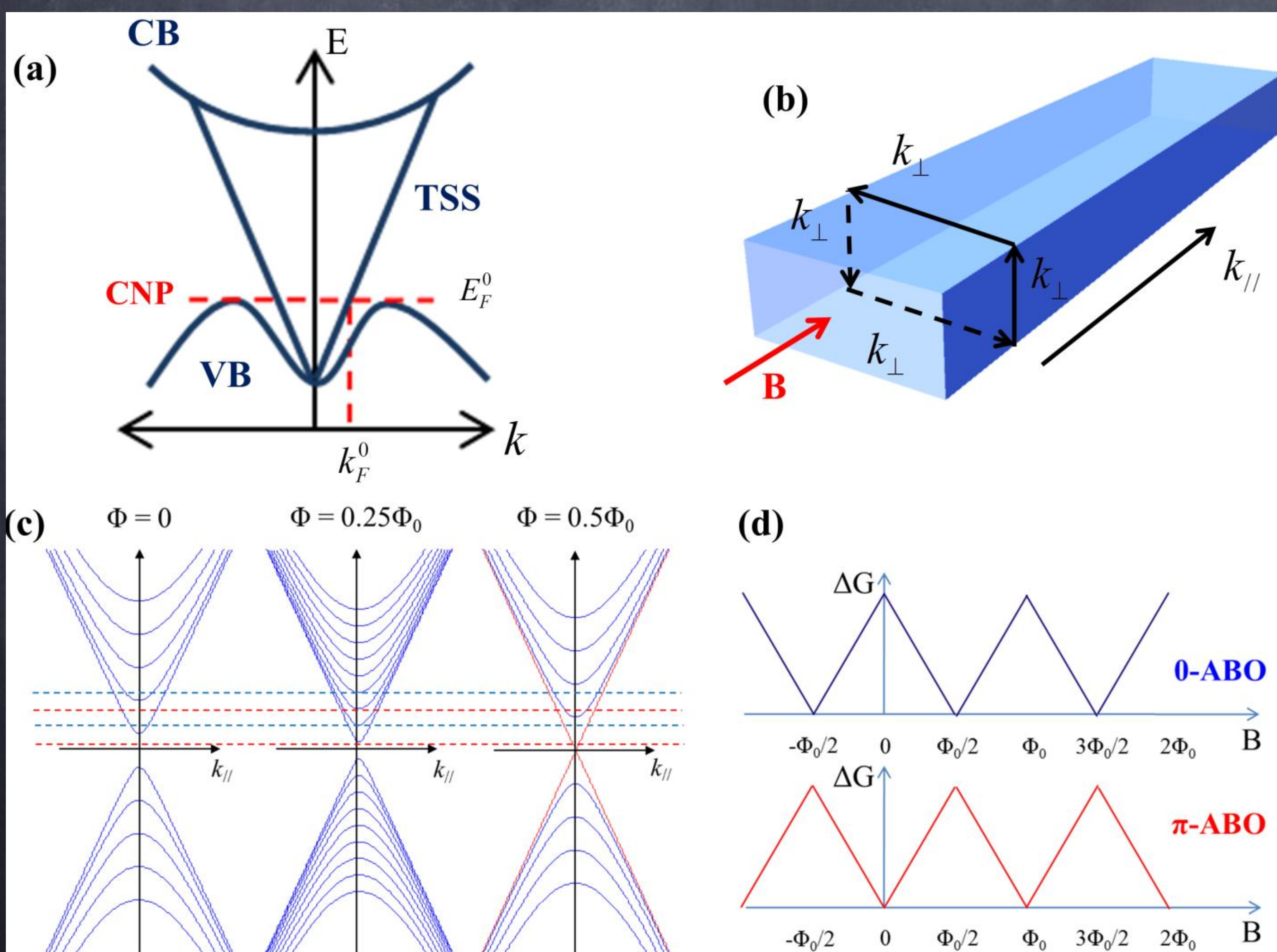
"Witten effect"

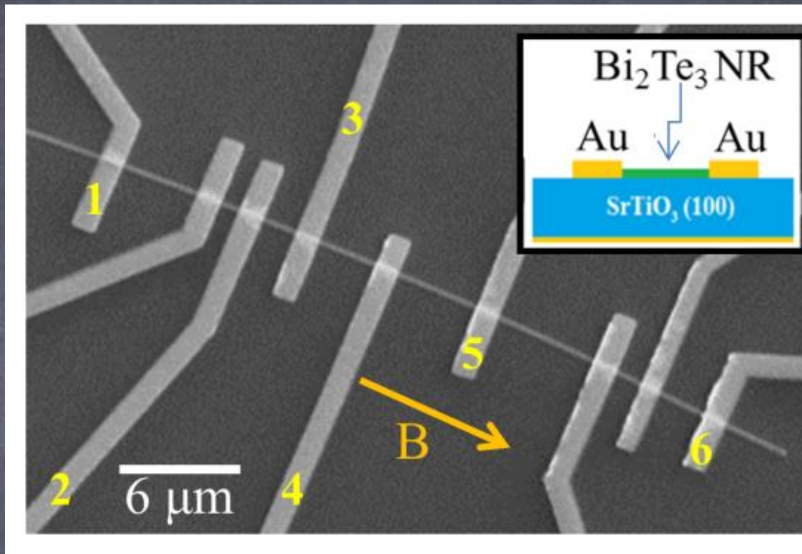


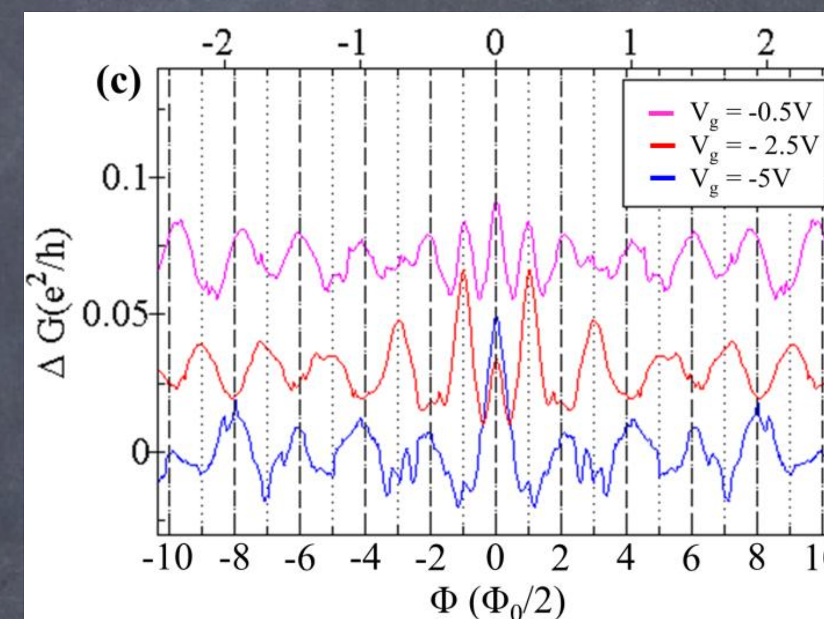
Experimental relevance:

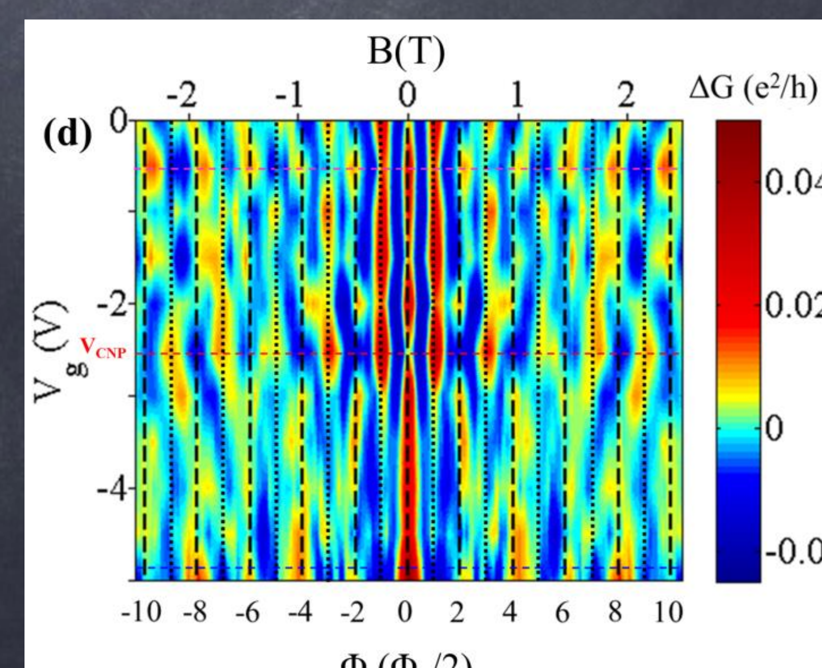
Magnetic field induced helical mode and topological transitions in a quasi-ballistic topological insulator nanoribbon with circumferentially quantized surface state sub-bands

Luis A. Jauregui[1,2], Michael T. Pettes[3,⊥], Leonid P. Rokhinson[4,1,2], Li Shi[3,5], Yong P. Chen[4,1,2,*]





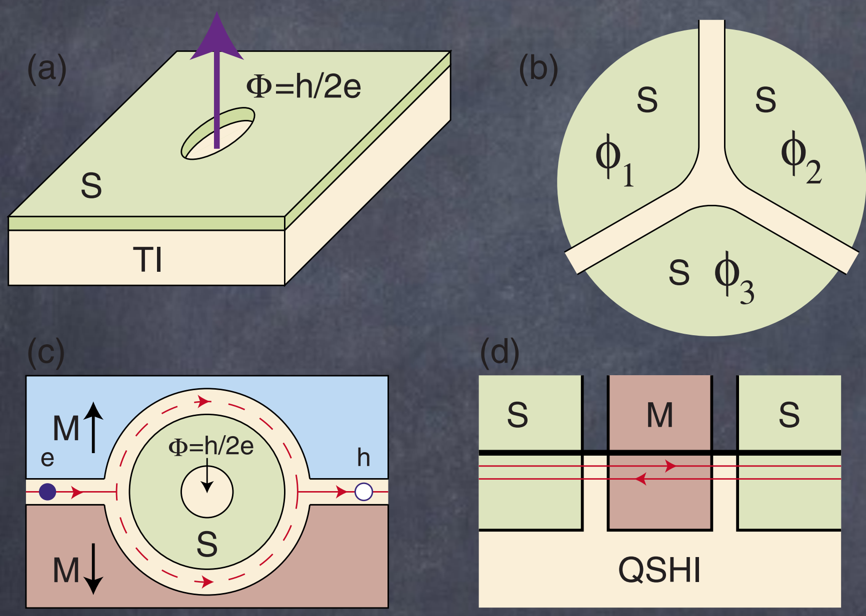




Exotic correlated surface states

Superconductivity

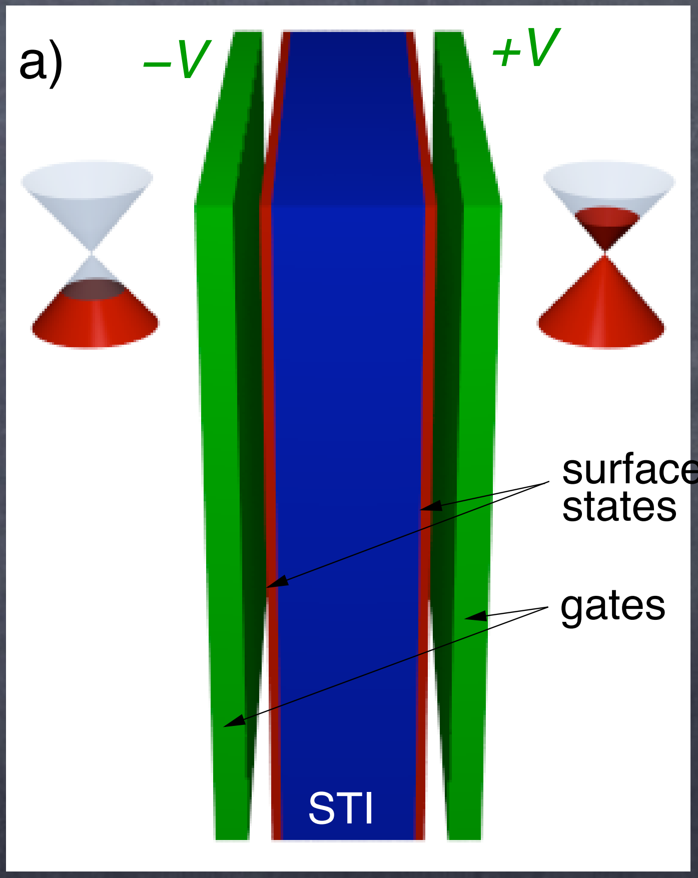
[Fu & Kane, PRL 2008]



Majorana fermions bound to vortices -> topological quantum computation

Exciton condensate

[Seradjeh, Moore & Franz, PRL 2009]



Fractional charge bound to vortices

Topological insulators: Closing Thoughts

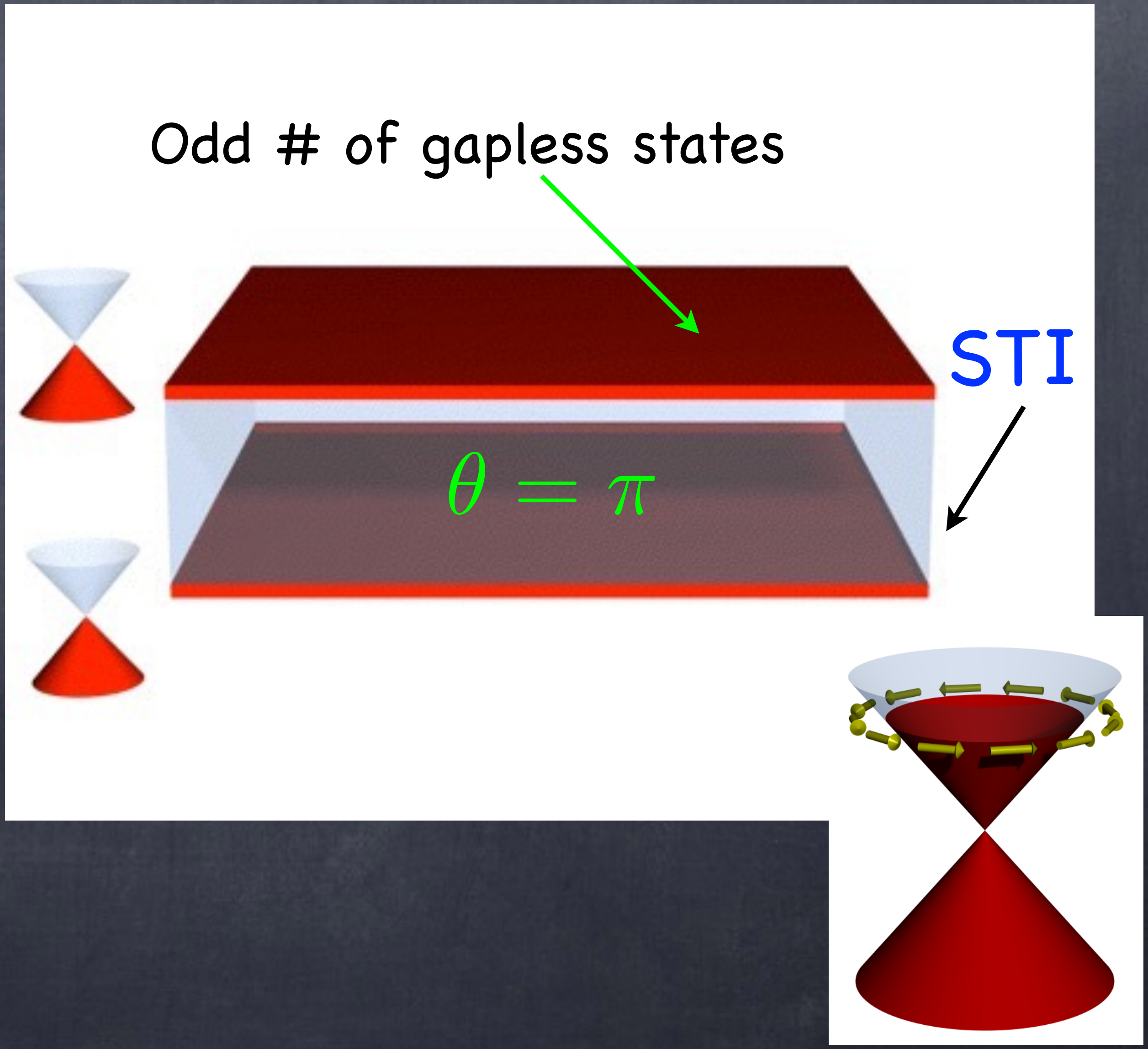
[For review see: Moore, Nature 2010; Hasan & Kane, Rev Mod Phys 2010]

- Time-reversal invariant band insulators with non-trivial band structure characterized by a Z_2-valued topological invariant.

- Topologically protected gapless surface states, robust to weak non-magnetic disorder.

- Variety of unusual surface phenomena: fractional quantum Hall effect, Majorana fermions, exciton condensate

- Axion term in the bulk electromagnetic response, Witten effect, wormhole effect, etc.



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