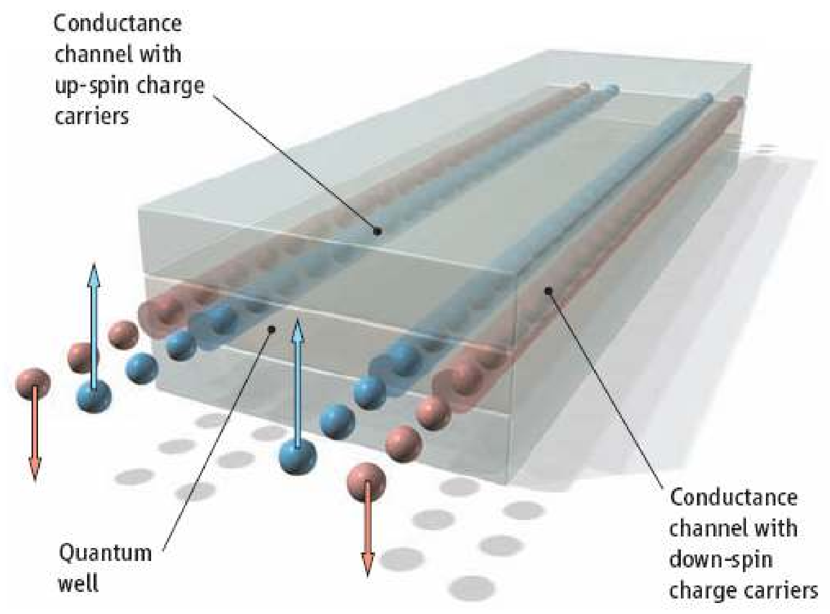
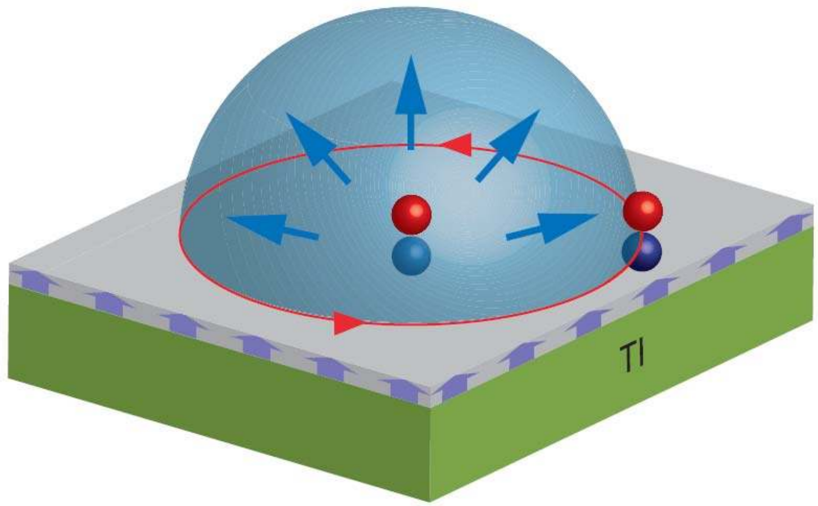
Topological Insulators and Superconductors





Tokyo 2010

Shoucheng Zhang, Stanford University

Colloborators

Stanford group: Xiaoliang Qi, Andrei Bernevig, Congjun Wu, Chaoxing Liu, Taylor Hughes, Sri Raghu, Suk-bum Chung

Stanford experimentalists: Yulin Chen, Ian Fisher, ZX Shen, Yi Cui, Aharon Kapitulnik, …

Wuerzburg colleagues: Laurens Molenkamp, Hartmut Buhmann, Markus Koenig Ewelina Hankiewicz, Bjoern Trauzettle

IOP colleagues: Zhong Fang, Xi Dai, Haijun Zhang, …

Tsinghua colleagues: Qikun Xue, Jinfeng Jia, Xi Chen,…

Outline

Models and materials of topological insulators

Topological field theory, experimental proposals

Topological Mott insulators

Topological superconductors and superfluids, experimental proposals

The search for new states of matter

The search for new elements led to a golden age of chemistry.

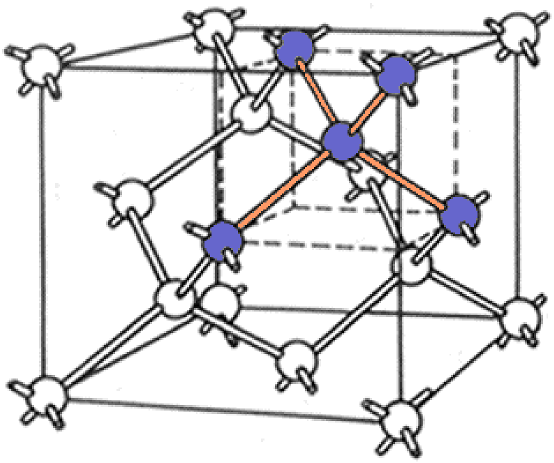
The search for new particles led to the golden age of particle physics.

In condensed matter physics, we ask what are the fundamental states of matter?

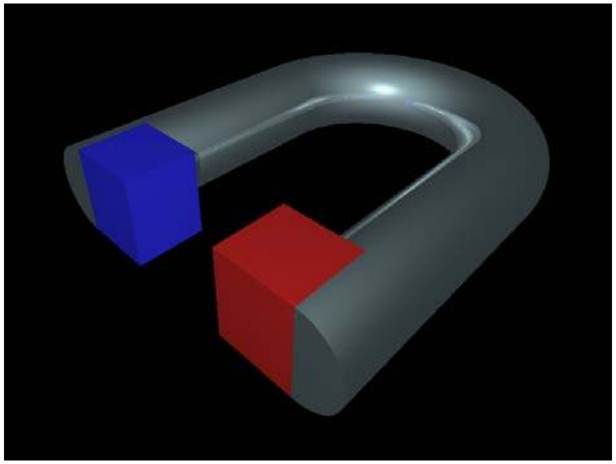
In the classical world we have solid, liquid and gas. The same H_2O molecules can condense into ice, water or vapor.

In the quantum world we have metals, insulators, superconductors, magnets etc.

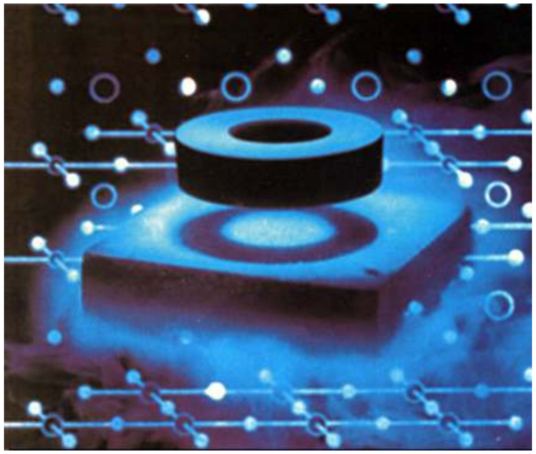
Most of these states are differentiated by the broken symmetry.



Crystal: Broken translational symmetry



Magnet: Broken rotational symmetry



Superconductor: Broken gauge symmetry

The quantum Hall state, a topologically non-trivial state of matter

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

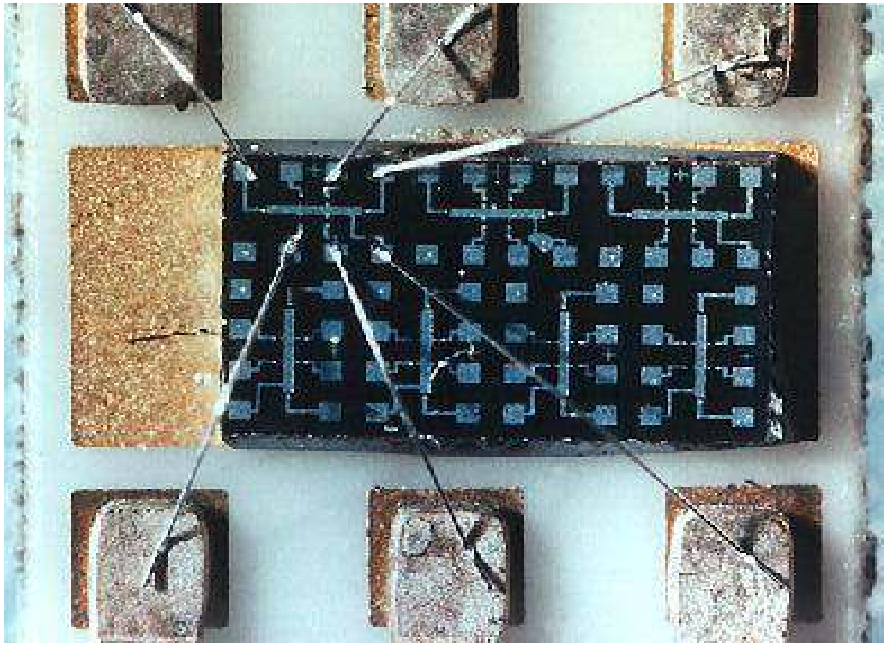
- TKNN integer= the first Chern number.

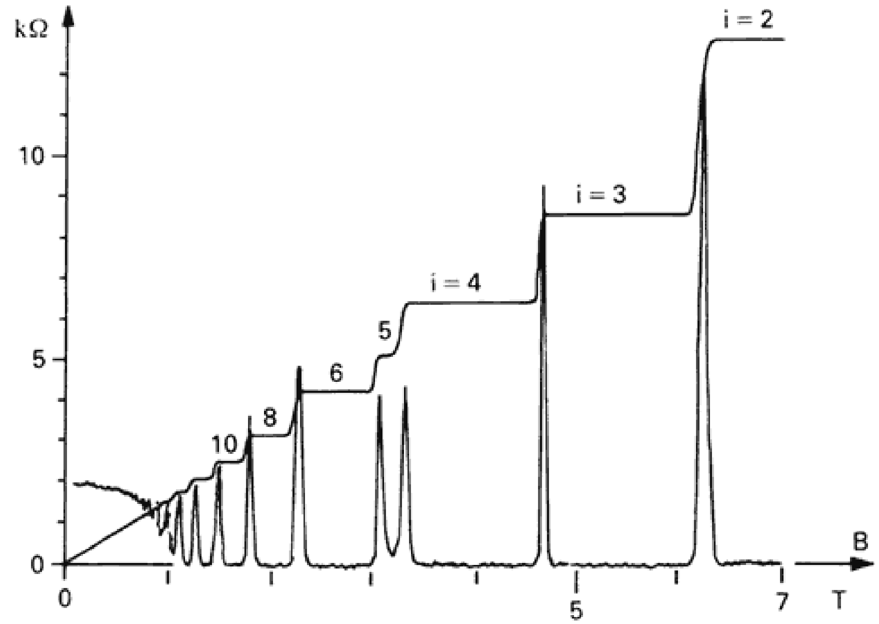
$$n = \int \frac{d^2k}{(2\pi)^2}\varepsilon^{\mu\nu}F_{\mu\nu}(k)$$

- Topological states of matter are defined and described by topological field theory:

$$S_{eff} = \frac{\sigma_{xy}}{2}\int d^2x dt \varepsilon^{\mu\nu\rho}A_\mu \partial_\nu A_\rho$$

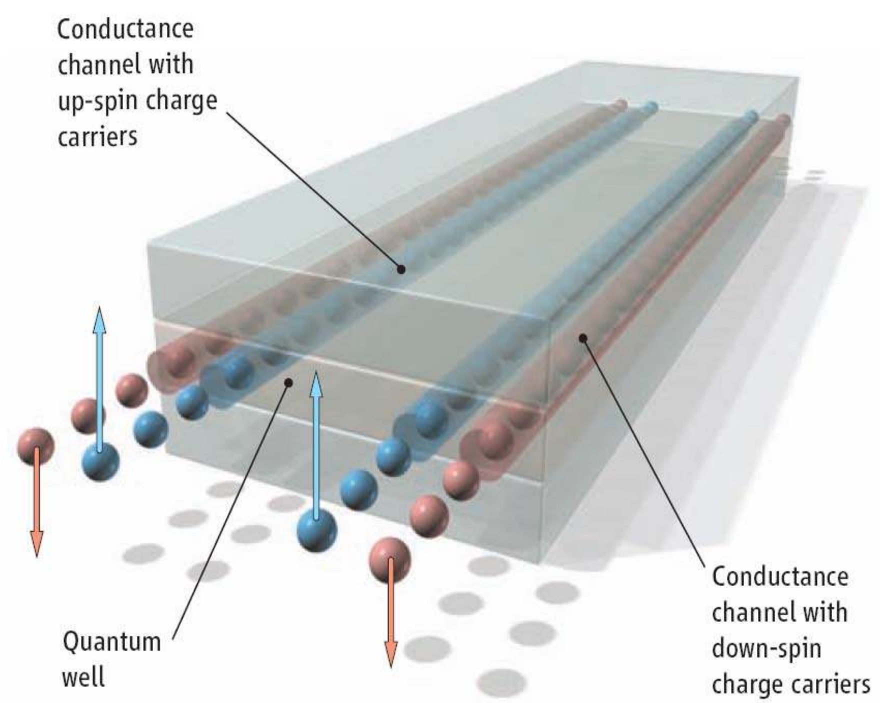
- Physically measurable topological properties are all contained in the topological field theory, e.g. QHE, fractional charge, fractional statistics etc…



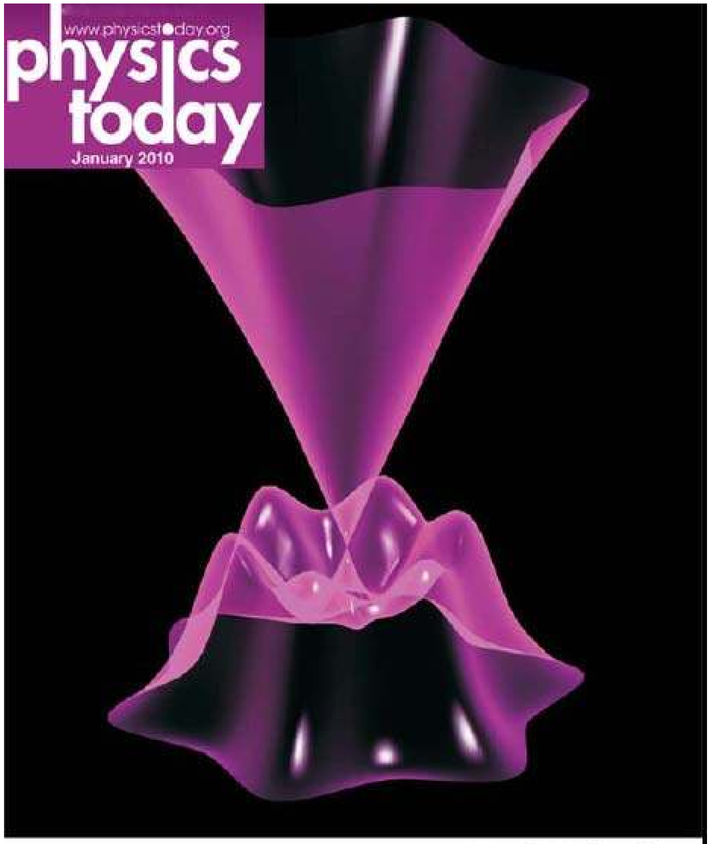


Discovery of the 2D and 3D topological insulator

HgTe Theory: Bernevig, Hughes and Zhang, Science **314**, 1757 (2006)
Experiment: Koenig et al, Science **318**, 766 (2007)
BiSb Theory: Fu and Kane, PRB **76**, 045302 (2007)
Experiment: Hsieh et al, Nature **452**, 907 (2008)
Bi2Te3, Sb2Te3, Bi2Se3 Theory: Zhang et al, Nature Physics 5, 438 (2009)
Theory and Experiment Bi2Se3: Xia et al, Nature Physics 5, 398 (2009),
Experiment BieTe3: Chen et al Science 325, 178 (2009)



Schematic of the spin-polarized edge channels in a quantum spin Hall insulator.



Topological insulators

Topological Insulator is a New State of Quantum Matter

Breakthrough of the Year

6 **ELECTRONS TAKE A NEW SPIN.** Chalk one up for the theorists. Theoretical physicists in California recently predicted that semiconductor sandwiches with thin layers of mercury telluride (HgTe) in the middle should exhibit an unusual behavior of their electrons called the quantum spin Hall effect (QSHE). This year, they teamed up with experimental physicists in Germany and found just what they were looking for.

PHYSICS

A New State of Quantum Matter

Experiments show that electron spins can flow without dissipation in a novel electrical insulator.

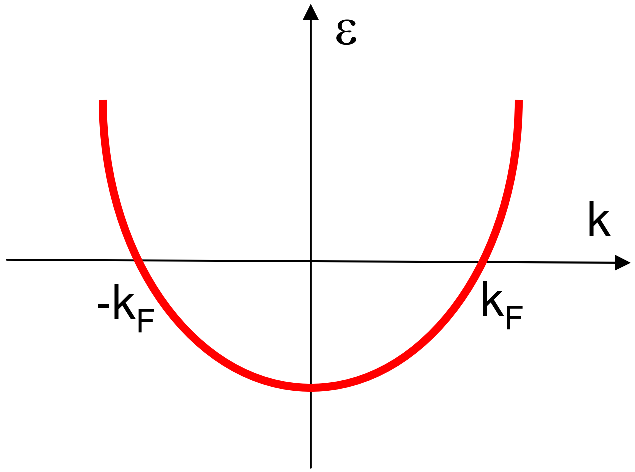
Naoto Nagaosa

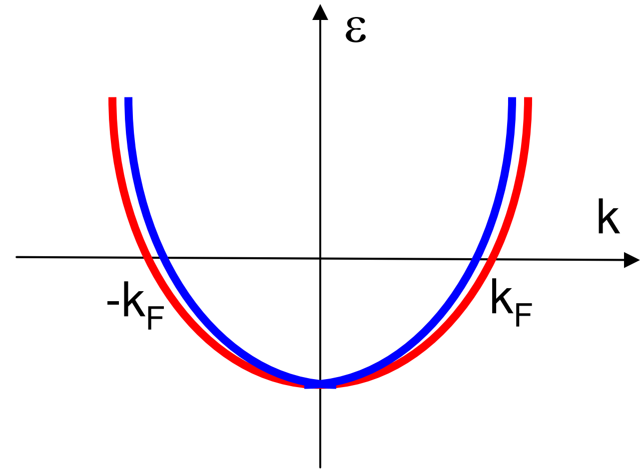
search & discovery

Quantum spin Hall effect shows up in a quantum well insulator, just as predicted

The effect, which occurs without a magnetic field, is a new and topologically distinct electronic state.

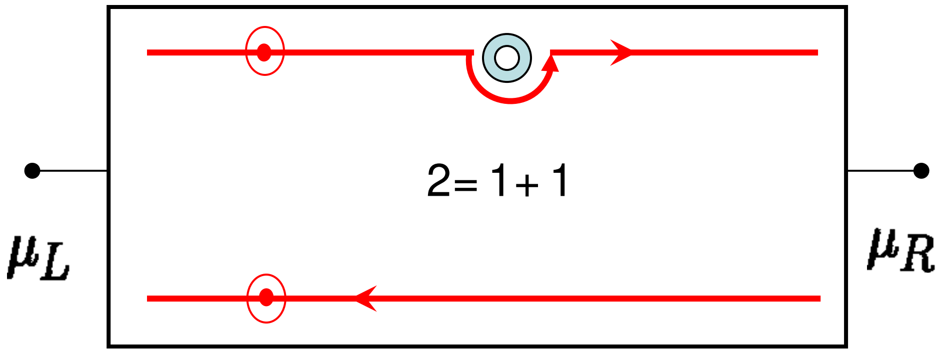
Chiral (QHE) and helical (QSHE) liquids in D= 1

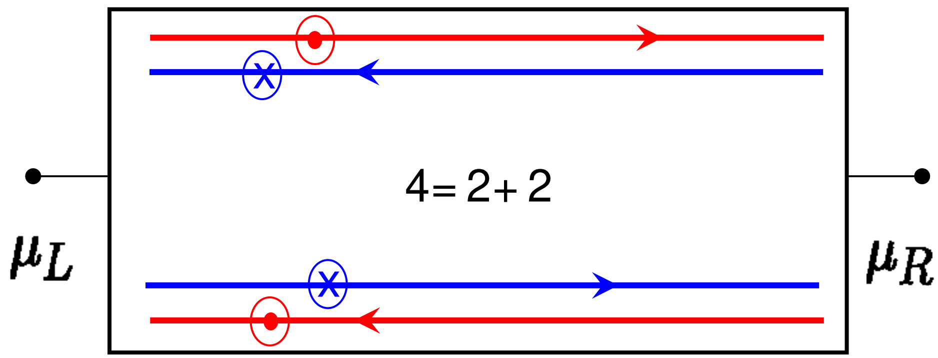




The QHE state spatially separates the two chiral states of a spinless 1D liquid

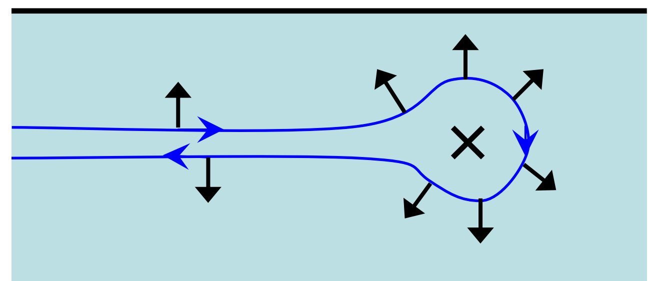
The QSHE state spatially separates the four chiral states of a spinful 1D liquid

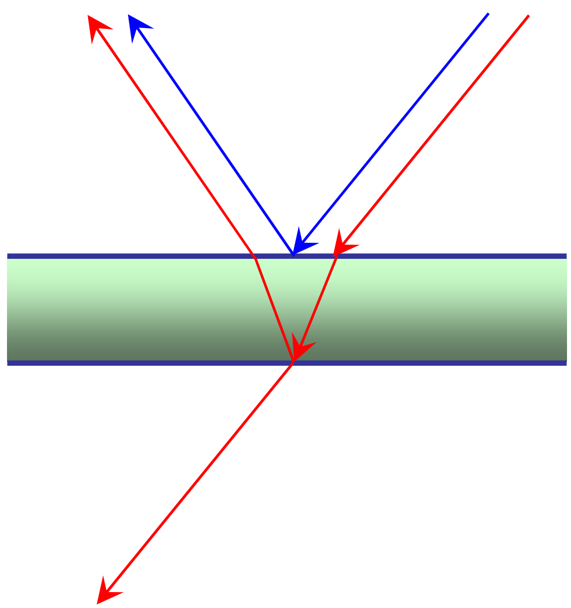


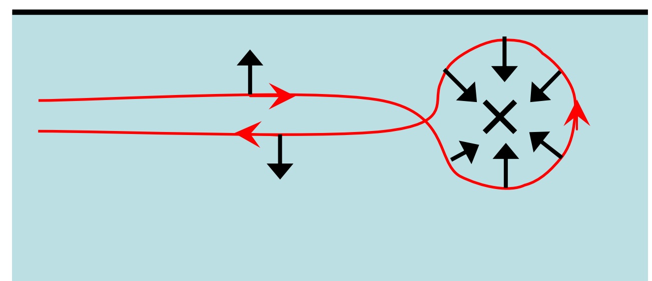


Kane and Mele (without Landau levels)
Benervig and Zhang (with Landau levels)

Quantum protection by $T^2 = -1$ (Qi&Zhang, Phys Today, Jan, 2010)







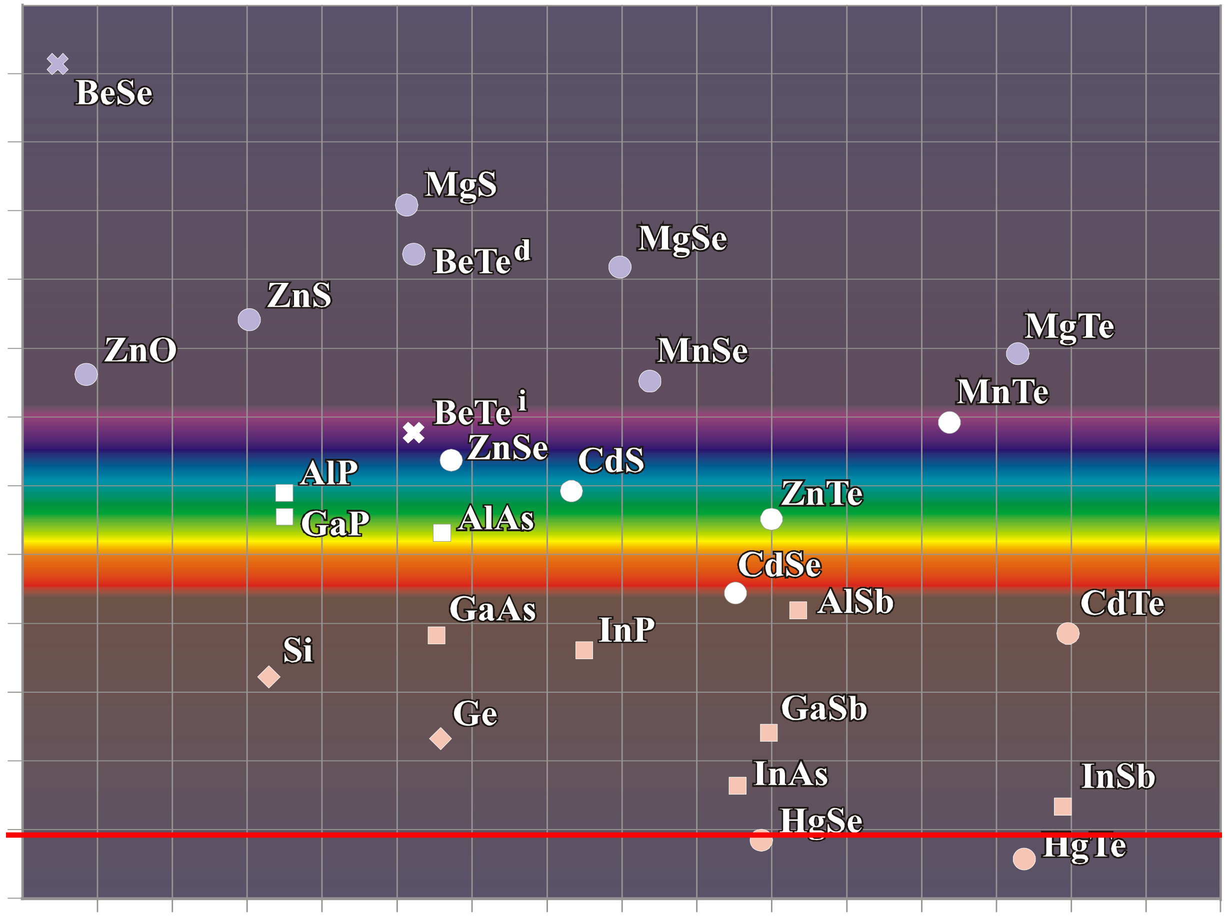
Transport experiments:
Molenkamp group
STM experiments:
Yazdani group, Kapitulnik group, Xue group

From topology to chemistry: the search for the QSH state

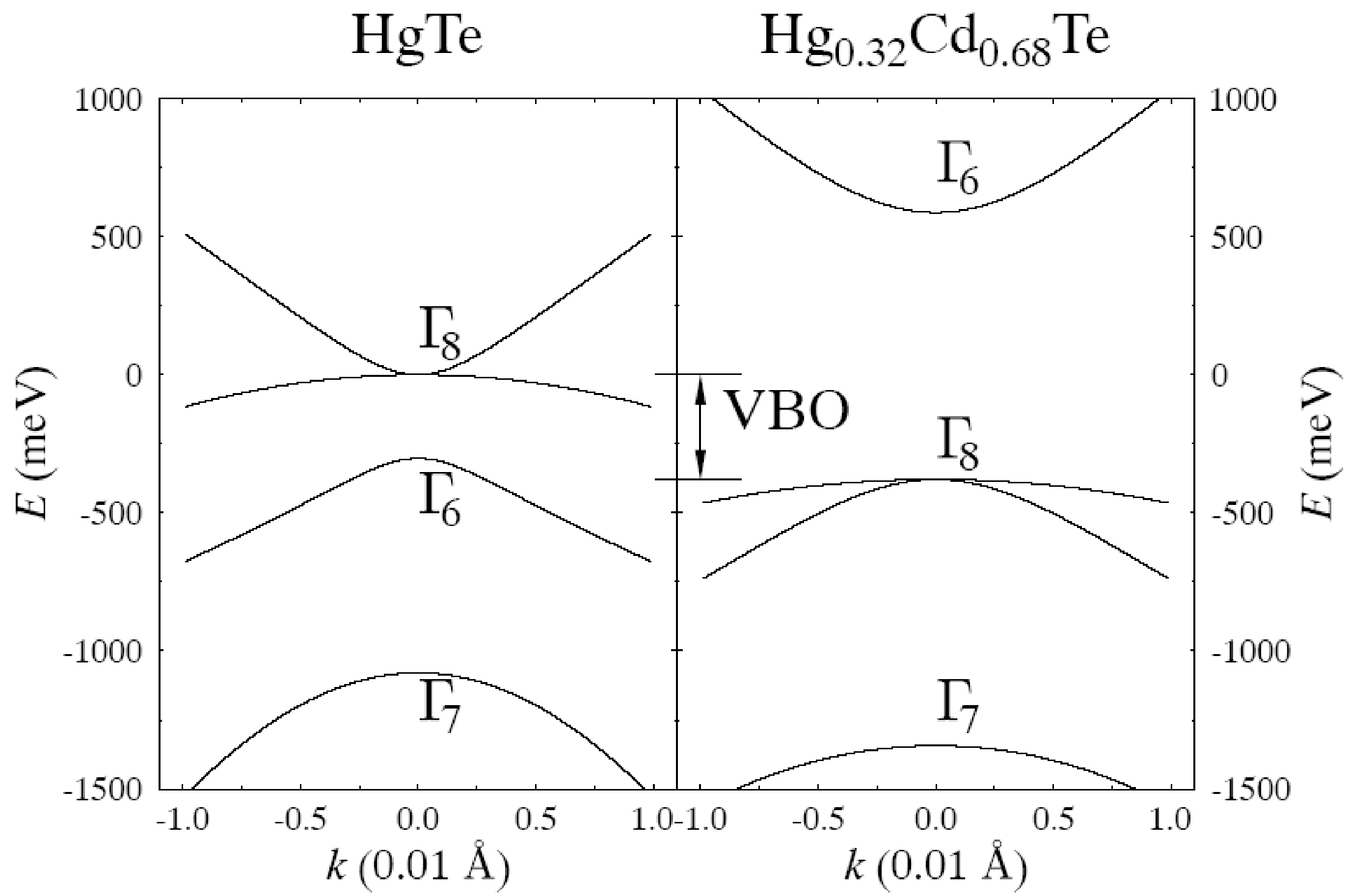
- Type III quantum wells work. HgTe has a negative band gap! (Bernevig, Hughes and Zhang, Science 2006)

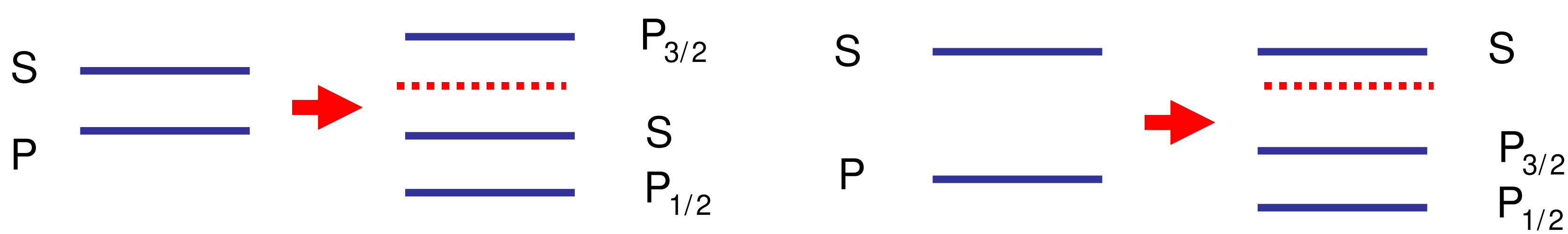
- Tuning the thickness of the HgTe/CdTe quantum well leads to a topological quantum phase transition into the QSH state.

- Sign of the Dirac mass term determines the topological term in field theory



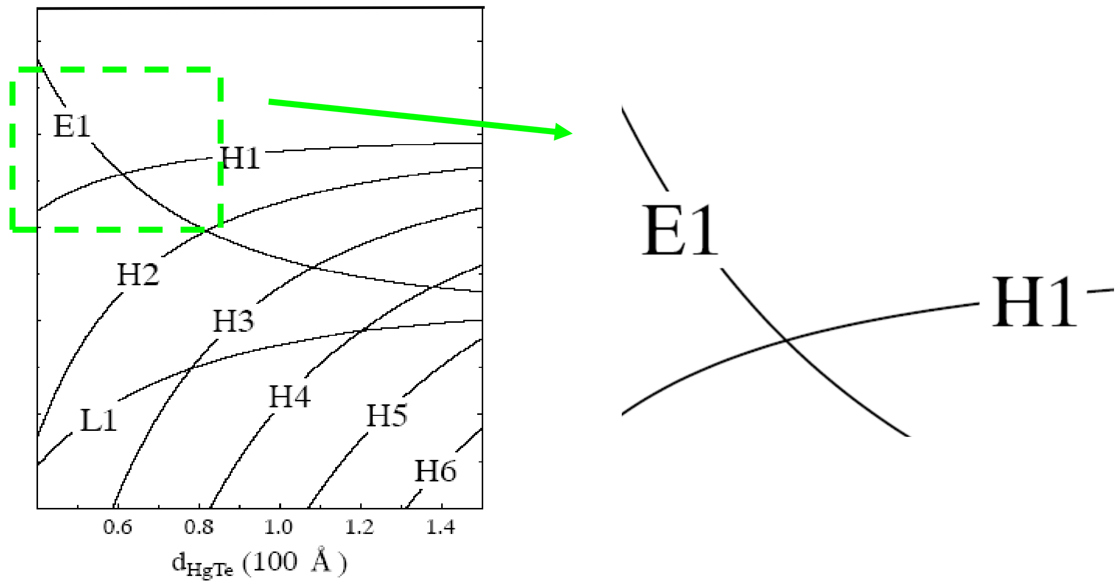
Band Structure of HgTe

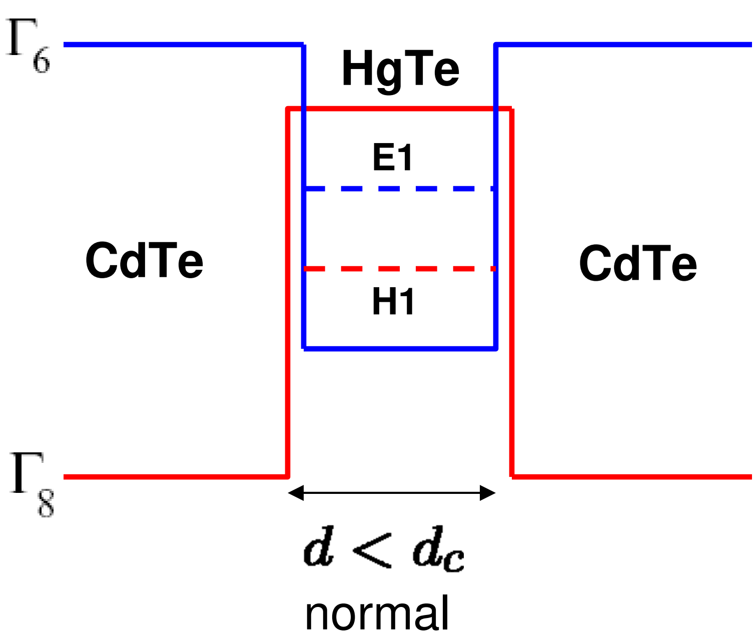


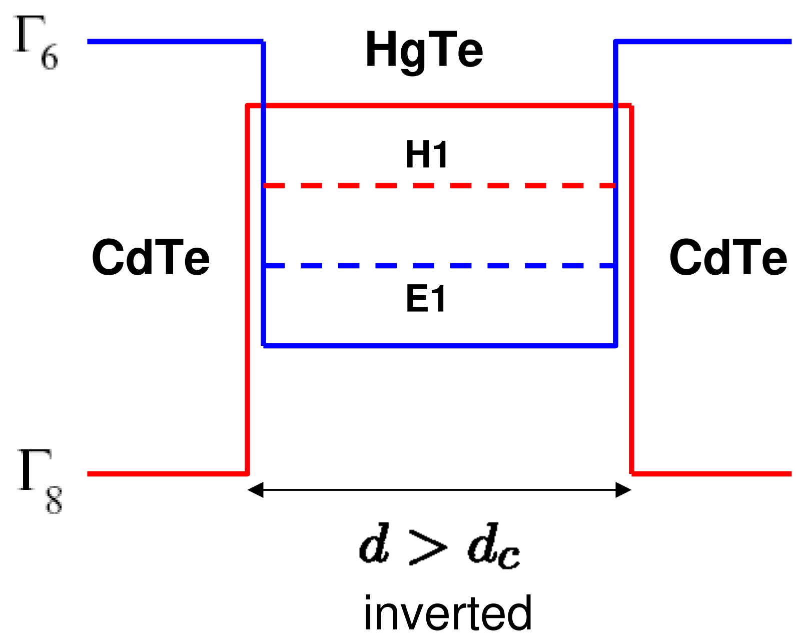


Band inversion in HgTe leads to a topological quantum phase transition

Let us focus on E1, H1 bands close to crossing point



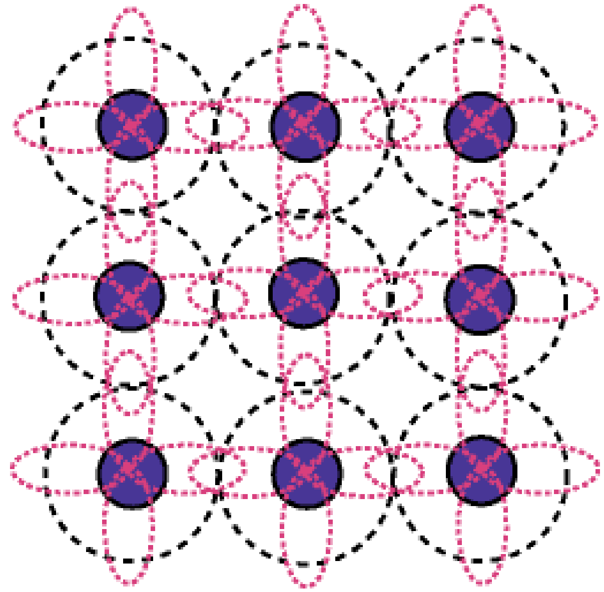




The model of the 2D topological insulator (BHZ, Science 2006)

Square lattice with 4-orbitals per site:

$$|s,\uparrow\rangle, |s,\downarrow\rangle, |(p_x + ip_y),\uparrow\rangle, |-(p_x - ip_y),\downarrow\rangle$$



Nearest neighbor hopping integrals. Mixing matrix elements between the s and the p states must be odd in k.

$$H_{eff}(k_x, k_y) = \begin{pmatrix} h(k) & 0 \\ 0 & h^*(-k) \end{pmatrix}$$

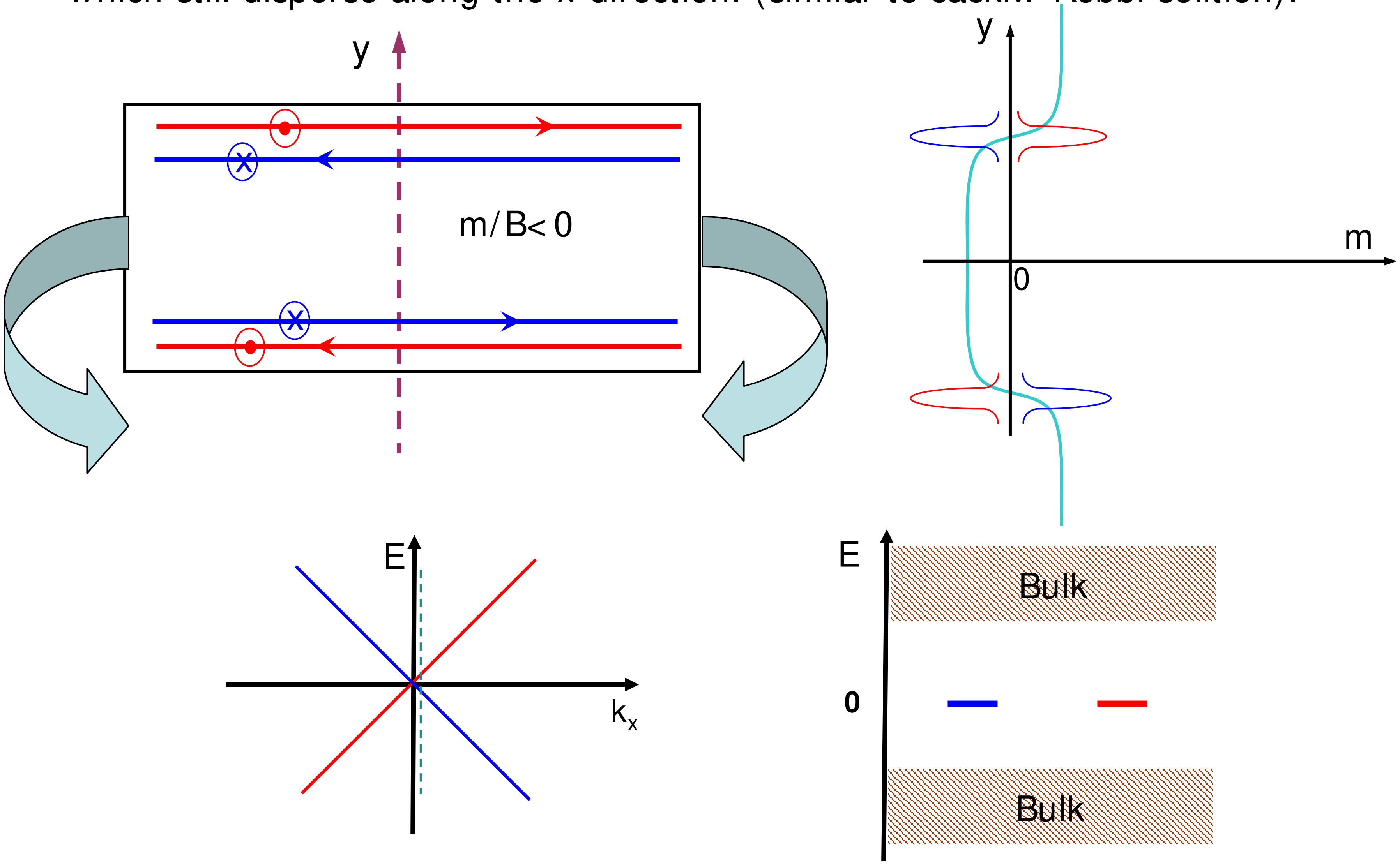
$$h(k) = \begin{pmatrix} m(k) & A(\sin k_x - i \sin k_y) \\ A(\sin k_x + i \sin k_y) & -m(k) \end{pmatrix} \equiv d_a(k)\tau^a$$

$$\Rightarrow \begin{pmatrix} m + Bk^2 & A(k_x - ik_y) \\ A(k_x + ik_y) & -m - Bk^2 \end{pmatrix}$$

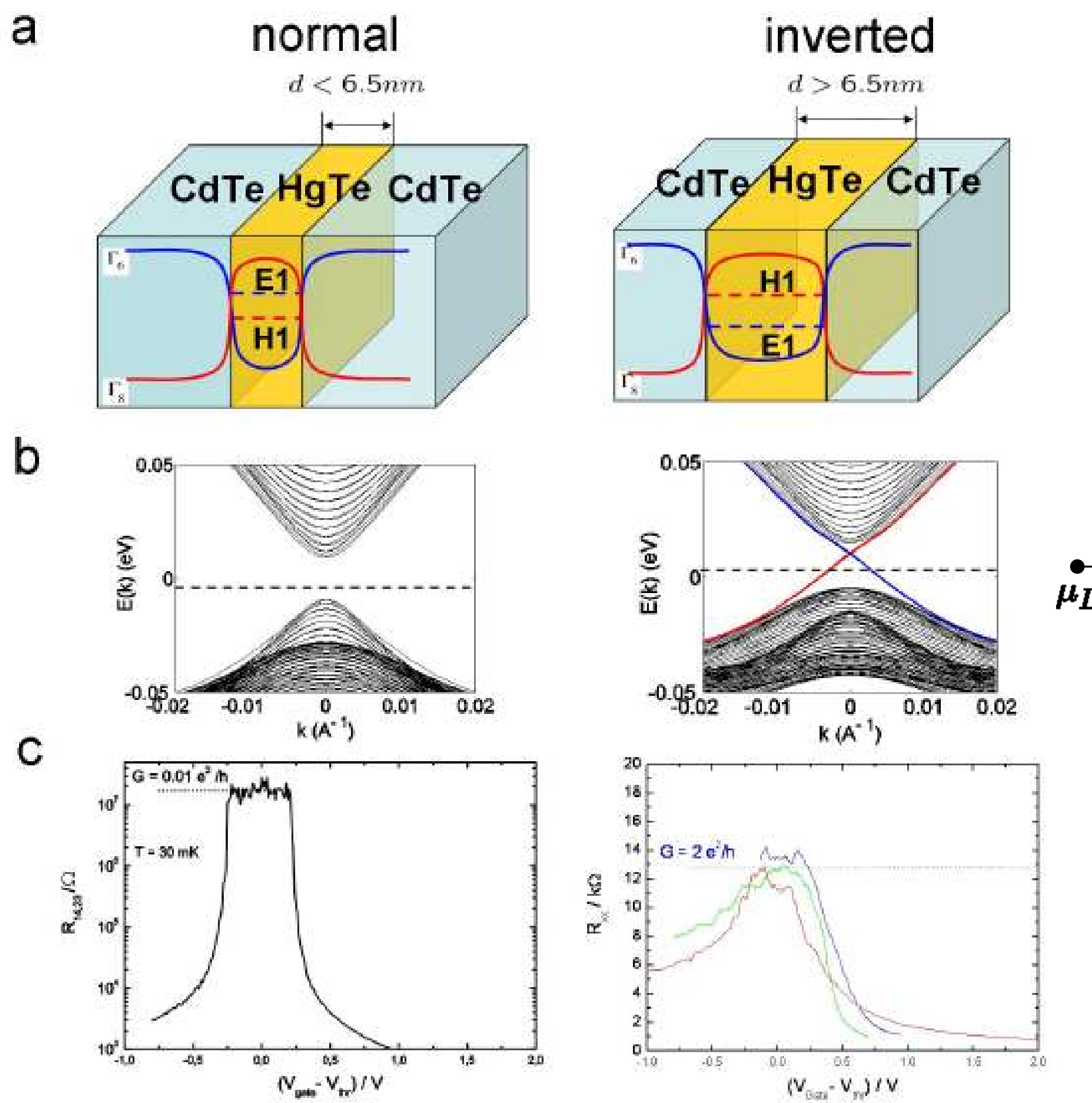
Similar to relativistic Dirac equation in 2+1 dimensions, with a mass term tunable by the sample thickness d! m/B<0 for d>d_c.

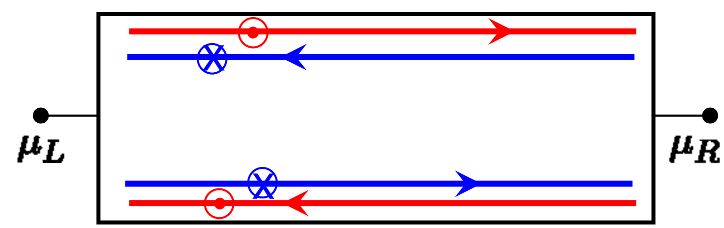
Mass domain wall

Cutting the Hall bar along the y-direction we see a domain-wall structure in the band structure mass term. This leads to states localized on the domain wall which still disperse along the x-direction. (similar to Jackiw-Rebbi solition).

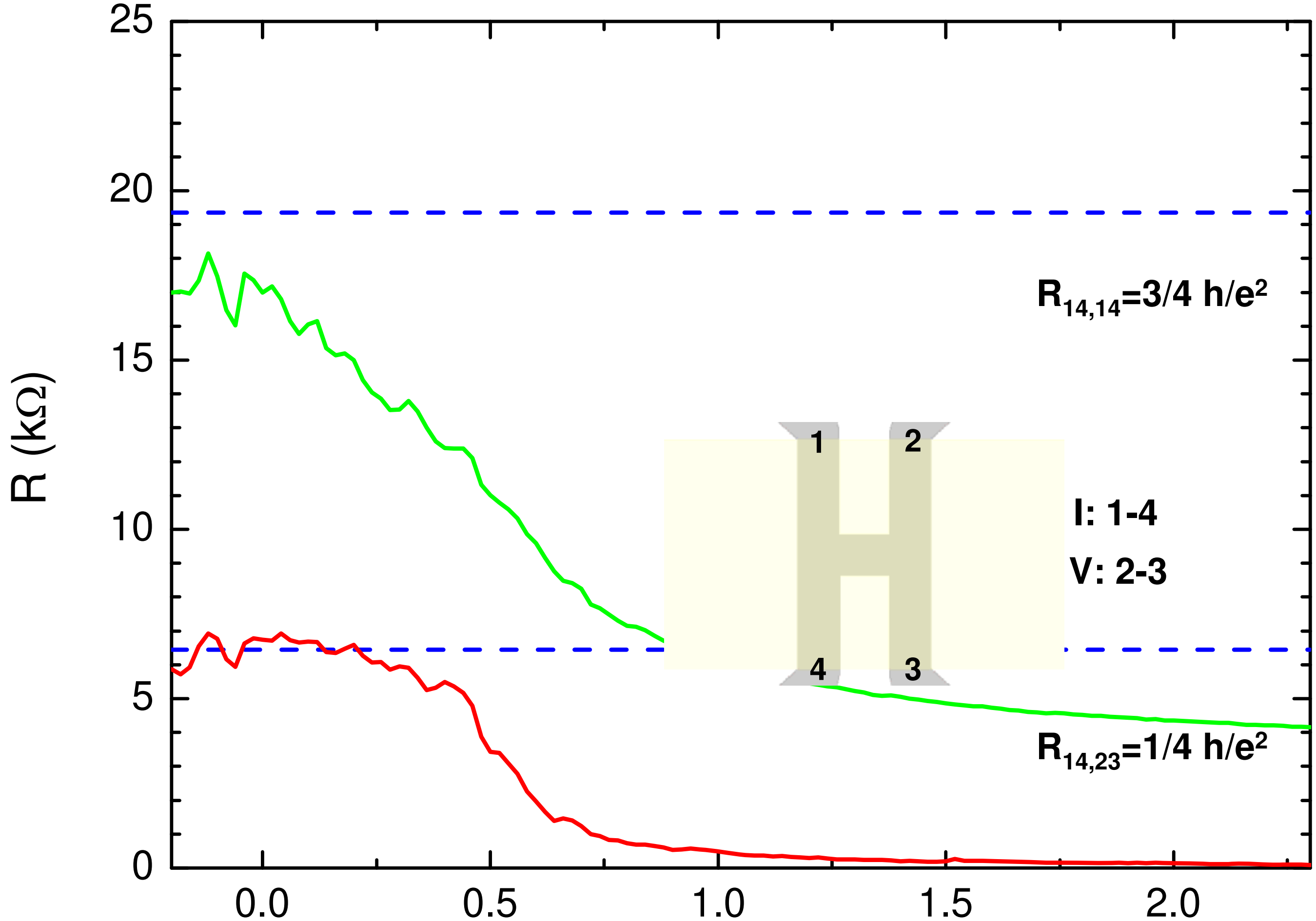


Experimental observation of the QSH edge state
(Konig et al, Science 2007)





Nonlocal transport in the QSH regime, (Roth et al Science 2009)



PHYSICS

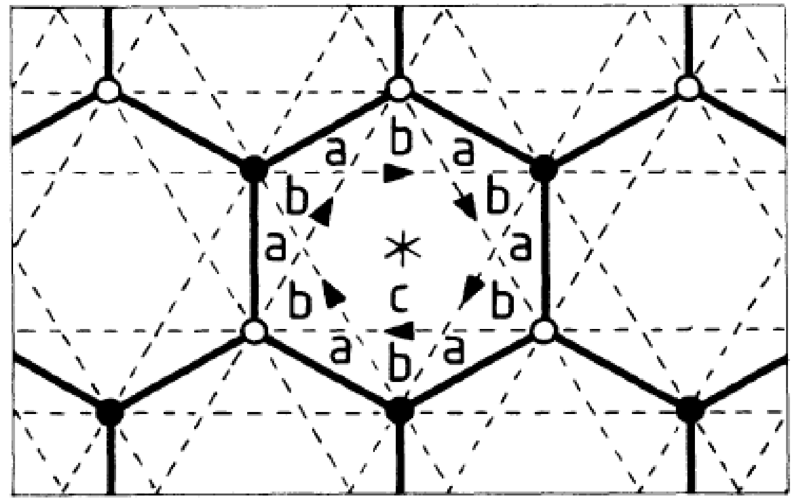
Edge-State Physics Without Magnetic Fields

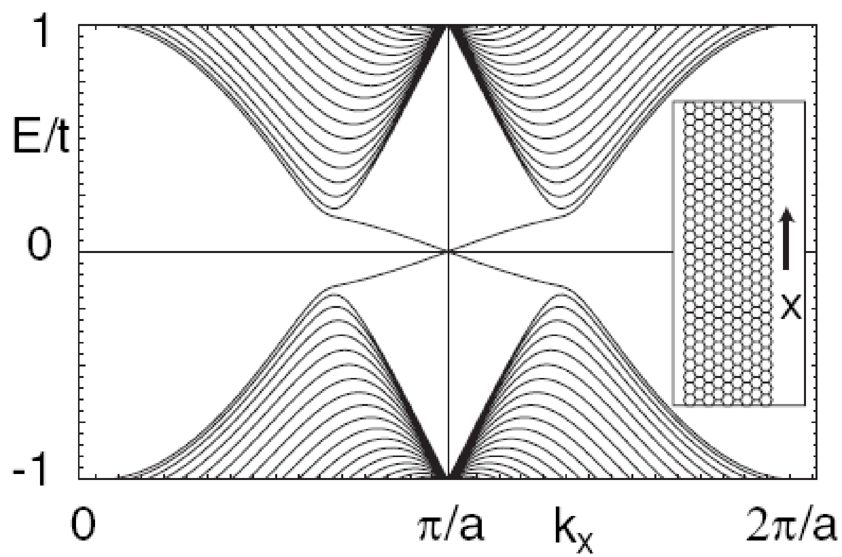
A novel class of materials called topological insulators allows spin physics to be probed without the need for magnetic fields.

Markus Büttiker

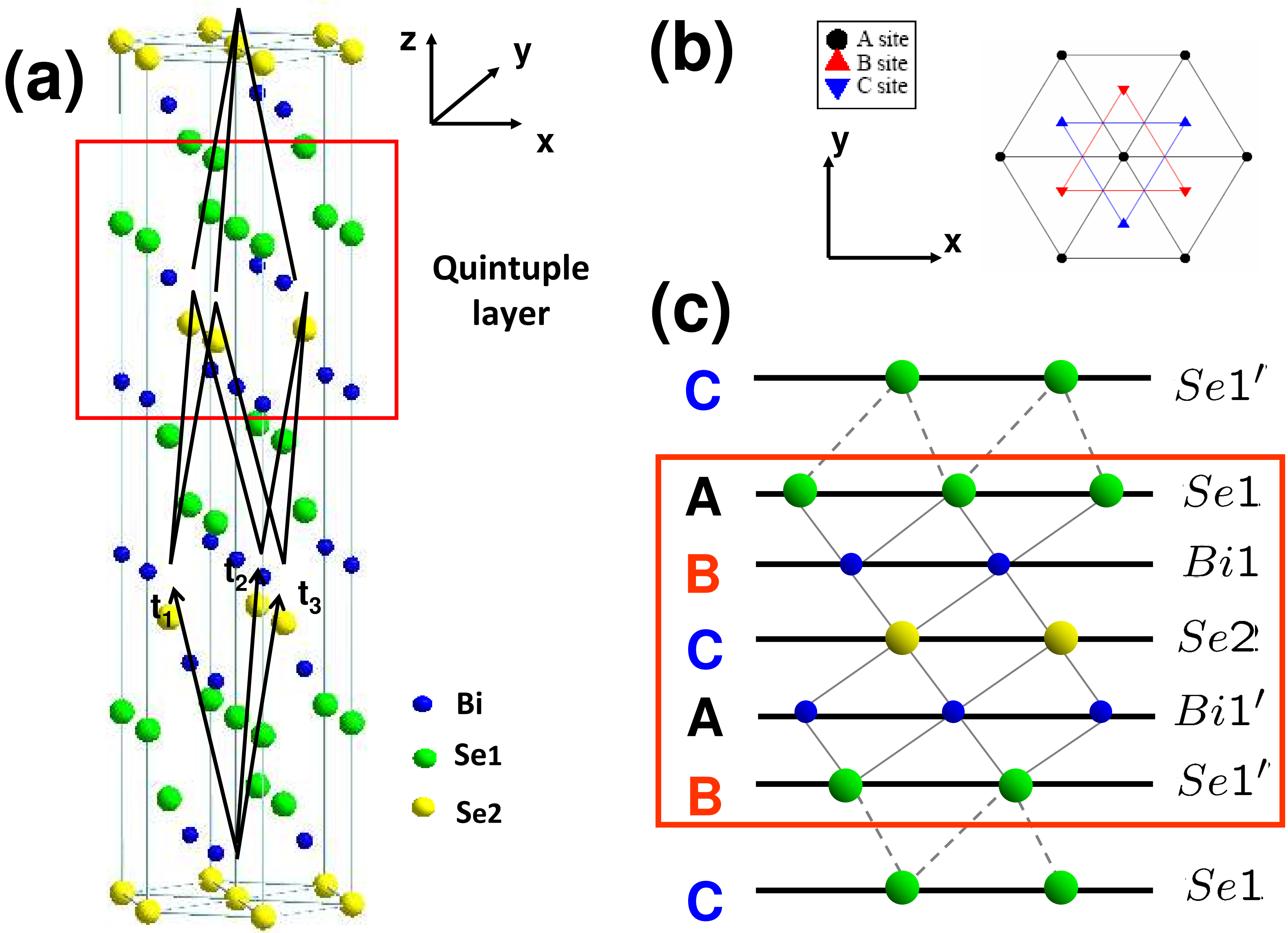
No QSH in graphene

- Bond current model on honeycomb lattice (Haldane, PRL 1988).
- Spin Hall insulator (Murakami, Nagaosa and Zhang 2004)
- Spin-orbit coupling in graphene (Kane and Mele 2005). They took atomic spin-orbit coupling of 5meV to estimate the size of the gap.
- Yao et al, Min et al 2006 showed that the actual spin-orbit gap is given by $\Delta^2_{so}/\Delta_{\pi\sigma} = 10^{-3}$ meV.
- Similar to the seasaw mechanism of the neutrino mass in the Standard Model!

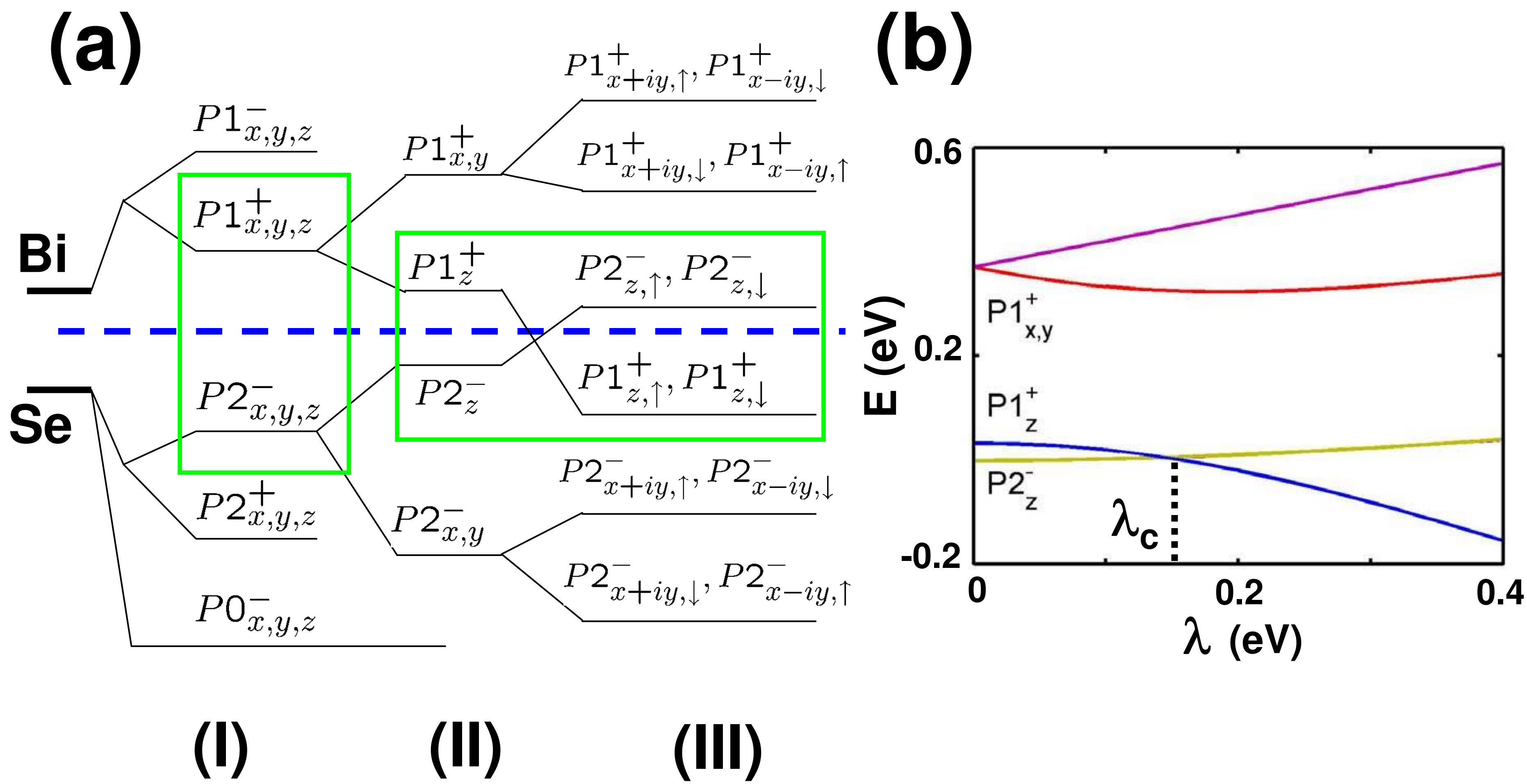




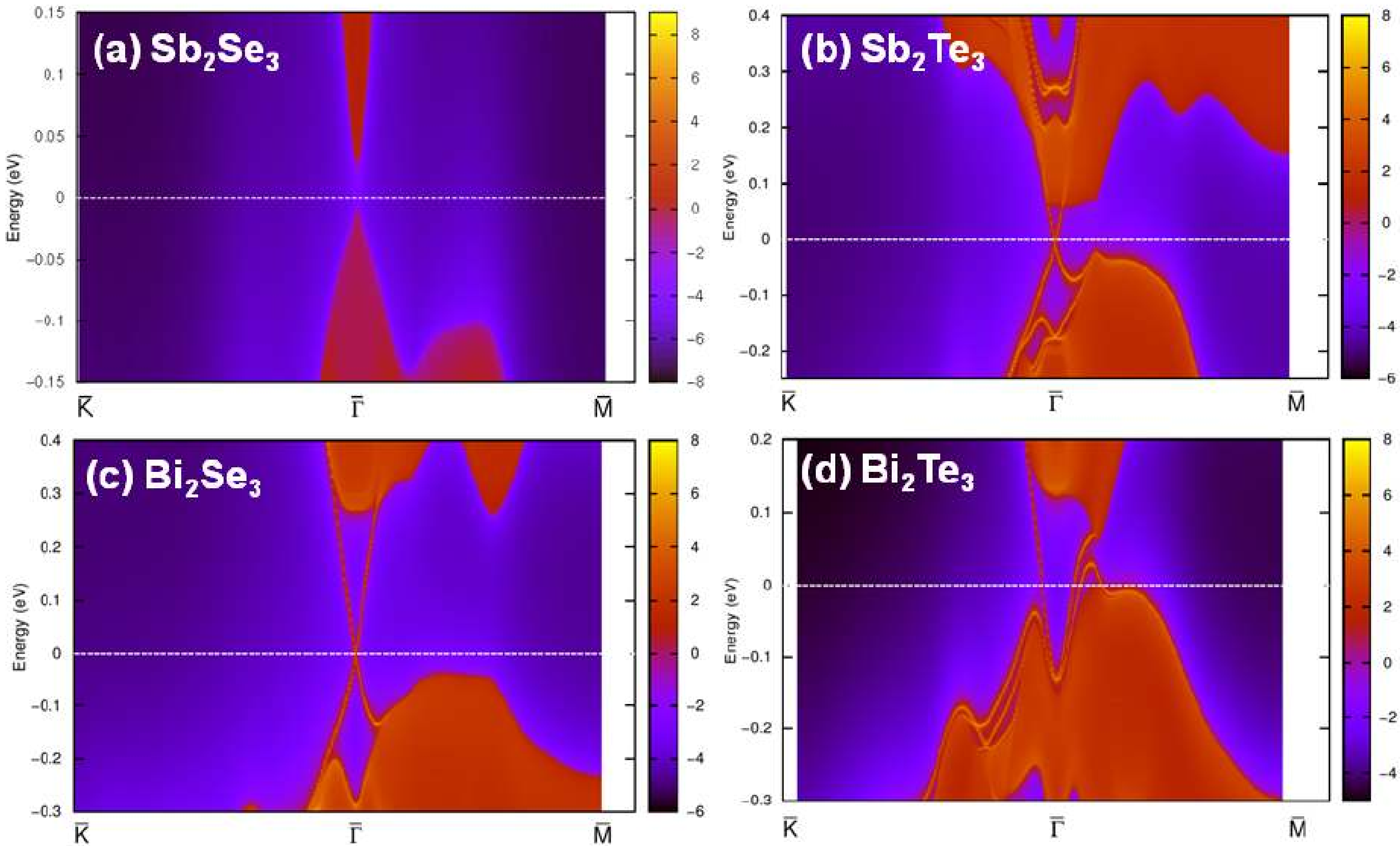
3D insulators with a single Dirac cone on the surface



Relevant orbitals of Bi2Se3 and the band inversion



Bulk and surface states from first principle calculations



Model for topological insulator Bi2Te3, (Zhang et al, 2009)

$$H(\mathbf{k}) = \epsilon_0(\mathbf{k})\mathrm{I}_{4\times 4} + \begin{pmatrix} \mathcal{M}(\mathbf{k}) & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -\mathcal{M}(\mathbf{k}) & A_2 k_- & 0 \\ 0 & A_2 k_+ & \mathcal{M}(\mathbf{k}) & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -\mathcal{M}(\mathbf{k}) \end{pmatrix} + o(\mathbf{k}^2)$$

Pz+, up, Pz-, up, Pz+, down, Pz-, down

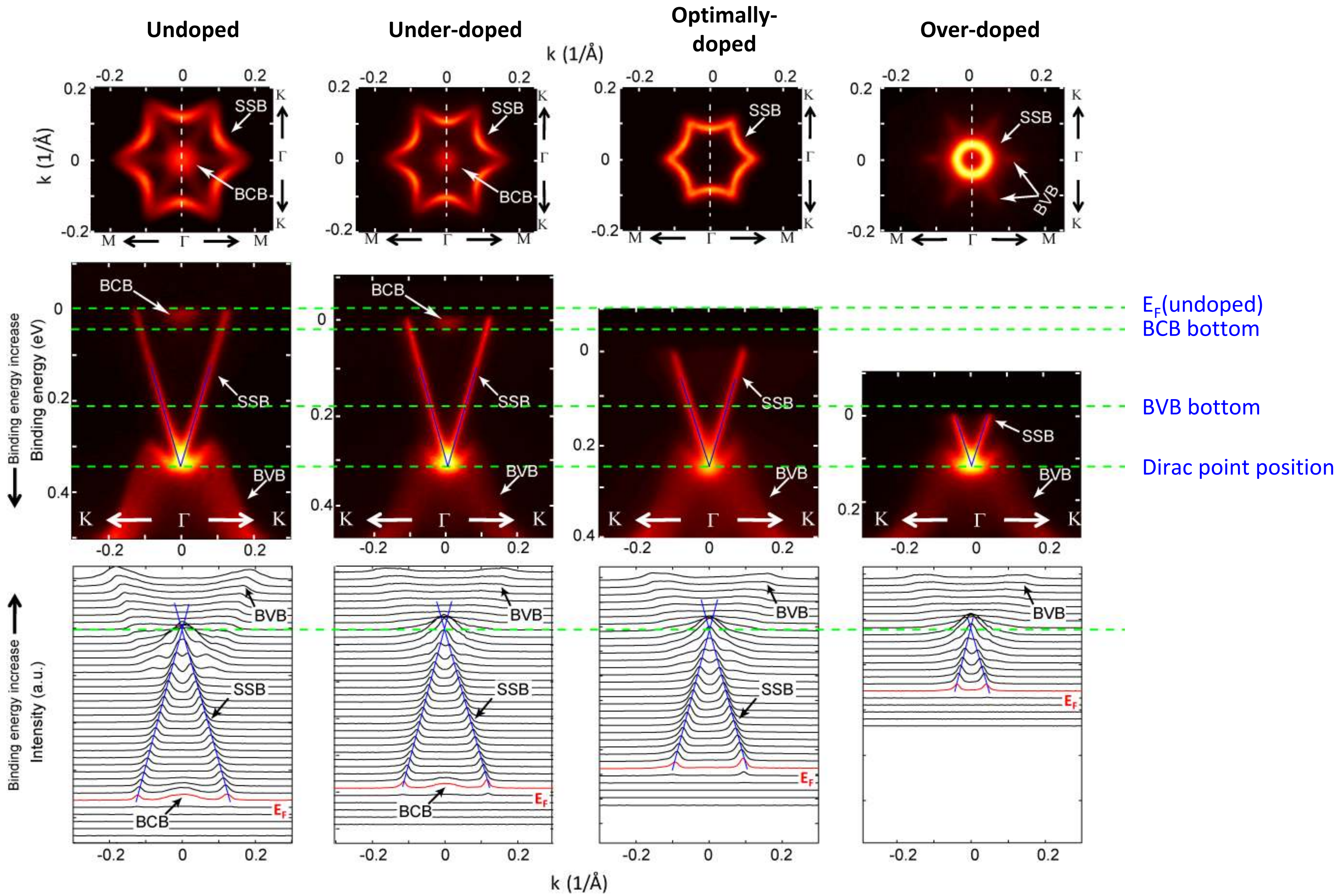
Single Dirac cone on the surface of Bi2Te3

$$H = \int d^2\mathbf{x}\psi^\dagger(\mathbf{x})\left[\hbar v_f(\hat{\mathbf{z}} \times (-i\nabla)) \cdot \boldsymbol{\sigma} - \mu\right]\psi(\mathbf{x}),$$

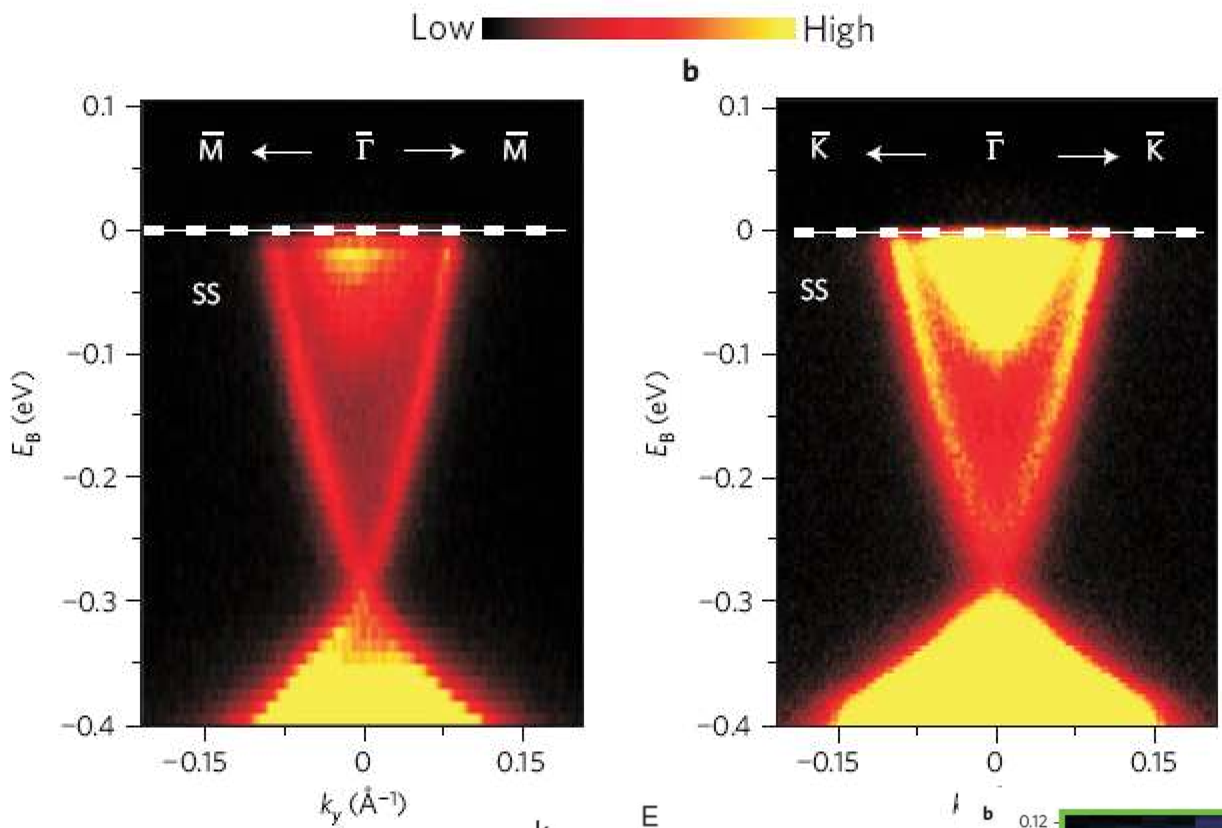
Surface of Bi2Te3 = ¼ Graphene !

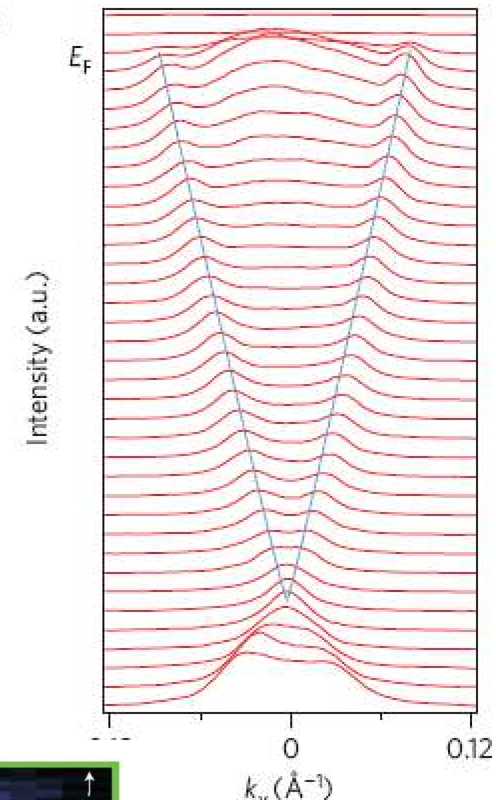
Arpes experiment on Bi2Te3 surface states, Shen group

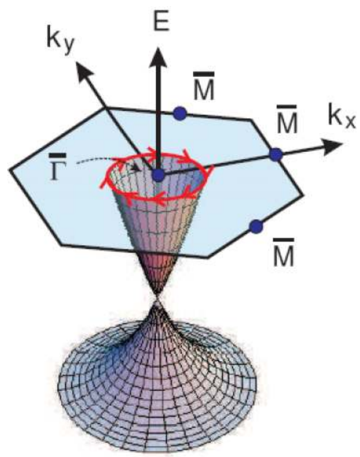
Doping evolution of the FS and band structure

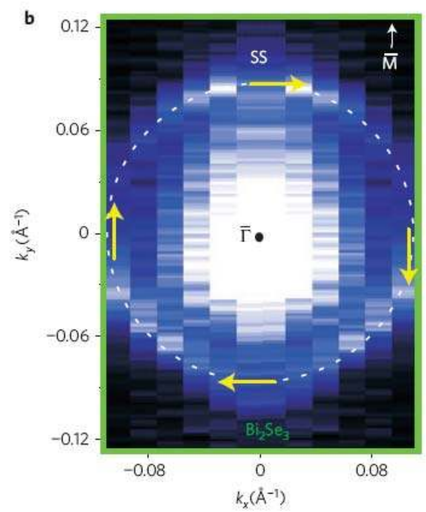


Arpes experiment on Bi2Se3 surface states, Hasan group









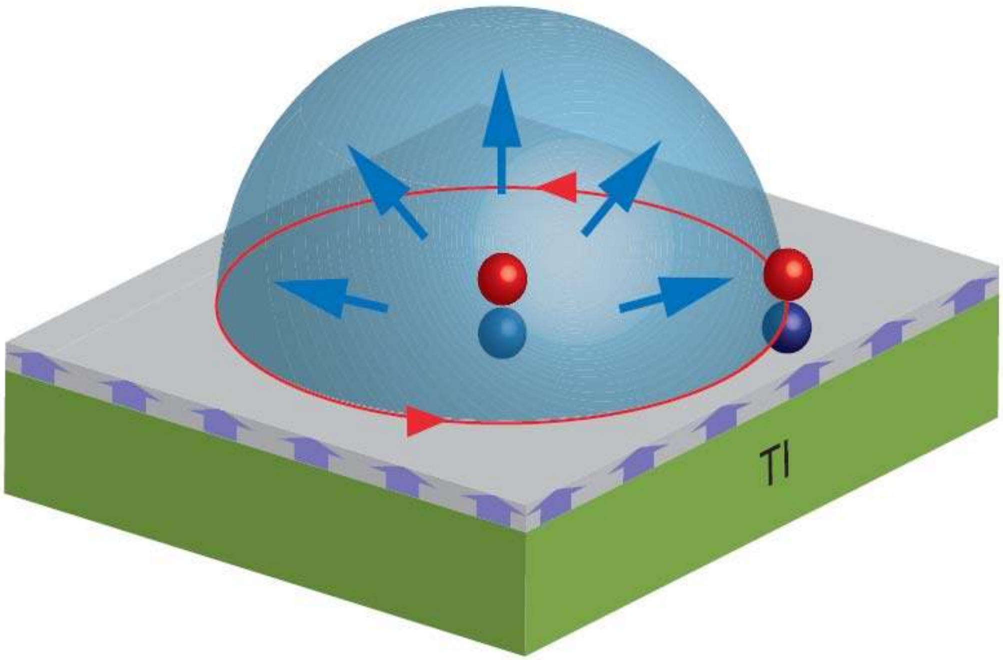
General definition of a topological insulator

- Topological field theory term in the effective action. Generally valid for interacting and disordered systems. Directly measurable physically. Relates to axion physics! (Qi, Hughes and Zhang)

$$S_0 = \frac{1}{8\pi}\int d^3x dt \left(\varepsilon \mathbf{E}^2 - \frac{1}{\mu}\mathbf{B}^2\right)$$

- For a periodic system, the system is time reversal symmetric only when
$\theta = 0$ => trivial insulator
$\theta = \pi$ => non-trivial insulator

- Z2 topological band invariant in momentum space based on single particle states.
(Fu, Kane and Mele, Moore and Balents, Roy)



$$S_\theta = \left(\frac{\theta}{2\pi}\right)\left(\frac{\alpha}{2\pi}\right)\int d^3x dt \mathbf{E}\cdot\mathbf{B}$$

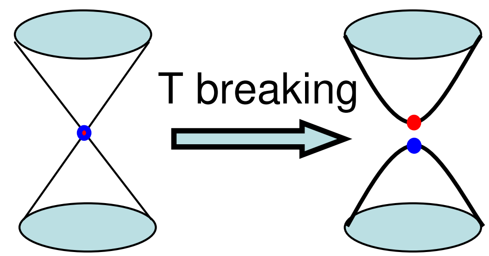
$$\alpha = \frac{e^2}{\hbar c}$$

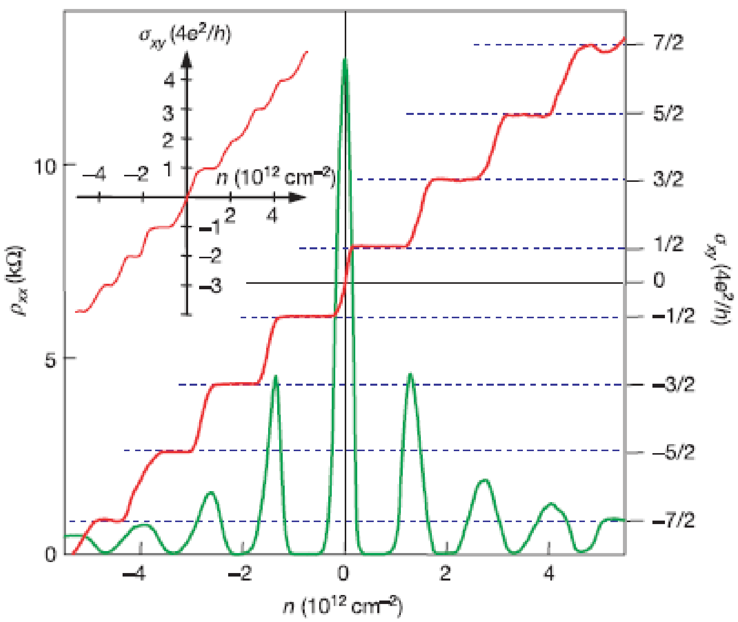
θ term with open boundaries

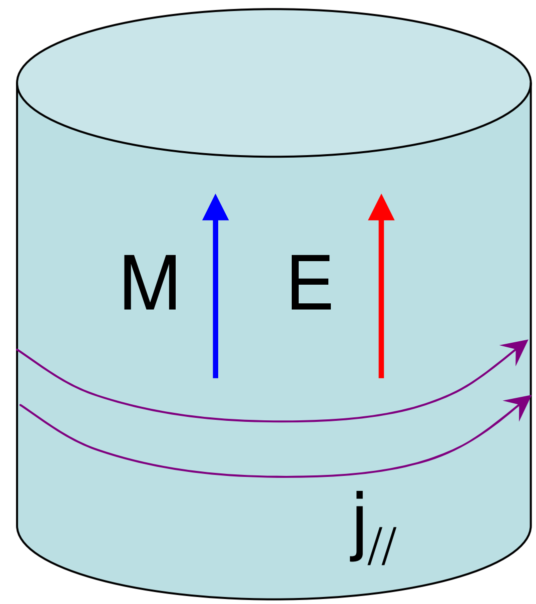
- θ= π implies QHE on the boundary with $\sigma_{xy} = \frac{1}{2}\frac{e^2}{h}$

$$S_\theta = \frac{\theta}{2\pi}\frac{\alpha}{16\pi}\int d^3x dt \epsilon_{\mu\nu\rho\tau}F^{\mu\nu}F^{\rho\tau} = \frac{\theta}{2\pi}\frac{\alpha}{4\pi}\int d^3x dt \partial^\mu(\epsilon_{\mu\nu\rho\sigma}A^\nu\partial^\rho A^\tau)$$

- For a sample with boundary, it is only insulating when a small T-breaking field is applied to the boundary. The surface theory is a CS term, describing the half QH.
- Each Dirac cone contributes σ_{xy}= 1/2e²/h to the QH. Therefore, θ=π implies an odd number of Dirac cones on the surface!







- Surface of a TI = ¼ graphene

Generalization of the QH topology state in d= 2 to time reversal invariant topological state in d> 2, in Science 2001

A Four-Dimensional Generalization of the Quantum Hall Effect

Shou-Cheng Zhang and Jiangping Hu

We construct a generalization of the quantum Hall effect, where particles move in four dimensional space under a $SU(2)$ gauge field. This system has a macroscopic number of degenerate single particle states. At appropriate integer or fractional filling fractions the system forms an incompressible quantum liquid. Gapped elementary excitation in the bulk interior and gapless elementary excitations at the boundary are investigated.

Time Reversal Invariant Topological Insulators

- Zhang & Hu 2001: TRI topological insulator in D=4. => Root state of all TRI topological insulators.
- Murakami, Nagaosa & Zhang 2004: Spin Hall insulator with spin-orbit coupled band structure.
- Kane and Mele, Bernevig and Zhang 2005: Quantum spin Hall insulator with and without Landau levels.
- Fu, Kane & Mele, Moore and Balents, Roy 2007: Topological band theory based on Z2
- Qi, Hughes and Zhang 2008: Topological field theory based on F F dual.

TRB Chern-Simons term in D=2: A_0=even, A_i=odd

$$S_{2D} = \int d^2k\, da(k) \int d^3x\, A(x) \wedge dA(x)$$

TRI Chern-Simons term in D=4: A_0=even, A_i=odd

$$S_{4D} = \int d^4k\, da(k) \wedge da(k) \int d^5x\, A(x) \wedge dA(x) \wedge dA(x)$$

Dimensional reduction

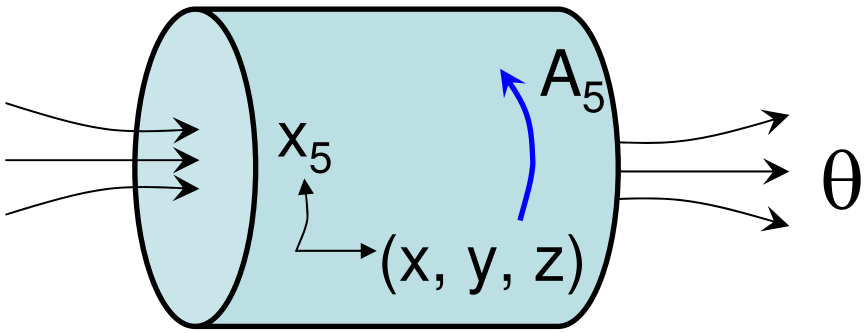
- From 4D QHE to the 3D topological insulator

Zhang & Hu, Qi, Hughes & Zhang

$$S_{4DQH} = \int d^4x dt \varepsilon^{\mu\nu\rho\sigma\tau} A_\mu F_{\nu\rho} F_{\sigma\tau}$$

$$\Rightarrow \int d^3x dt \left(\int dx_5 A_5(x,t)\right) \varepsilon^{\nu\rho\sigma\tau} F_{\nu\rho} F_{\sigma\tau}$$

$$\Rightarrow S_{3D} = \int d^3x dt\, \theta(x,t) \varepsilon^{\nu\rho\sigma\tau} F_{\nu\rho} F_{\sigma\tau}$$



- From 3D axion action to the 2D QSH

$$S_{3D} = \int d^3x dt \varepsilon^{\nu\rho\sigma\tau} A_\nu \partial_\rho \theta \partial_\sigma A_\tau$$

$$\Rightarrow \int d^2x dt \varepsilon^{\rho\sigma\tau} \left(\int dz A_z(x,t)\right) \partial_\rho \theta \partial_\sigma A_\tau$$

$$\Rightarrow S_{2D} = \int d^2x dt \varepsilon^{\rho\sigma\tau} \partial_\sigma \varphi \partial_\rho \theta A_\tau$$

$$J_{2D}^{\ \mu} = \frac{e}{2\pi^2} \varepsilon^{\mu\rho\sigma} \partial_\sigma \varphi \partial_\rho \theta$$

$$\Leftrightarrow J_{1D}^{\ \mu} = \frac{e}{2\pi} \varepsilon^{\mu\sigma} \partial_\sigma \varphi$$

Goldstone & Wilzcek

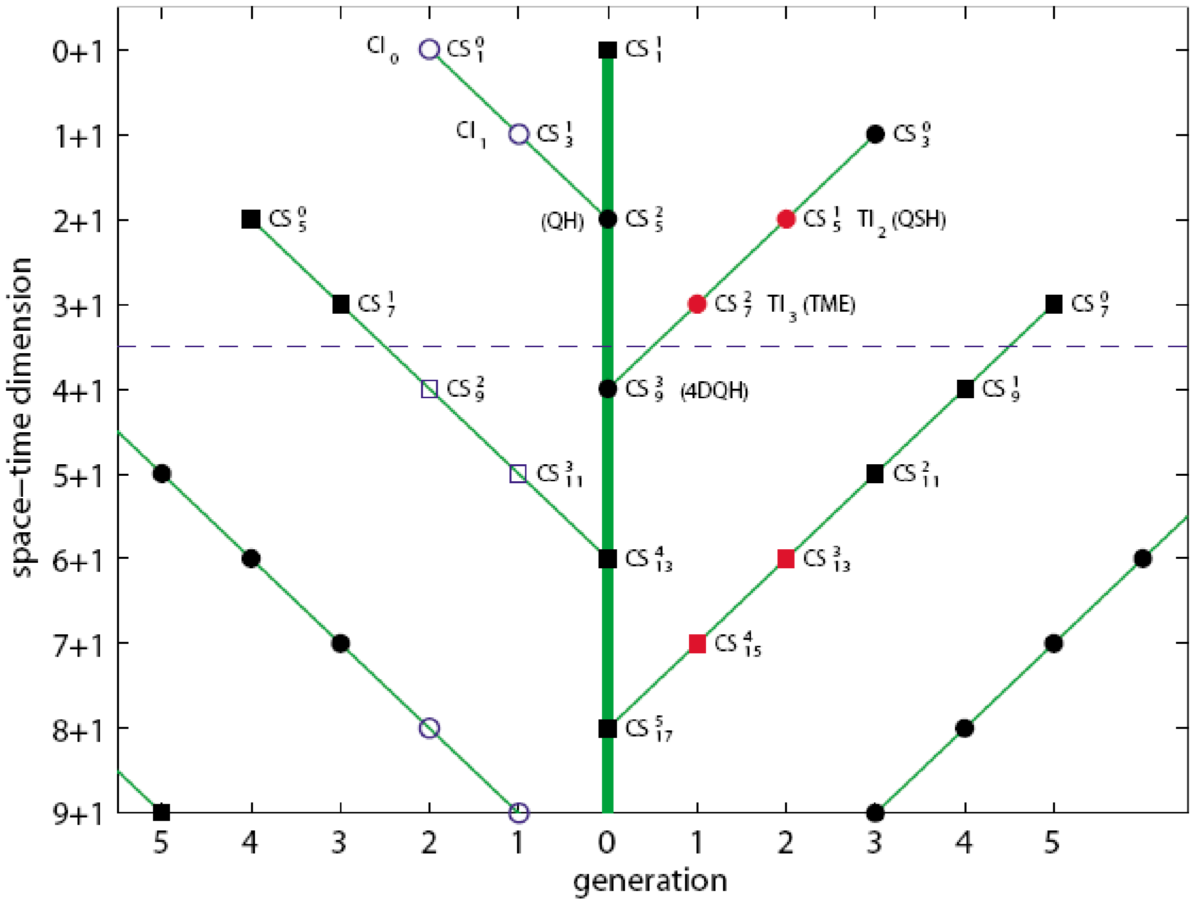
Topological field theory and the family tree

- Topological field theory of the QHE: (Thouless et al, Zhang, Hansson and Kivelson)

$$S=\int d^2k\, da(k)\int d^3x\, A(x)\wedge dA(x)$$

- Topological field theory of the TI: (Qi, Hughes and Zhang, 2008)

$$S=\int d^3k\,(a(k)\wedge da(k)+..)\int d^4x\, dA(x)\wedge dA(x)$$



- More extensive and general classification soon followed (Kitaev, Ludwig et al)

Equivalence between the integral and the discrete topological invariants (Wang, Qi and Zhang, 0910.5954)

$$P_3 = \frac{1}{16\pi^2}\int d^3\mathbf{k}\epsilon^{ijk}\mathrm{Tr}\{[f_{ij}(\mathbf{k}) - \frac{2}{3}ia_i(\mathbf{k})\cdot a_j(\mathbf{k})]\cdot a_k(\mathbf{k})\}$$

$$2P_3(\mathrm{mod}\,2) = -\frac{1}{24\pi^2}\int d^3\mathbf{k}\epsilon^{ijk}\mathrm{Tr}[(B\partial_i B^\dagger)(B\partial_j B^\dagger)(B\partial_k B^\dagger)]\,(\mathrm{mod}\,2)$$

$$\begin{aligned} B_{\alpha\beta}(-\mathbf{k}) &= \langle \mathbf{k},\alpha|\Theta,-\mathbf{k},\beta\rangle \\ &= -\langle -\mathbf{k},\beta|\Theta,\mathbf{k},\alpha\rangle \\ &= -B_{\beta\alpha}(\mathbf{k}) \end{aligned}$$

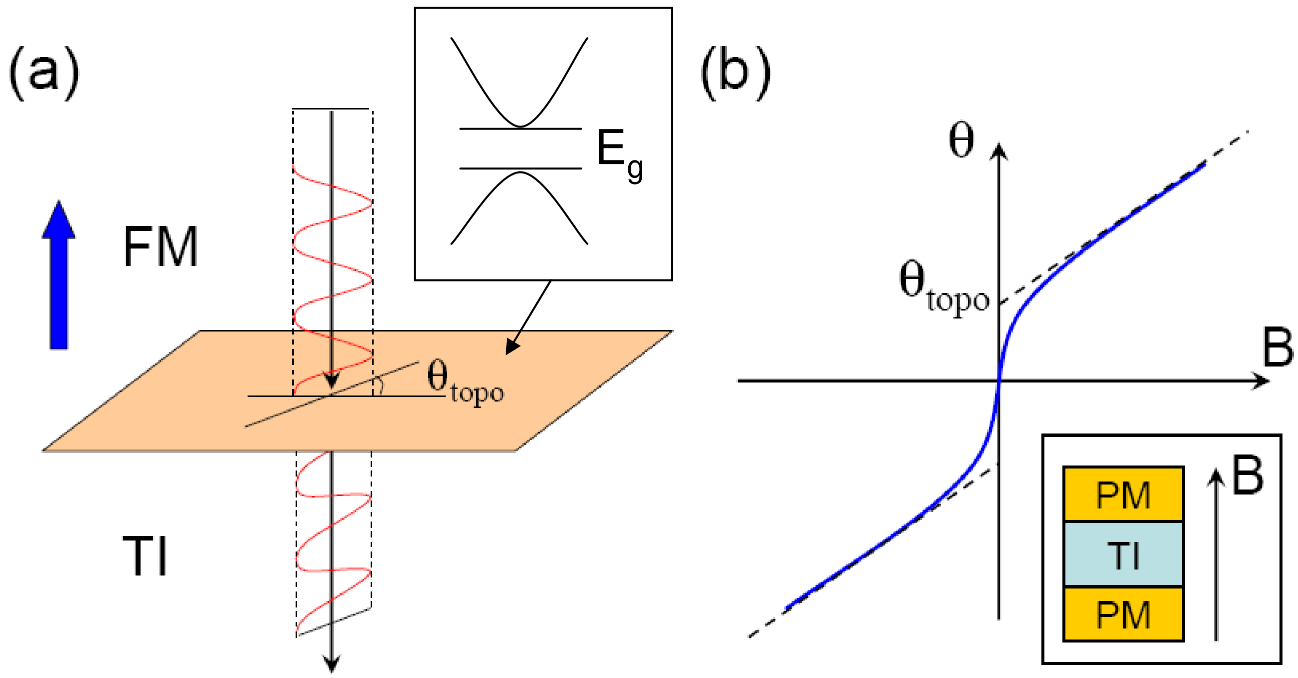
$$A_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad A_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

$$(-1)^{2P_3} = (-1)^{\sum_{m=1}^{N}\deg_2(g_m)} = \prod_m (-1)^{n_m}$$

LHS=QHZ definition of TI, RHS=FKM definition of TI

Low frequency Faraday/ Kerr rotation

(Qi, Hughes and Zhang, PRB78, 195424, 2008)



Adiabatic Requirement:

$$\hbar\omega \ll E_g$$

(surface gap)

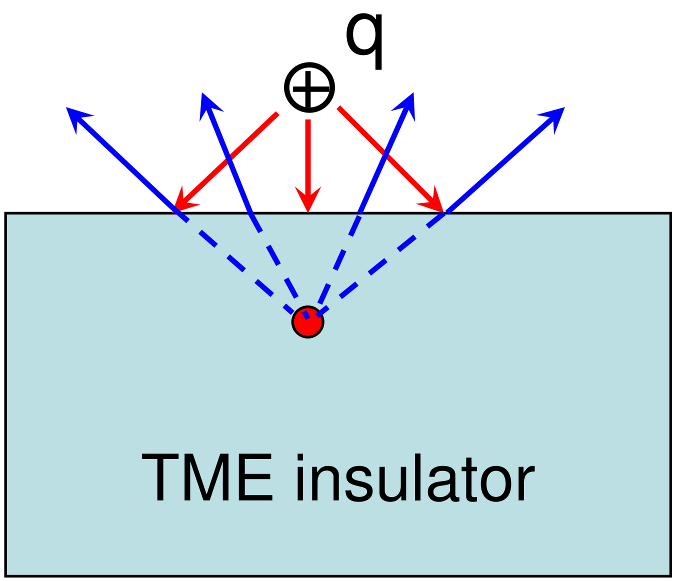
$$\theta(B) = uB + \mathrm{sgn}(B)\arctan\left(\frac{(2n-1)\alpha}{\sqrt{\epsilon/\mu}+\sqrt{\epsilon'/\mu'}}\right)$$

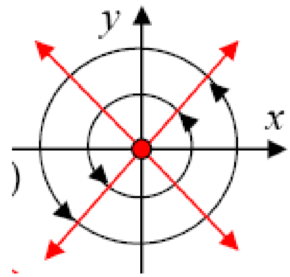
normal contribution

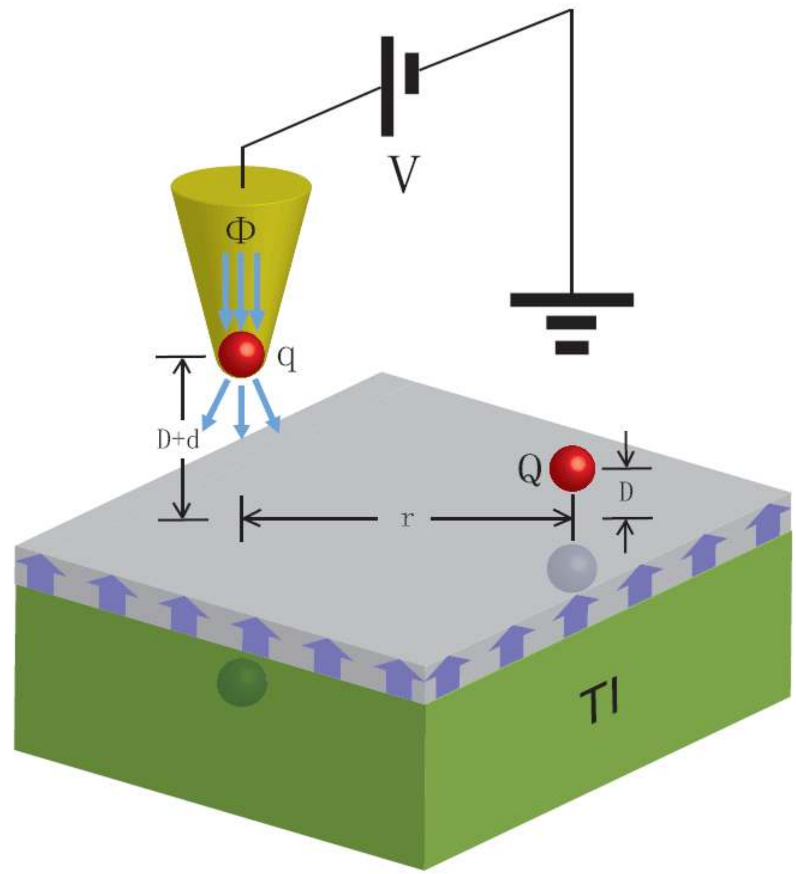
Topological contribution

$\theta_{topo} \approx 3.6 \times 10^{-3}$ rad

Seeing the magnetic monopole thru the mirror of a TME insulator, (Qi et al, Science 323, 1184, 2009)







$$g = \frac{\alpha P_3}{1+\alpha^2 P_3^2} q$$

higher order feed back

(for μ=μ', ε=ε')

similar to Witten's dyon effect

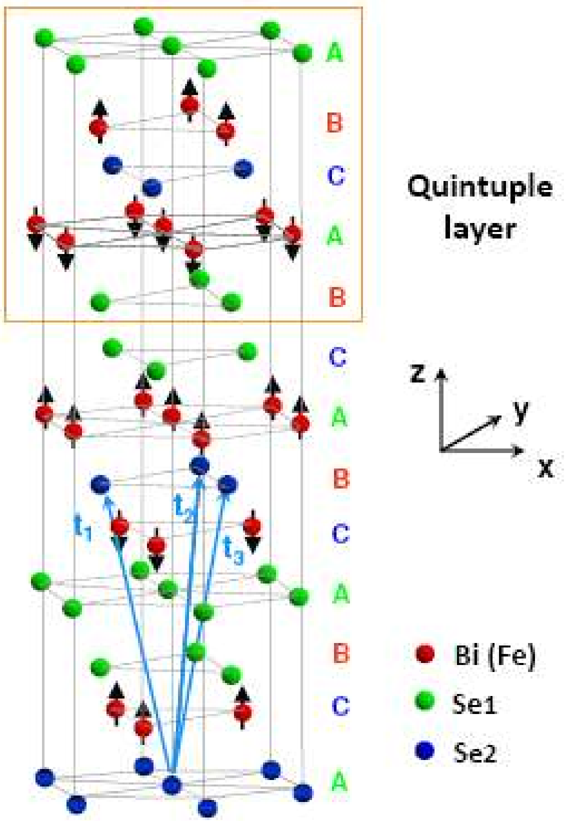
Magnitude of B:
$10^6 V/m \rightarrow 0.25G$

Dynamic axions in topological magnetic insulators
(Li et al, Nature Physics 2010)

$$\theta = \frac{1}{4\pi}\int d^3k \epsilon^{ijk} Tr\left[A_i \partial_j A_k + \frac{2}{3} A_i A_j A_k\right]$$

- Hubbard interactions leads to anti-ferromagnetic order

$$H = H_0 + U\sum_i (n_{iA\uparrow}n_{iA\downarrow} + n_{iB\uparrow}n_{iB\downarrow}) + V\sum_i n_{iA}n_{iB}$$

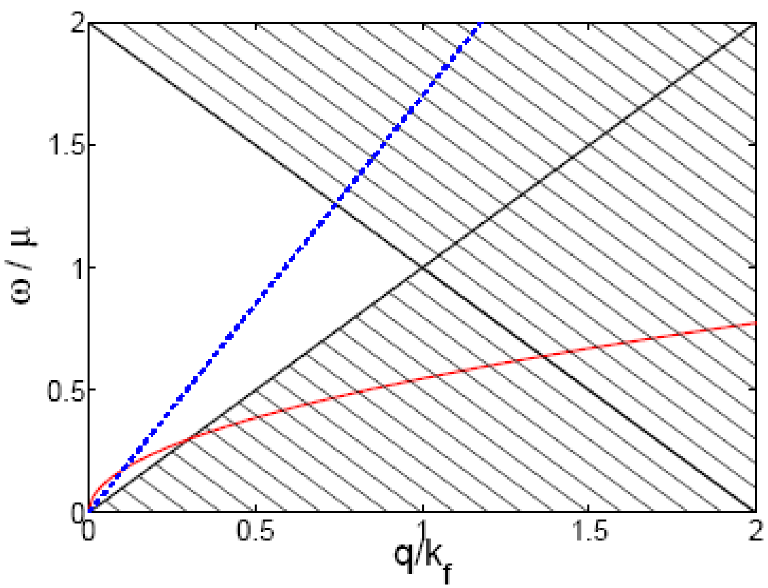


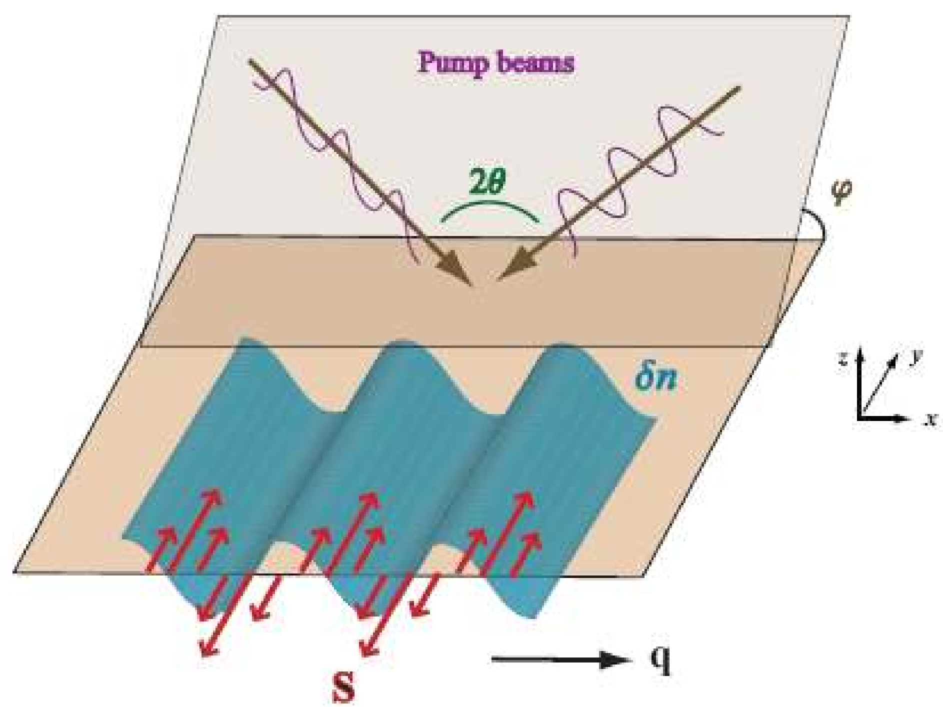
- Effective action for dynamical axion

$$\begin{aligned}
\mathcal{S}_{\rm tot} &= \mathcal{S}_{\rm Maxwell} + \mathcal{S}_{\rm topo} + \mathcal{S}_{\rm axion} \\
&= \frac{1}{8\pi}\int d^3x dt (\epsilon \mathbf{E}^2 - \frac{1}{\mu}\mathbf{B}^2) \\
&+ \frac{\alpha}{4\pi^2}\int d^3x dt\, (\theta_0 + \delta\theta)\, \mathbf{E}\cdot\mathbf{B} \\
&+ g^2 J \int d^3x dt \left[(\partial_t \delta\theta)^2 - (v_i \partial_i \delta\theta)^2 - m^2 \delta\theta^2\right]
\end{aligned}$$

Spin-plasmon collective mode (Raghu et al, 0909.2477)

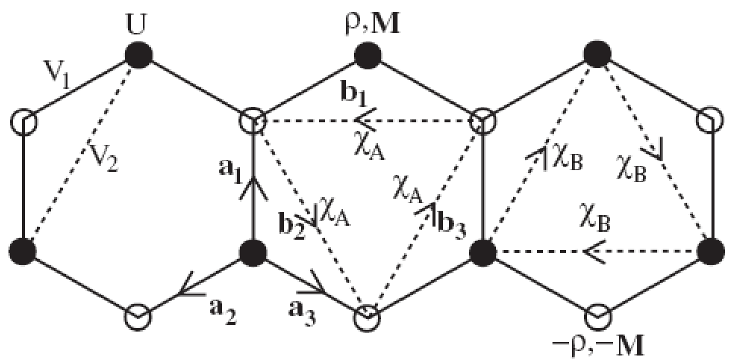
- General operator identity: $\mathbf{j}(\mathbf{x}) = \psi^\dagger(\mathbf{x}) v_f \left(\boldsymbol{\sigma} \times \hat{\mathbf{z}}\right) \psi(\mathbf{x}) \equiv v_f \mathbf{S}(\mathbf{x}) \times \hat{\mathbf{z}}$
- Density-spin coupling: $\partial_t n_{\mathbf{q}} = -iqs^T_{\mathbf{q}}.$ $\quad \frac{s_T}{n} = \sqrt{\frac{\alpha k_f}{2q}}$

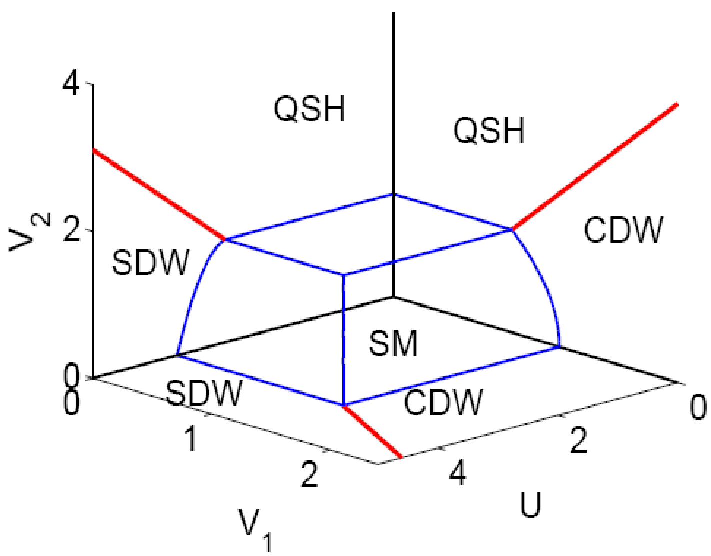




Topological Mott insulators

- Dynamic generation of spin-orbit coupling can give rise to TMI (Raghu et al, PRL 2008).
- Interplay between spin-orbit coupling and Mott physics in 5d transition metal Ir oxides, Nagaosa, SCZ et al PRL 2009, Balents et al, Franz et al.
- Topological Kondo insulators (Coleman et al)





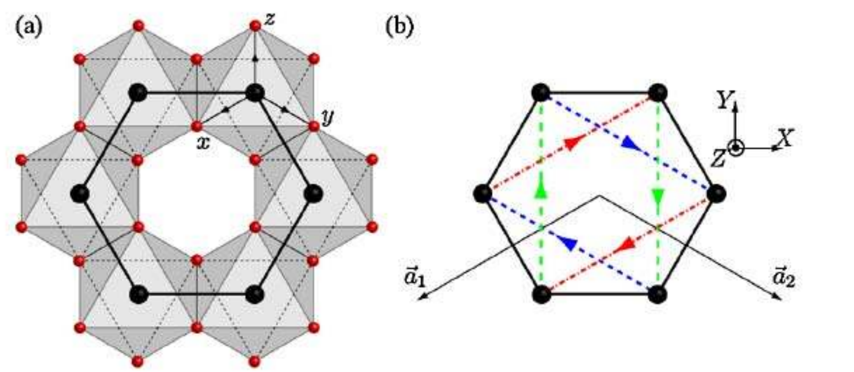
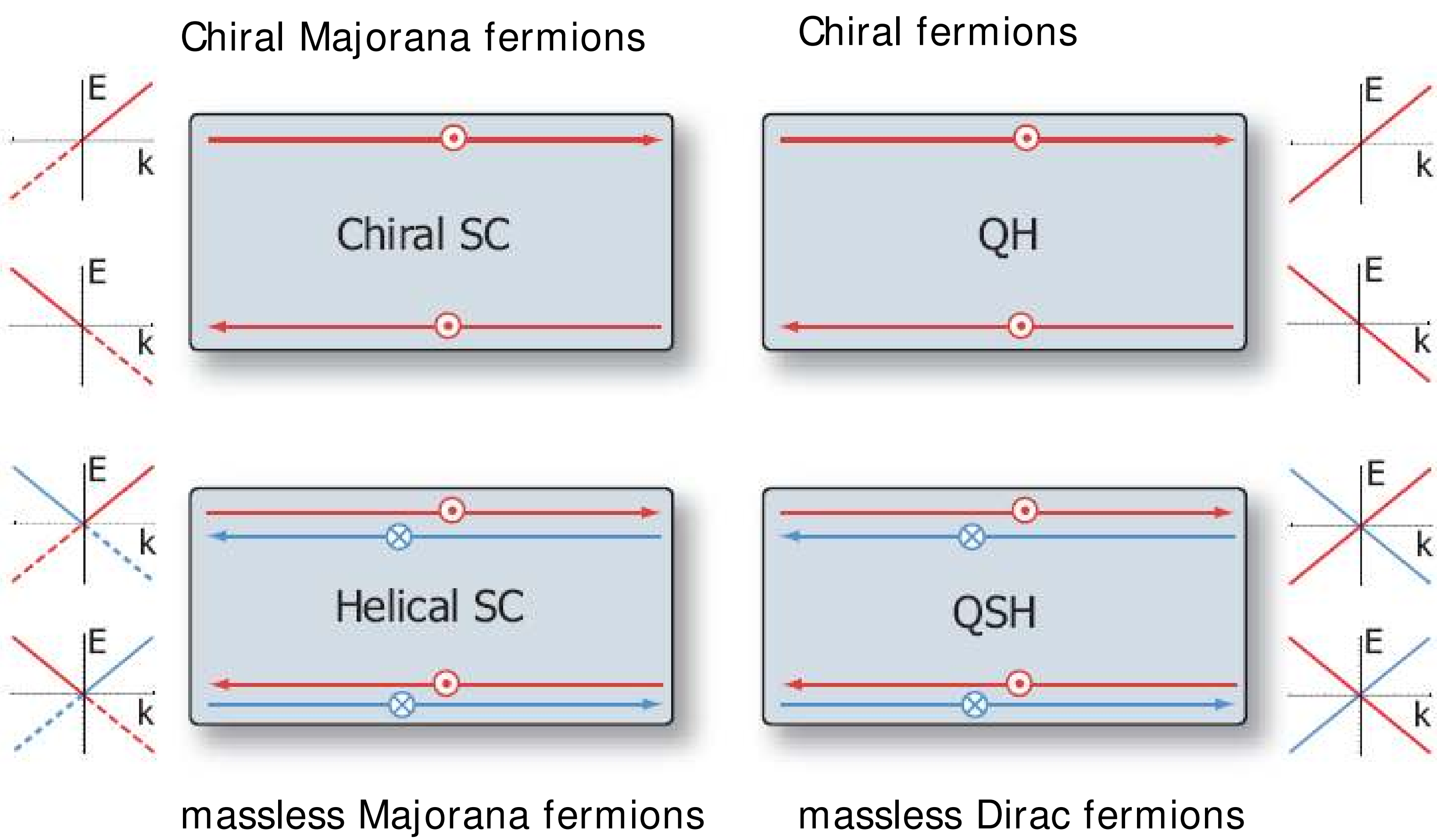


FIG. 1 (color online). (a) The honeycomb lattice of Ir atoms in Na_2IrO_3 viewed from the c axis. A large black circle shows an Ir atom surrounded by six O atoms (red small circles). (b) The transfer integrals on the honeycomb lattice. A black solid line shows $-t$, while blue short-dashed, red dash-dotted, and green long-dashed arrows indicate $it'\sigma_x$, $it'\sigma_y$, $it'\sigma_z$, respectively.

Topological insulators and superconductors

Full pairing gap in the bulk, gapless Majorana edge and surface states



Qi, Hughes, Raghu and Zhang, PRL, 2009

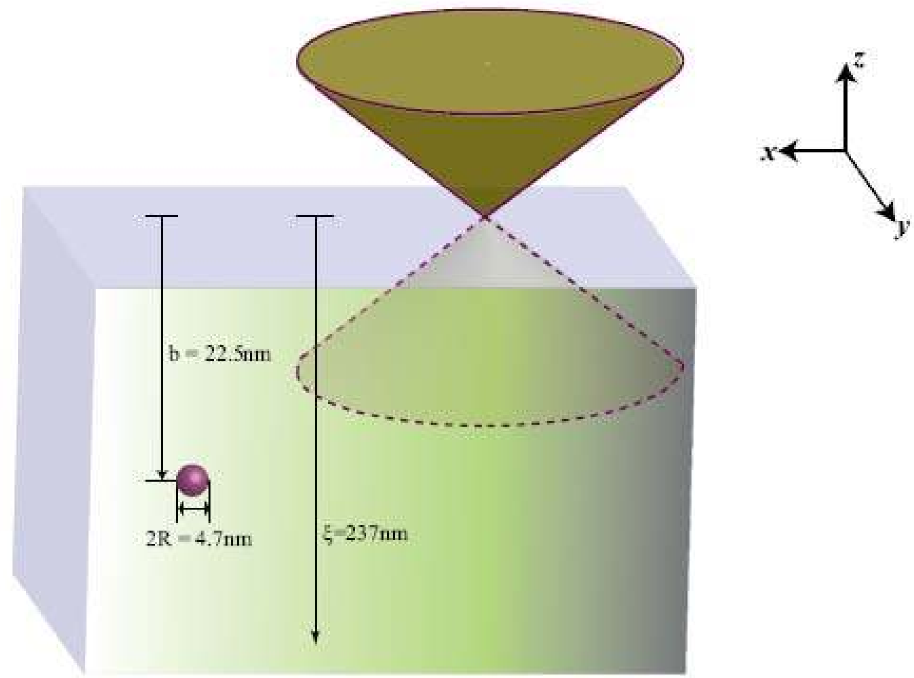
Probing He3B as a topological superfluid (Chung and Zhang, 2009)

The BCS-BdG model for He3B ⇔ Model of the 3D TI by Zhang et al

$$\hat{\mathcal{H}}_{BdG} = \begin{bmatrix} \epsilon_{\mathbf{p}} - E_F & 0 & -\frac{\Delta}{p_F}\hat{p}_- & \frac{\Delta}{p_F}\hat{p}_x \\ 0 & \epsilon_{\mathbf{p}} - E_F & \frac{\Delta}{p_F}\hat{p}_x & \frac{\Delta}{p_F}\hat{p}_+ \\ -\frac{\Delta}{p_F}\hat{p}_+ & \frac{\Delta}{p_F}\hat{p}_x & -\epsilon_{\mathbf{p}} + E_F & 0 \\ \frac{\Delta}{p_F}\hat{p}_x & \frac{\Delta}{p_F}\hat{p}_- & 0 & -\epsilon_{\mathbf{p}} + E_F \end{bmatrix}$$

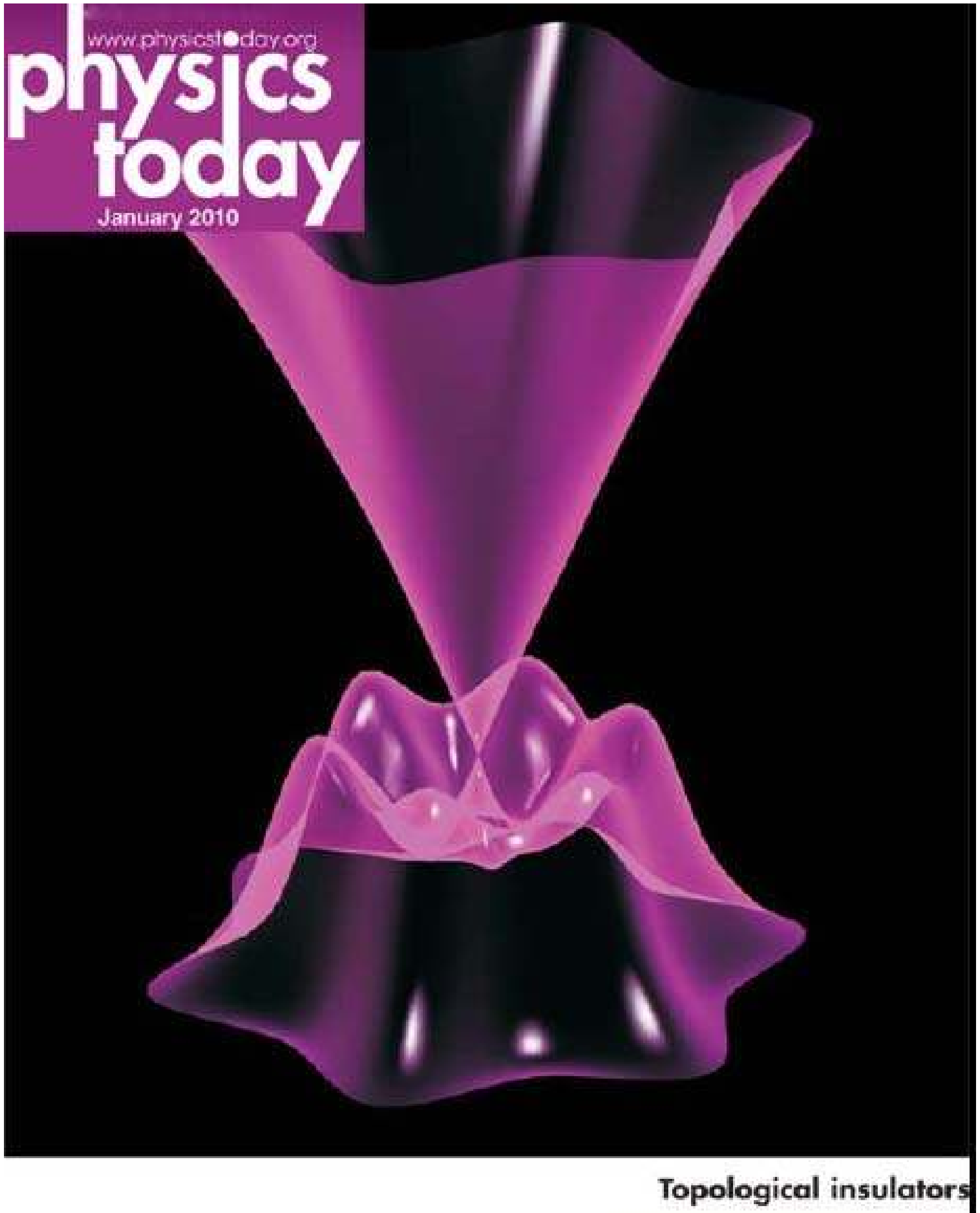
Surface Majorana state:

$$\mathcal{H}_{surf} = v_F \boldsymbol{\sigma} \cdot (\hat{\mathbf{z}} \times \mathbf{p})$$



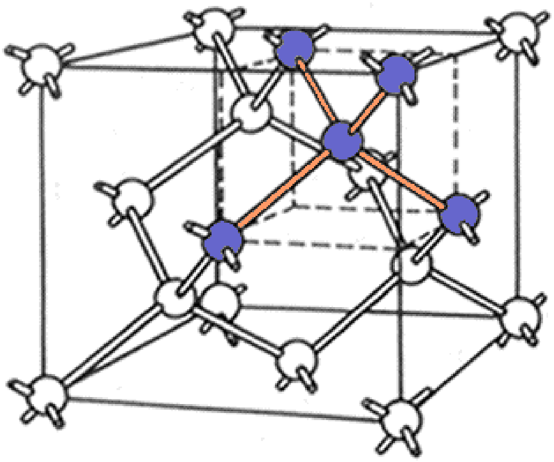
Qi, Hughes, Raghu and Zhang, PRL, 2009
Schnyder et al, PRB, 2008
Kitaev
Roy

General reading

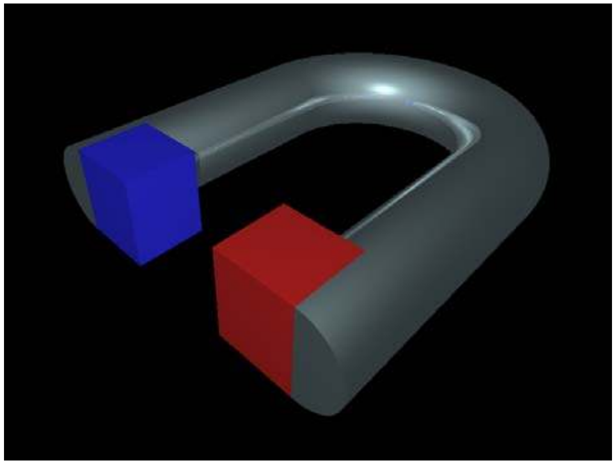


For a video introduction of topological insulators and superconductors, see ***http://www.youtube.com/watch?v=Qg8Yu-Ju3Vw***

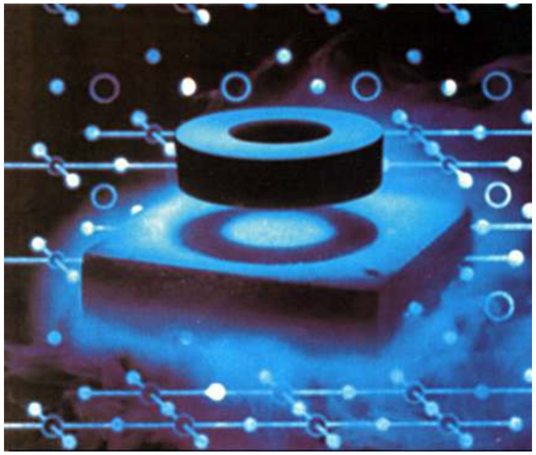
Summary: discovery of new states of matter



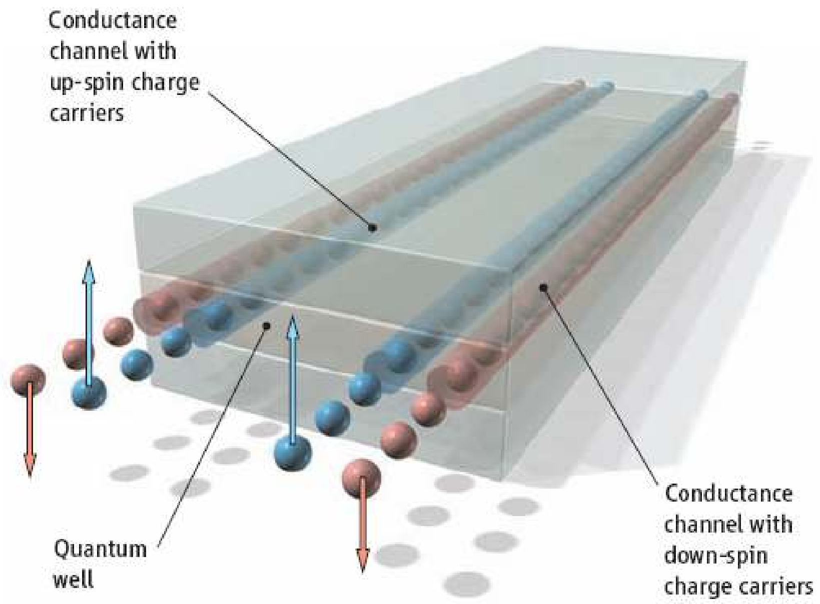
Crystal



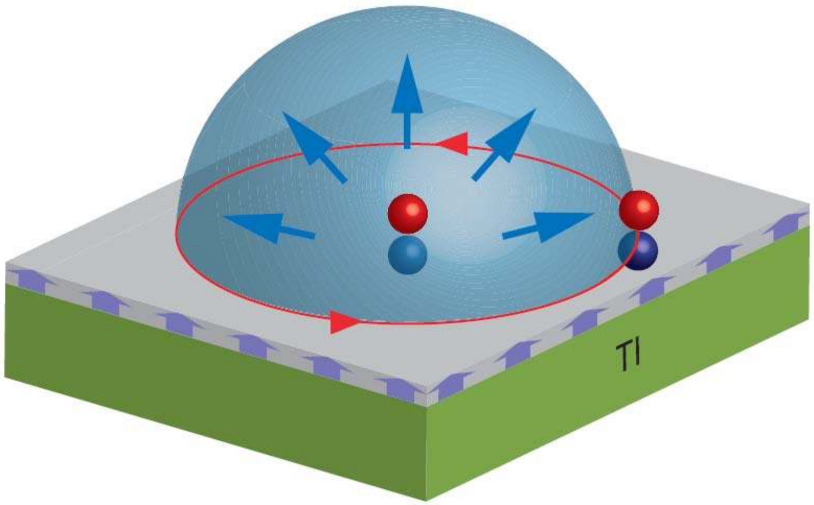
Magnet



s-wave superconductor



Quantum Spin Hall



Topological insulators