Topological phases of quantum matter

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`Geometric phases in optics and topological matter'

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2016 Nobel prize in physics awarded to David Thouless, Duncan Haldane and Michael Kosterlitz

- For theoretical discoveries of topological phase transitions and topological phases of matter

- Although first to mention topological phases, not really the first Nobel prize for topological phases
- First, 1982 - Nobel to Klaus von Klitzing for 'discovery of quantised Hall effect'
- Second, 1998- Robert Laughlin, Horst Stormer and Daniel Tsui for ` discovery of a new form of quantum fluid with fractionally charged excitations'
- Can expect many more in the future!

arXiv number 1807.10271

The (“High-Quality”) Topological Materials In The World

TQC we then develop codes to check which materials in ICSD are topological. Out of 26938 stoichiometric materials in our filtered ICSD database, we find 2861 topological insulators (TI) and 2936 topological semimetals (2505 and 2560 non-f electron, respectively). Our method is *uniquely* capable to show that *none* of the TI's found exhibit fragile topology. We partition the topological

Conclusion We found that roughly 24% of the materials in the world are topological. Roughly 12% are topological insulators. With these findings, we now enter an important era of topological material design. One important future research direction is be to compute and discover the physical properties of our large set of materials. Slab calculations should be performed for all our topological insulator compounds, in order to reveal their surface states. Compounds whose topological character

- Thus expect many new phenomena and many more Nobel prizes for topological materials

M. G. Vergniory, L. Elcoro, C. Felser, B.A. Bernevig and Z.Wang

Plan of the talk

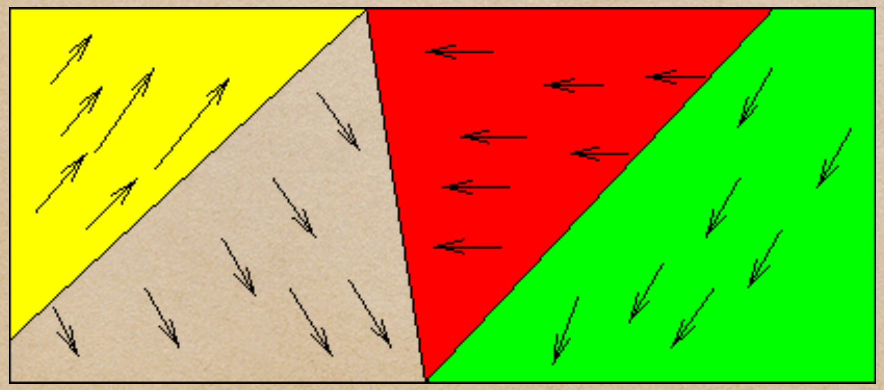
- I - Introduction
- II - Quantum Hall effect, TKNN quantisation
- III - Edge states, recognition of bulk-boundary correspondence
- Topological insulators and topological superconductors
- Current day generalisations and prospects

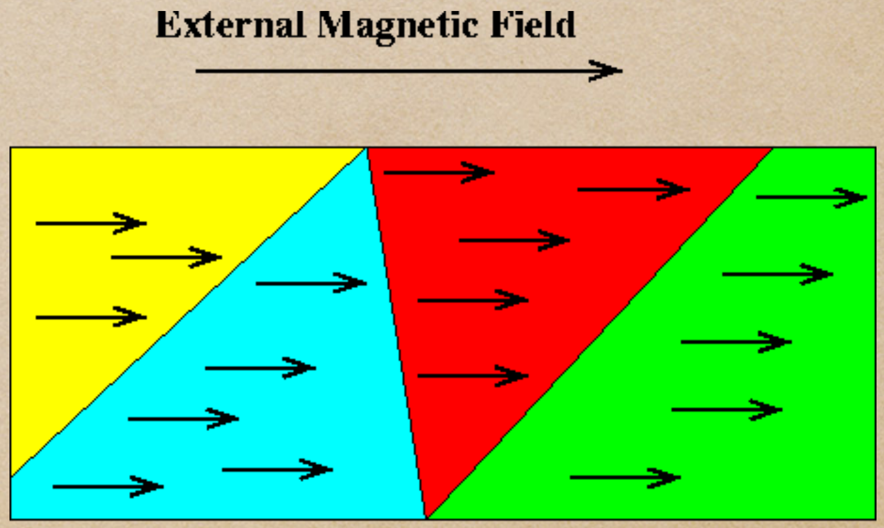
I- Introduction

What are phases of matter?

- All of you are familiar with states of matter like gas, liquid, and solid
- If you reduce the temperature of water, it freezes, becomes solid
- If you increase temperature of water, it boils and turns into vapour

- Phase = collection of particles with some property that distinguishes them from other phases
- Earlier phases classified in terms of symmetries -e.g. ferromagnets break the rotational symmetry in the spin space





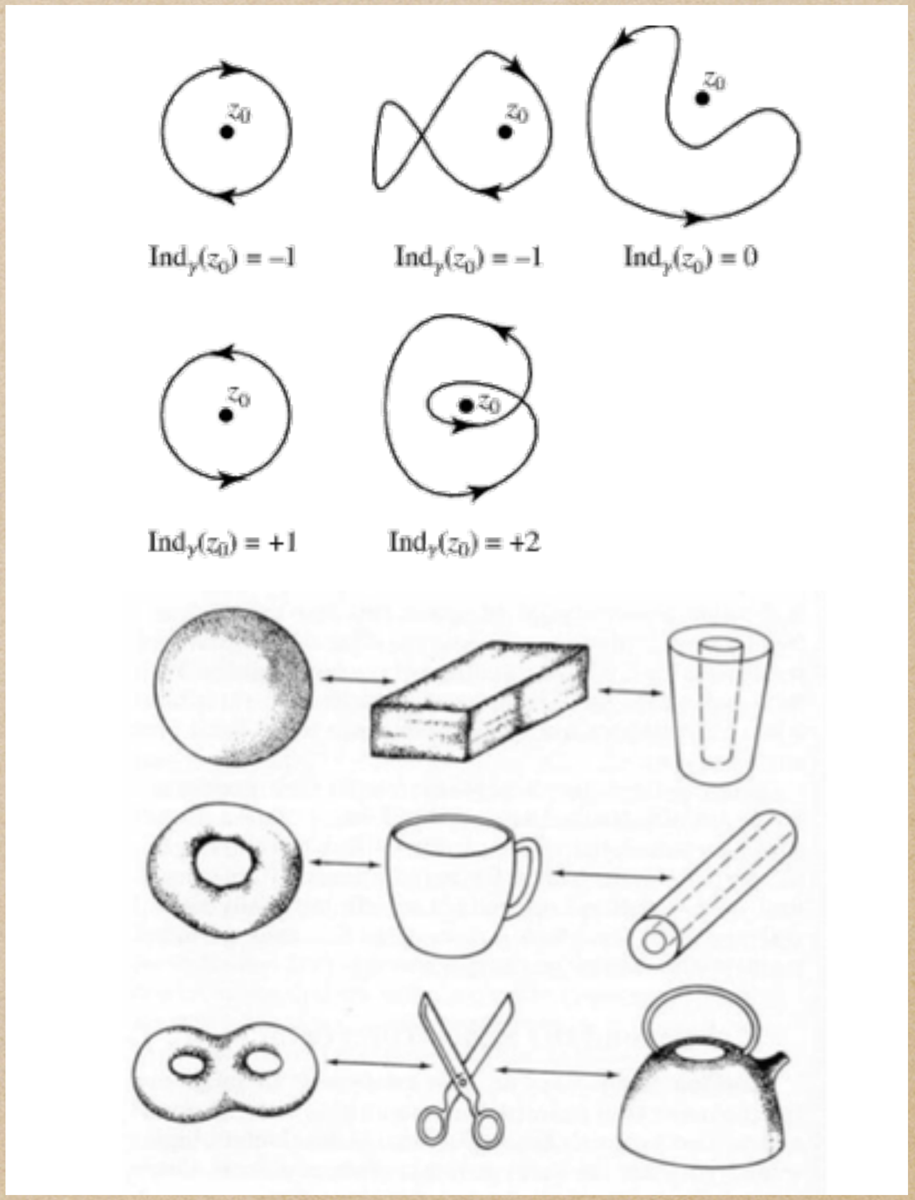
- In the last 10-15 years, a paradigm shift in the way of classifying phases - now based on topology - more correctly on the interplay of topology and symmetry

Why are topological phases interesting?

- New phases of matter always exciting!
- Topological phases have excitations, which can obey unusual statistics
- Anyonic, and also non-abelian statistics - expected to be relevant in making quantum computers
- Various exotic excitations such as monopoles, dyons, axions, etc may actually be found in these phases - in low energy condensed matter systems

What is Topology ?

- Topology is a branch of mathematics dealing with shapes
- Topological implies not changed by small perturbations, depends on the system as a whole
- For example, only whether or not z_0 is enclosed and how many times and in which direction



- More technically,
  Mappings from one space (e.g., 2D space with one point z_0 removed) to the space of wave functions are classified by a topological invariant - the winding number
- Similarly other mappings classified by a number

- For a quantum condensed matter system, the space turns out to be something called a Brillouin zone, which could for instance be a torus in momentum space
- Topological classification is of mappings of Brillouin zone (BZ) to space of gapped single particle Hamiltonians (wavefunctions for every band define a map from BZ to space of physical states)

Definition of topological phases

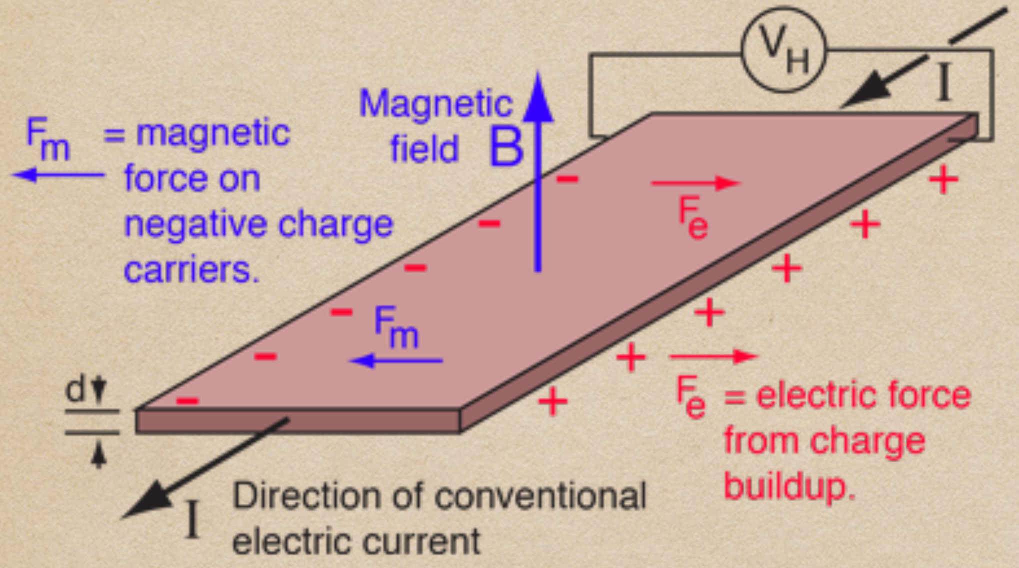
- Topological phases have some physical property to which an integer can be assigned which depends only on global properties and cannot be destroyed by impurities or disorder

- For example, conductance in the quantum Hall effect

- To change the topological phase, need to make a `hole in the surface' - do something drastic
- In real physical systems, idea is that as long as the system has a mass gap, physical states can be changed slightly and the topological invariant will not change - `topological protection'
- But when the system becomes massless or gapless, then even small changes can make a big difference- topological invariant no longer protected

II - First topological phase - 35 years ago Integer quantum Hall effect

Conventional Hall effect



$$\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}$$

$$F_y = 0 \rightarrow E_y = v_x B_z$$

$$V_H = E_y W \text{ and } v_x = \frac{I_x}{ndWq}$$

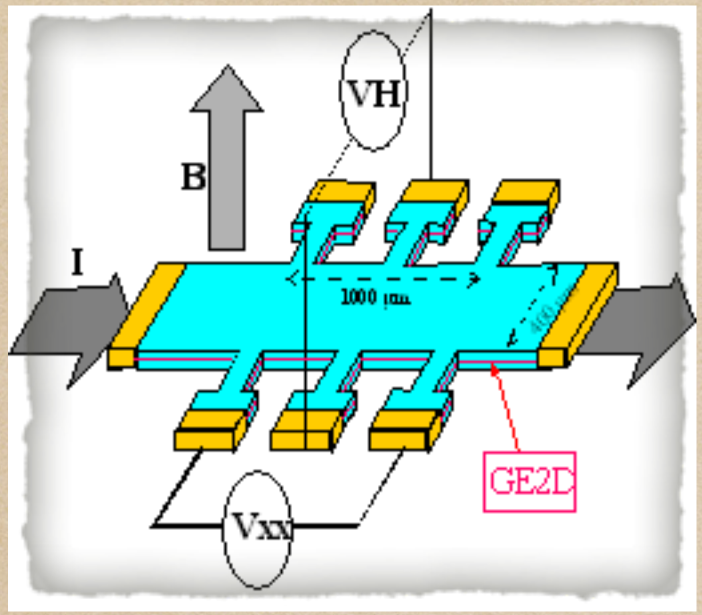
- In the steady state, charges are not moving perpendicular to the current, leads to charge build up and Hall voltage proportional to magnetic field

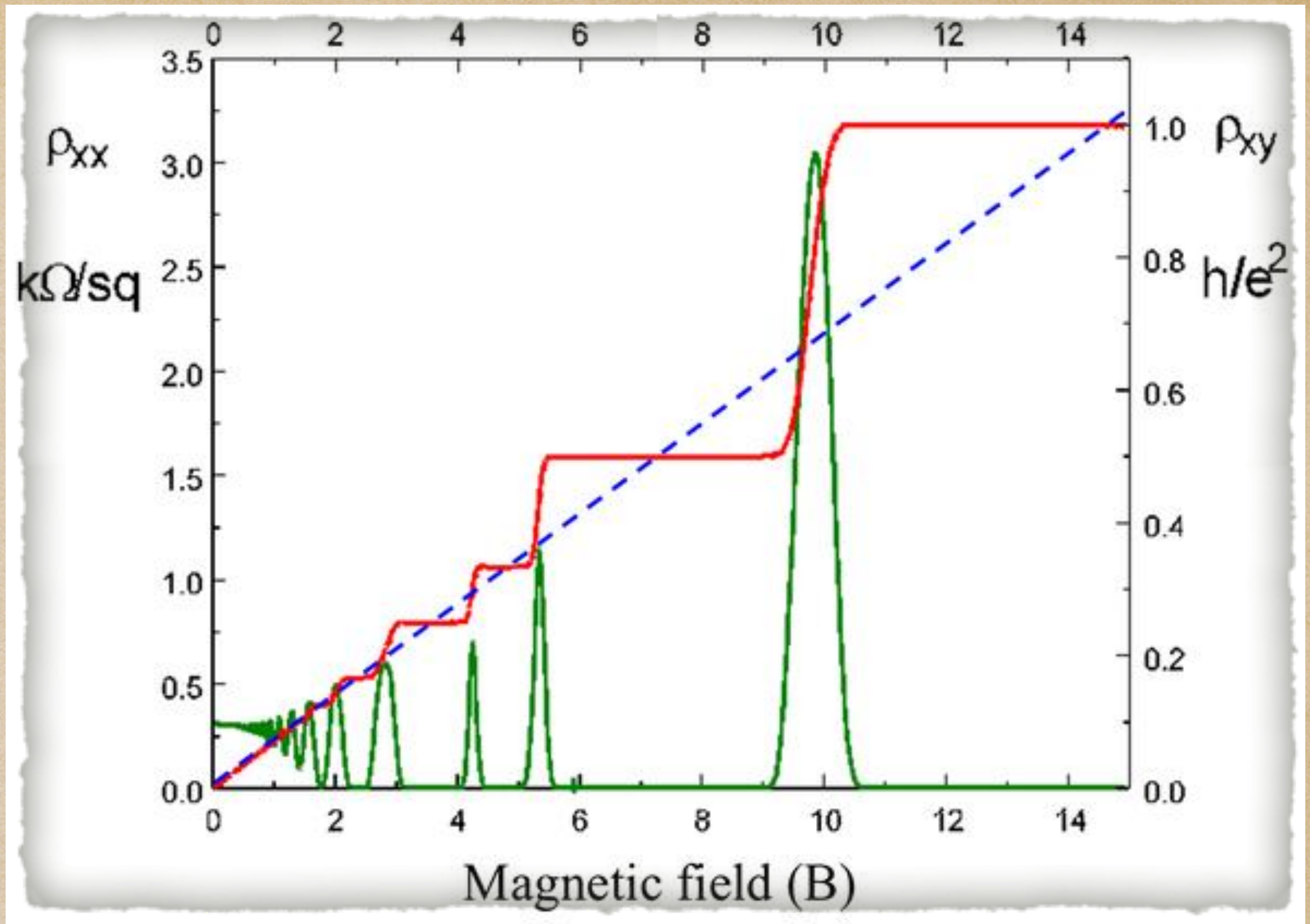
$$V_H = \frac{I_x B_z}{ndq} \qquad \rightarrow \rho_{xy} = \frac{V_H}{I_x} = \frac{B_z}{ndq}$$

Integer quantum Hall effect- 1982

von Klitzing, 1982

- Phenomenon that occurs in two dimensional electron systems at low temperatures and in the presence of strong magnetic fields
- Hall conductance quantised in terms of integers
- Longitudinal resistance is zero except when Hall current changes from one integer to another





- Experimentally, find that Hall conductance quantised in units of e^2/h . The unit of resistance now called von Klitzing is given by

h/e^2 = 25.812807557 (18) - standard of resistance

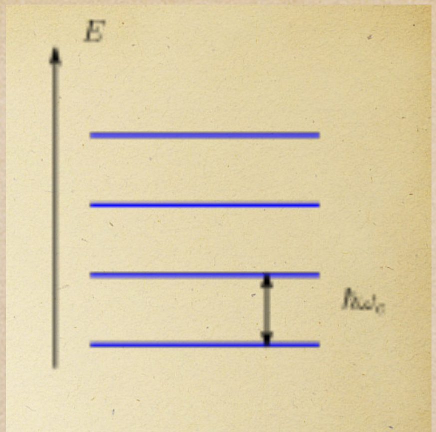
Quantum problem of single electron moving in a perpendicular magnetic field

- Quantum mechanical problem to solve is for an electron moving in two dimensions in a magnetic field in the z-direction $\mathbf{A} = (B_z y, 0, 0)$

$$H\psi(x,y) = \frac{(\mathbf{p} - e\mathbf{A})^2}{2m}\psi(x,y) = E_{n,p_x}\psi(x,y)$$

- Solutions are highly degenerate Landau levels

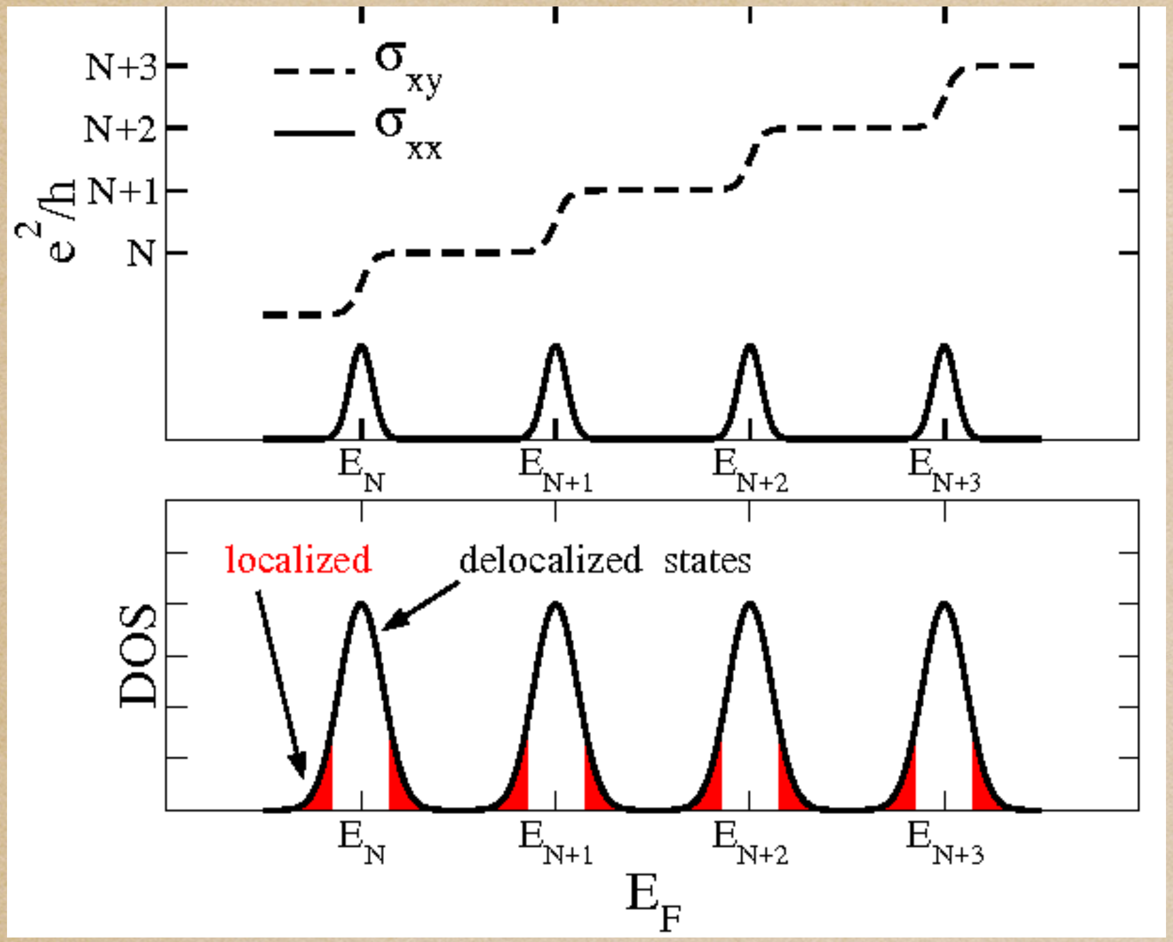
$$E_{n,p_x} = (n + 1/2)\hbar\omega, \quad \omega = eB_z/m$$



$$\omega = eB/m$$

- So when you put electrons in Landau levels, you get gaps in the energy, so you may think that it should be an insulator. But it is not!

- As we already know classically, the electrons drift when we apply a magnetic field, and one gets the Hall current perpendicular to the electric field



$$E_N = (N + 1/2)\hbar\omega$$

$$\omega = eB/m$$

$$\text{degeneracy} = \frac{B}{hc/e} = eB/hc$$

$$\nu = \frac{N}{eB/hc}$$

- Degenerate Landau levels spread out into localised states and extended states because of disorder

- When the density of electrons is such that integer number of Landau levels is filled, state is stable, gap to excitations
- Due to disorder, there are states in the gap but they do not conduct electricity (localised)
- Only states near centre of band carry current which is quantised

Halperin,1982

- Remarkable fact is that the quantisation is so extra-ordinarily accurate $\sigma_{xy} = ne^2/h$ with $n =$ integer (measured accuracy, 1 part in billion)

- Measurement made in complex, macroscopic many-body state, with impurities, at different temperatures, different sized and shaped materials, etc

- How does this happen? Answer - topological protection

Topological explanation of the quantisation

- Thouless recognised that the Hall current is related to a topological quantum number (like the winding number)

- Wave-functions for each Landau band define a map from the Brillouin zone (2-torus) to the space of physical states

- Can compute a number called Chern number (or TKNN number) for each Landau band

- Wave-functions for each Landau band define a map from the Brillouin zone (2-torus) to the space of physical states

- Phase of wave-function winds as we move around the Brillouin zone - captured by magnetic potential $\mathcal{A}_i(\mathbf{k}) = -i < u_k|\partial_{k^i}|u_k >$

- Integrating the magnetic field over the Brillouin zone gives the Chern number of the band

- $$C_\alpha = \frac{1}{2\pi}\int d^2k\ \mathcal{F}^\alpha_{xy} \qquad \mathcal{F}(\mathbf{k}) = \nabla \times \mathbf{A}(\mathbf{k})$$

- Conductance $\sigma_{xy} = \frac{e^2}{h}\sum_\alpha C_\alpha$ where C_α is the Chern number and the sum is over all filled bands

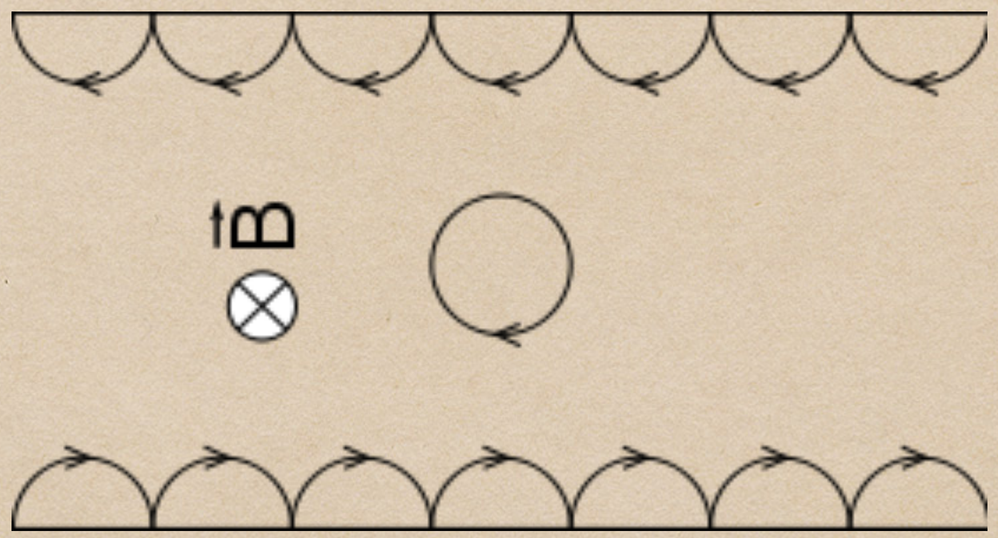
- This explains the extra-ordinary accuracy of the conductance quantisation - related to an integer which does not change in the presence of impurities - depends only on number of filled Landau levels

TKNN, PRL, 1982

III - Edge states and bulk-boundary correspondence

- What is the consequence of the fact that every quantum Hall state has a topological number attached to it?
- Most important is what happens at the boundary between different topological states

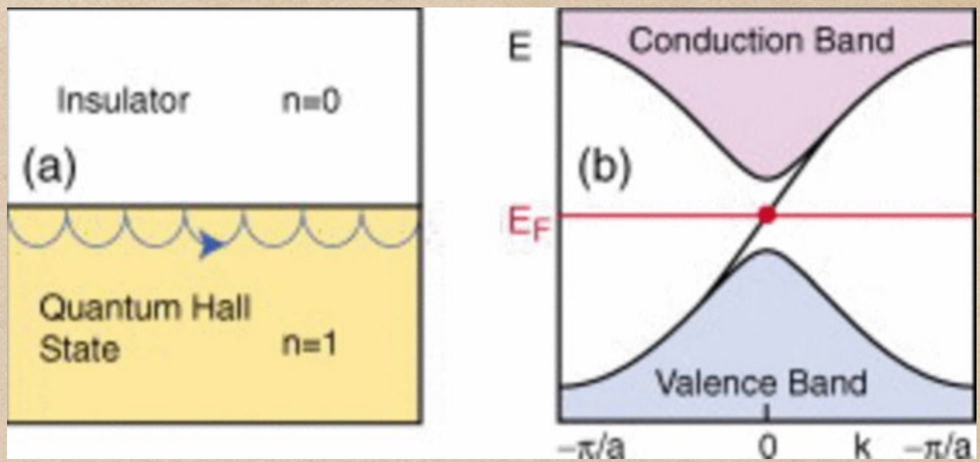
Semi-classical argument

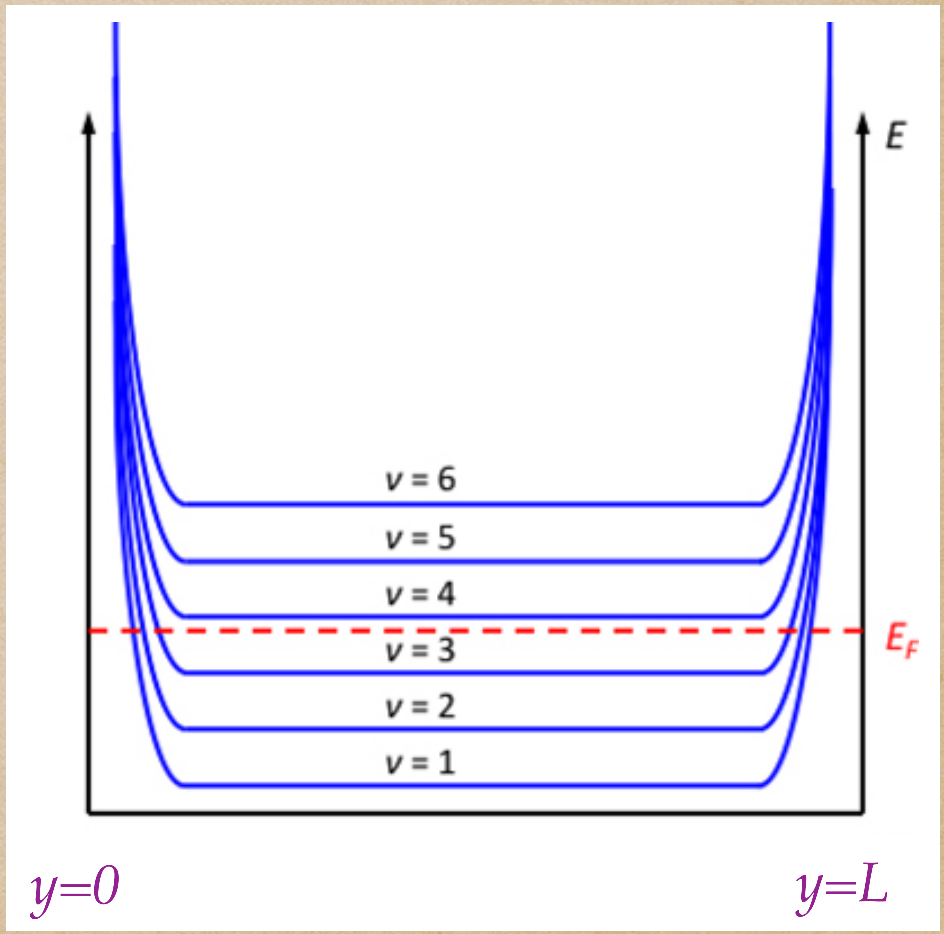


- If sample has an edge, a semi-classical picture implies electrons move in Landau orbits in the bulk, but have skipping orbits at the edges - implies one way transport at the edges
- So bulk is insulating and transport occurs at the edges

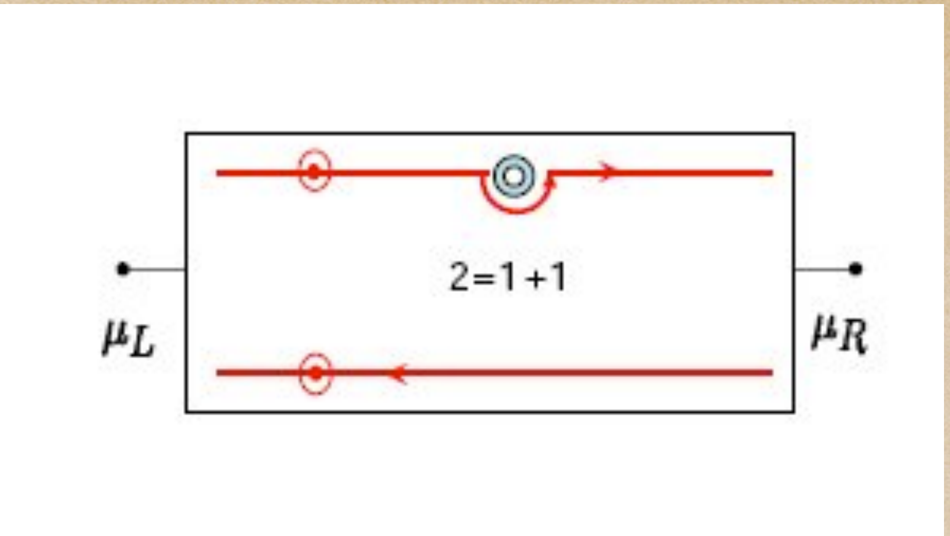
Quantum mechanical - bulk edge correspondence

- Quantum mechanically, the edge states are `chiral Dirac fermions' at top and bottom edges
- In real space, bulk spectrum consists of degenerate Landau levels which bend at the edges due to the confining potential
- One edge state per Landau level at the edge
- velocity $v_x = \dfrac{1}{eB}\dfrac{\partial E}{\partial y}$



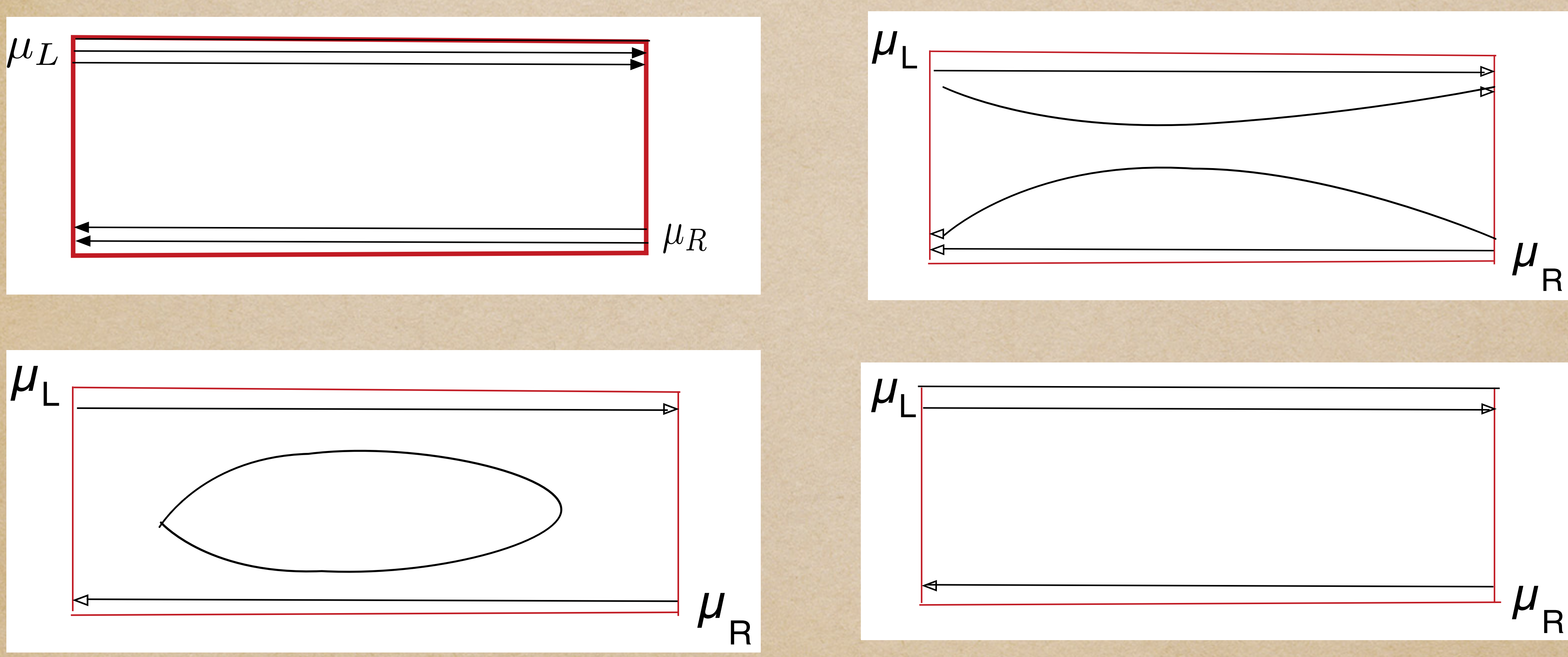


- Bulk-boundary correspondence
  Chern number in the bulk = number of edge states (related to index theorems in mathematics)



- The direction of flow at both edges is uni-directional, fixed by sign of magnetic field and <u>only edge states carry current</u>.
- Because of spatial separation of left and right movers at the edges, no possibility of back-scattering due to impurities
- Explains robustness and accuracy of quantum Hall effect and why it is not affected by impurities or disorder

- Can argue that when the system evolves from one IQH state to another, the number edge states change.
- Cannot happen when the bulk remains insulating - else the invariant cannot change



- The bulk gap has to close , implies current through the bulk, when the Chern invariant changes

- So main points of topological phase
  (a) bulk is an insulator and the current in only carried by edge states

- (b) quantised transport since there is no back-scattering

- The quantum Hall effect was initially seen to occur in two dimensional (2DEG) formed in a layer of AlGaAs sandwiched between GaAs material
- In recent times, quantum Hall effect seen in other 2D materials like graphene as well

- But this topological transport in IQHE happens at very low temperatures and very high magnetic fields
- The recognition that topological phases can exist in bands, even without the need for magnetic fields is what has led to the whole new revolution of topological materials in the last decade

IV- Topological materials Post -2005

The topological revolution 10-15 years ago - Topological insulators

- Realisation that strong magnetic fields were not required for topological phases
- Prediction of insulating materials with metallic surface states without magnetic field or time-reversal breaking - these were the topological insulators
- Haldane, prl(1988); Kane-Mele, prl (2005); Bernevig, Zhang, Wu, Hughes, (2006) ; R. Roy, archives (2006); Moore and Balents, prl (2007); Fu,Kane and Mele, prl (2007); Konig et al, science (2007); hasan et al, nature (2008).

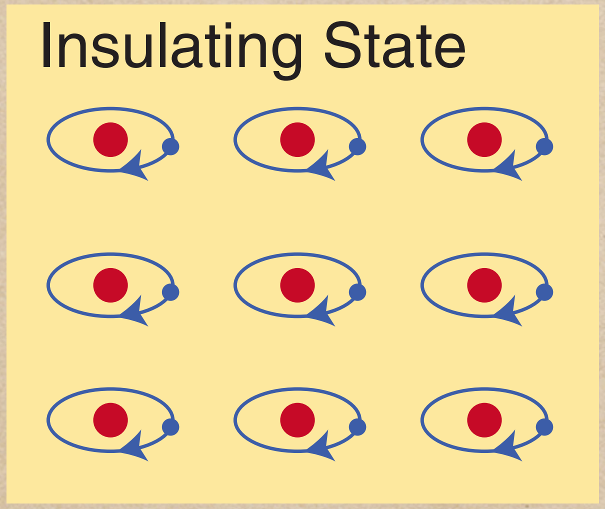
- Materials with strong spin-orbit coupling can `behave' like a quantum Hall state
- Insulating in the bulk but with conducting edge states - rather like block of wood covered with a metal, except that it is made of a single material - these are Topological insulators
- Joke - (R. Shankar from Yale) -`Do not stand on a topological insulator to change a light bulb'

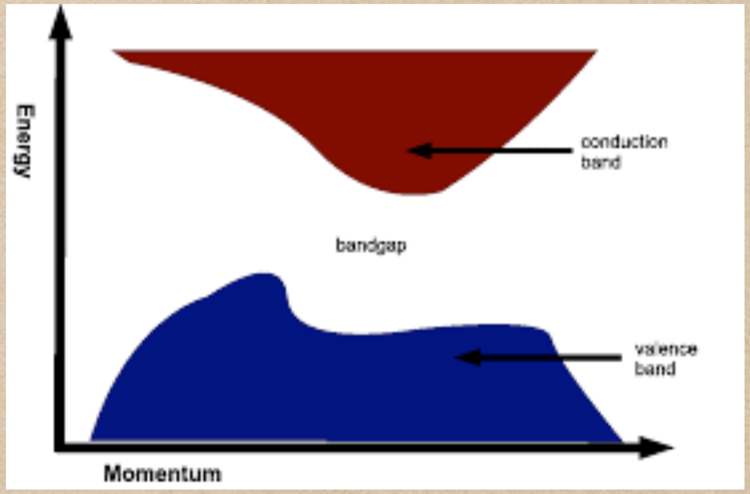
- Not discovered earlier for many reasons, including need for sophisticated instruments that can map local density of states to know which states carry current
- Theoretically, require understanding of Berry phases and structures of mappings of Brillouin zone to the Hamiltonian - more information than just the dispersion (energy of the states)
- <u>Predicted first</u>, and then experimentally observed - unlike the quantum Hall effect

Topological band theory

- Most basic and most `boring' state of matter - insulators
- Electrons are bound to atoms and cannot conduct electricity
- Atomic states broaden into bands and occupied states form valence band and unoccupied states form conduction band
- Can gradually move from atomic insulator to band or covalent insulator - topologically equivalent

- Size of the band - gap or shape does not matter - topologically equivalent to trivial insulator

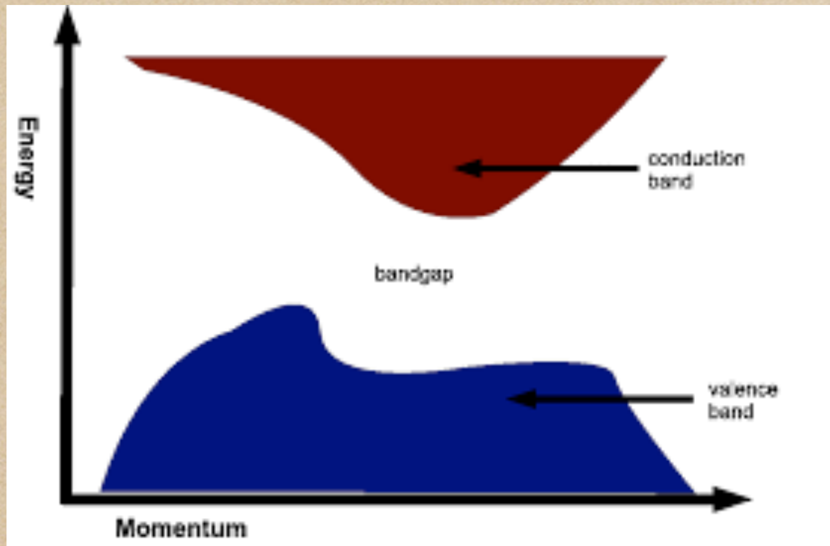


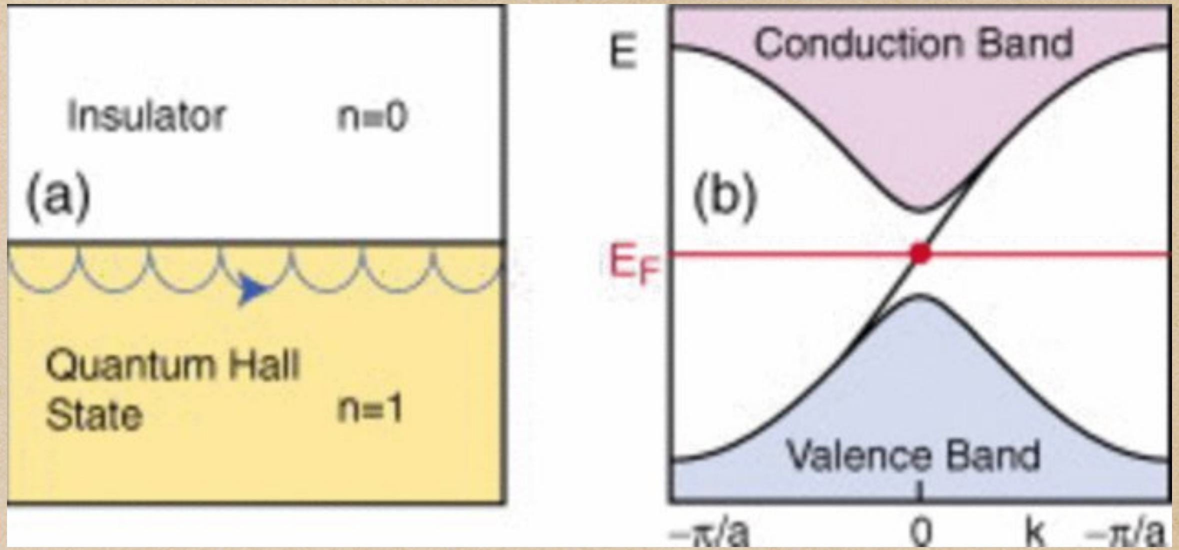


Adiabatic continuity and topology

- Insulators are topologically equivalent if they can be continuously deformed into each other while keeping the energy gap fixed
- Just like the donut can be deformed into a coffee cup continuously

- Are there phases that are not topologically equivalent to the trivial band insulator?
- If an orange is the analog of the trivial phase, then the donut is the analog of the non-trivial phase which cannot be adiabatically connected to an orange

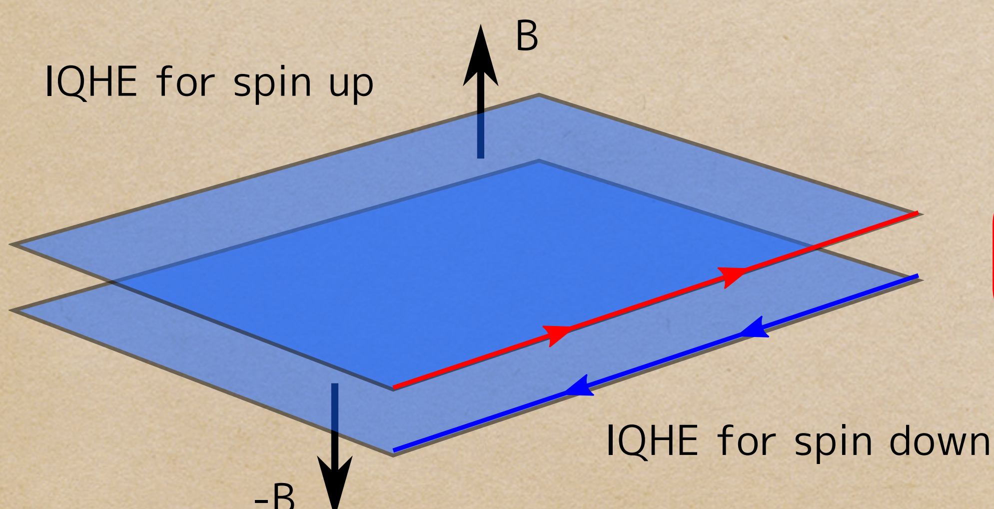


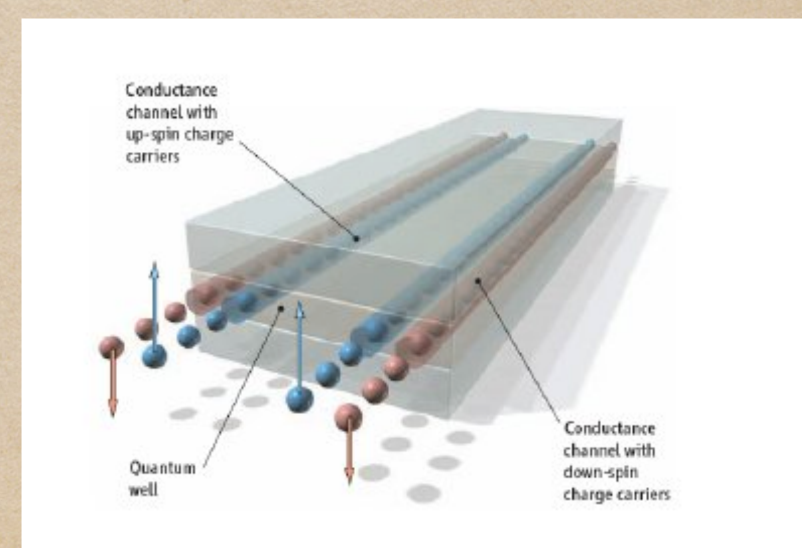


- Have found the quantum Hall phases which are topological, but they need strong magnetic field and break time-reversal invariance
- Are there topological phases with unbroken time reversal invariance?

Quantum spin Hall effect

- Independent and opposite IQHE for spin up and spin down electrons - no net magnetic field
- $\sigma_{xy,\uparrow} - \sigma_{xy,\downarrow}$ Is quantised as an integer modulo 2



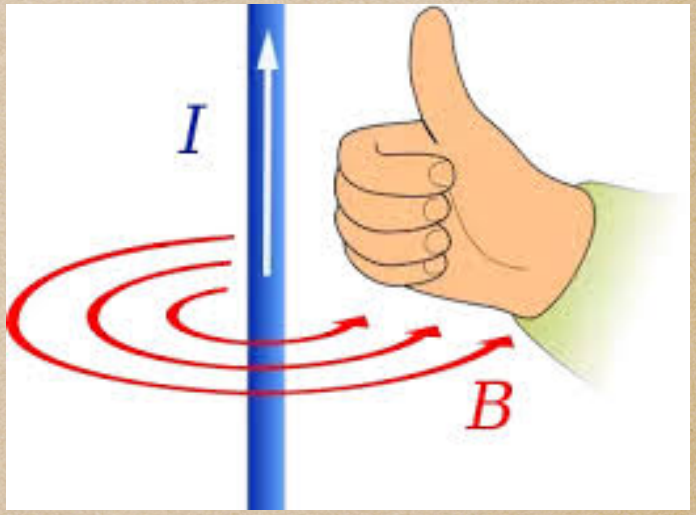


Topological insulators

- Interestingly, even without S_z conservation, for time-reversal invariant systems with 1/2 integer spins, the two classes survive
- But can no longer interpret it as independent QHE for spin up and spin down electrons
- Why does this happen?

Time reversal symmetry

- Microscopic Laws of physics remain the same when you evolve a system backwards in time. But under reversal of direction of time $\mathbf{B} \to -\mathbf{B}$
- Right moving edge states go to left moving edge states
- Spin up electrons go to spin down electrons



Kramer's theorem

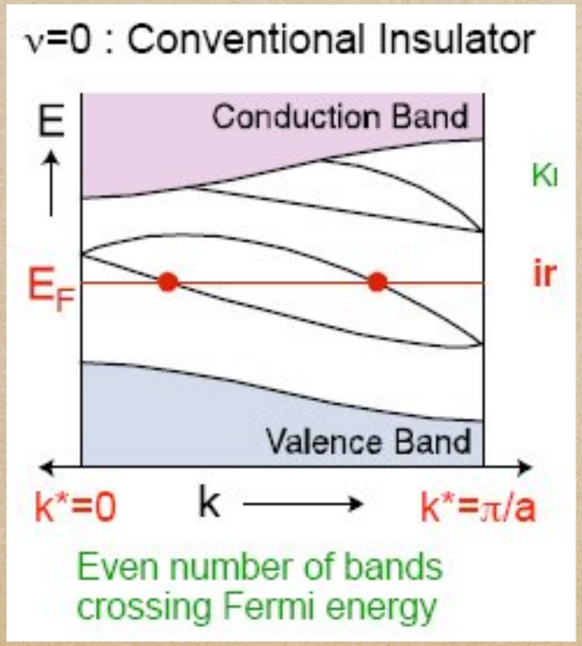
- For time-reversal invariant systems, $[T, H] = 0$
  for spin 1/2 particles, the time-reversal operator is anti-unitary $T^2 = -1$

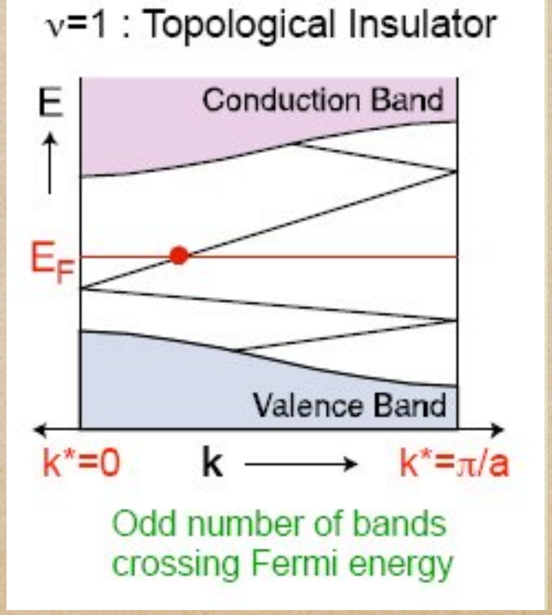
- All time-reversal invariant states are doubly degenerate. Proof : if they were the same state, then $T|\psi >= e^{i\phi}|\psi >$

- $$T^2|\psi >= Te^{i\phi}|\psi >= e^{-i\phi}T|\psi >= e^{-i\phi}e^{i\phi}|\psi >= |\psi >$$

- But this contradicts the statement $T^2 = -1$

- Energy bands are TR invariant and hence doubly degenerate at $k = 0$ and $k = \pi$
- Hence, there are two classes of possibilities for the states in an insulating gap - second case has at least one state crossing the Fermi level, whereas first case has even number of levels crossing Fermi level



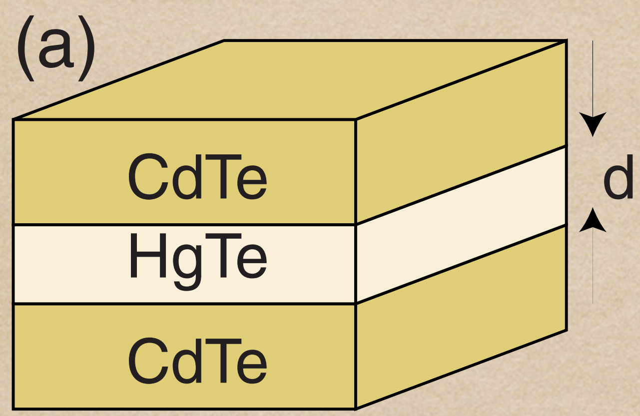


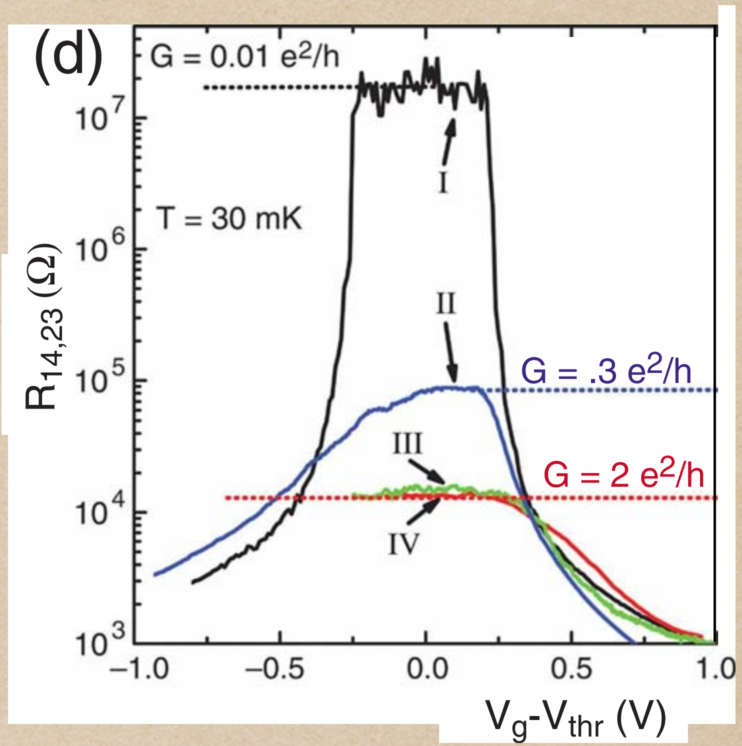
What are the consequences ?

- Essentially expect to see edge states like in the quantum Hall problem - 2 states of opposite chirality at each edge - time-reversed partners states

- Expect two terminal conductance of $2e^2/h$ for a rectangular 2D sample - one edge at top and one edge at bottom moving in same direction

Real material and experiments in 2D





- When thickness d is very small, not a TI and conductance not quantised (samples I and II)
- III and IV, thickness d is large enough and conductance is quantised

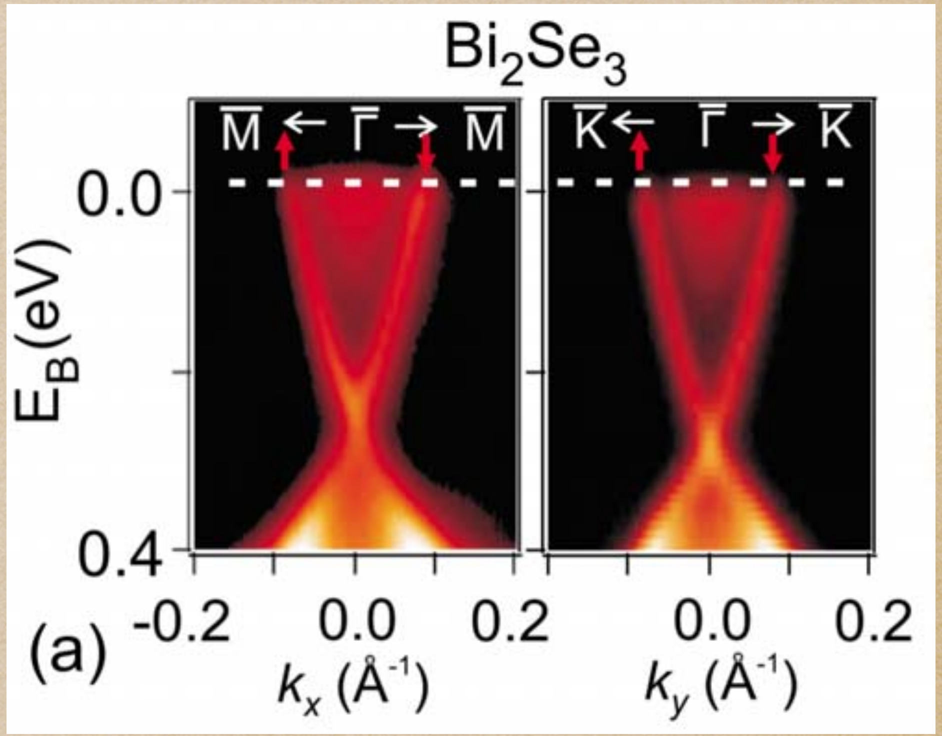
Konig *et al*, 2008

3D topological insulators

- Topological insulators can exist in three dimensions as well
- Then, surface states replace edge states as current carrying states and the bulk states are insulating
- Turns out that the electrically conducting states on the surface are `Dirac cones' - excitations that obey the Dirac equation instead of the usual Schrodinger equation that normal electrons obey

Real materials and experiments in 3D

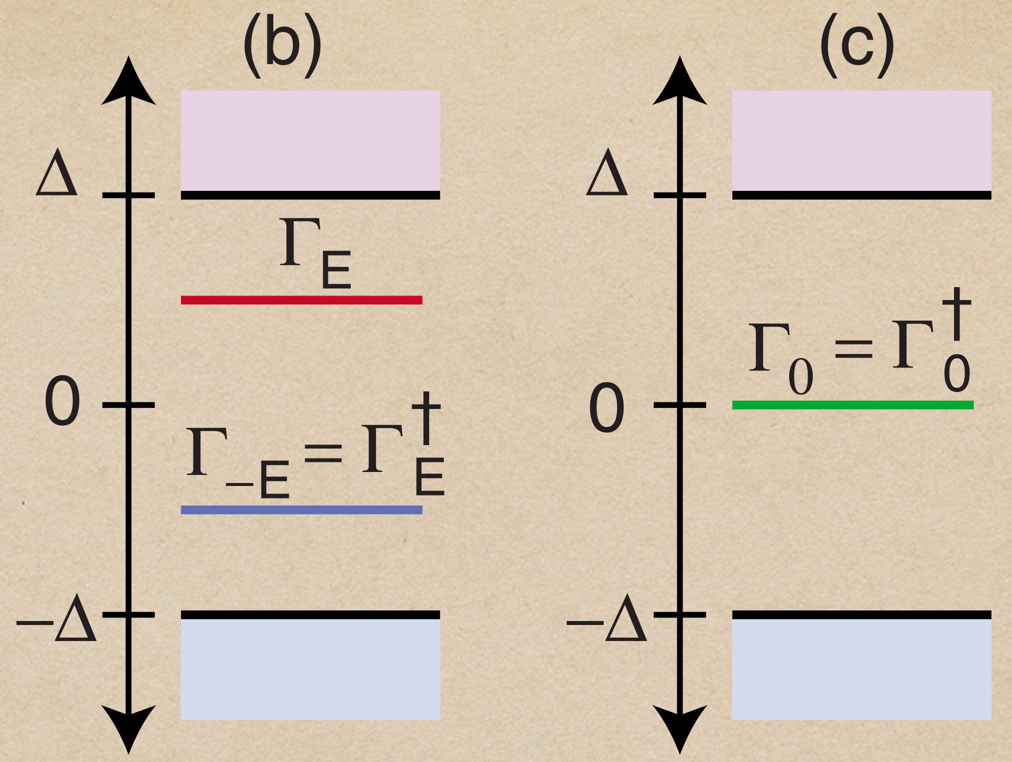
- Material called Bismuth Selenide - insulator, but has surface states
- ARPES (picture of energy as a function of momentum) and showed that surface states exist and formed Dirac cone as expected



Taniguchi *et al*, PRL, 2010

Topological superconductors

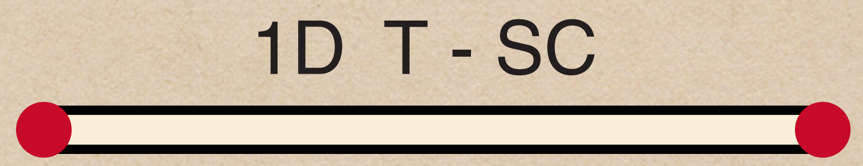
- Superconductors are like insulators, and can have valence bands and conduction bands
- Gap to bulk excitations exist, but can have edge states
- Only difference between topological insulators and superconductors - topological superconductors are particle-hole symmetric (excitations are Boguliobons or Boguliobov-de Gennes quasiparticles)



- Conduction band is a `mirror image' of the valence band - adding an electron to the conduction band is the same as removing an electron from the valence band (particle-hole symmetry)

- At zero energy, both these processes are the same - Majorana modes

One dimensional topological insulator



- Can have a state at zero energy. Can't move it away from zero energy because it does not have a partner

- Zero energy particle is its own antiparticle - Majorana mode

Kitaev, 2001

Majorana modes

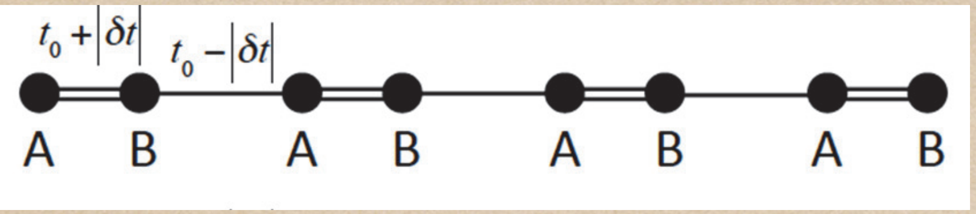
- Majorana modes give a new way of storing and manipulating quantum information
- The two Majorana modes at two ends define a single qubit of information non-locally
- So it can be immune from decoherence

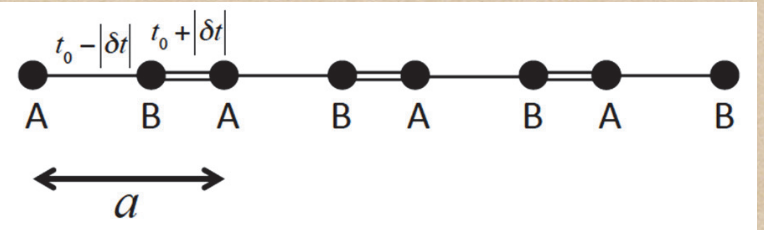
- These excitations obey non-abelian statistics under exchange (More exotic particles than fermions (antisymmetric under exchange), bosons (symmetric under exchange), or even anyons (non-trivial phase under exchange)
- Could be relevant as building blocks in making quantum computers

Explicit models in one dimension

One dimensional topological insulator

Su-Schrieffer-Heeger model

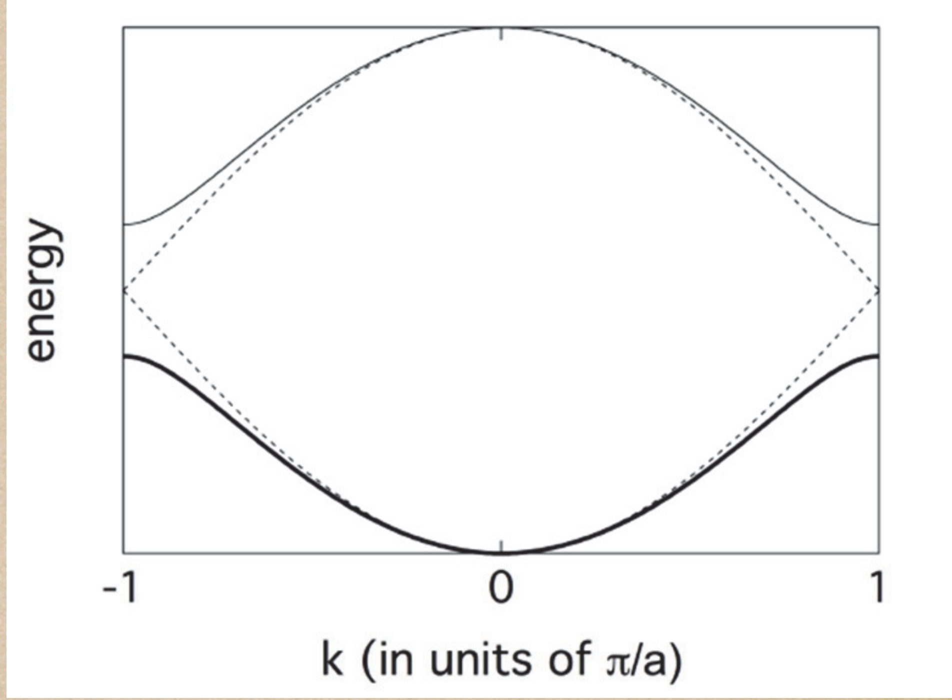




- Model of alternating long and short bonds with periodic boundary conditions and with 2N atoms - 2 band model

$$H = \Sigma_i [(t_0 + \delta t) c^\dagger_{A,i} c_{B,i} + (t_0 - \delta t) c^\dagger_{A,i+1} c_{B,i} + h.c.]$$

- We can solve by Fourier transforming to write the model as a 2 component model in momentum space as



$$H = \Sigma_i H_{ab}(k) c^\dagger_{ak} c_{bk}$$

$$H(k) = \mathbf{d}(k) \cdot \vec{\sigma}$$

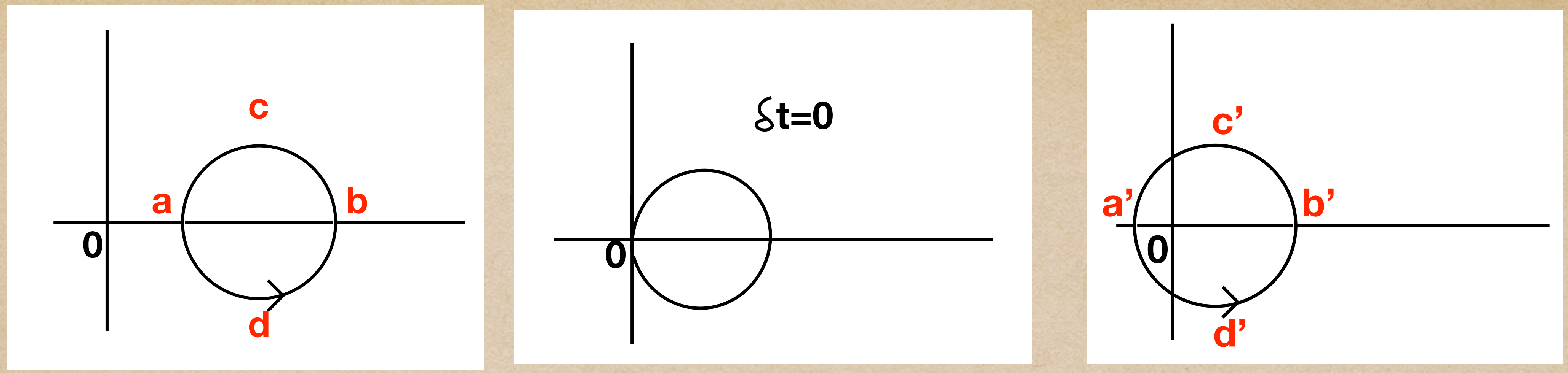
$$d_x(k) = (t_0 + \delta t) + (t_0 - \delta t) \cos ka$$

$$d_y(k) = (t_0 - \delta t) \sin ka$$

$$d_z = 0$$

-

- Can compute the topological invariant explicitly by integrating the Berry connection for the lower energy band over the first BZ
- But can also see the two topological phases pictorially
- Since atoms at A and B are the same, extra symmetry giving rise to $d_z = 0$, so $\vec{d}$ is constrained to lie on a plane



$$a = 2\delta t, d = (t_0 + \delta t)\hat{x} - (t_0 - \delta t)\hat{y}$$
$$b = 2t_0, c = (t_0 + \delta t)\hat{x} + (t_0 - \delta t)\hat{y}$$

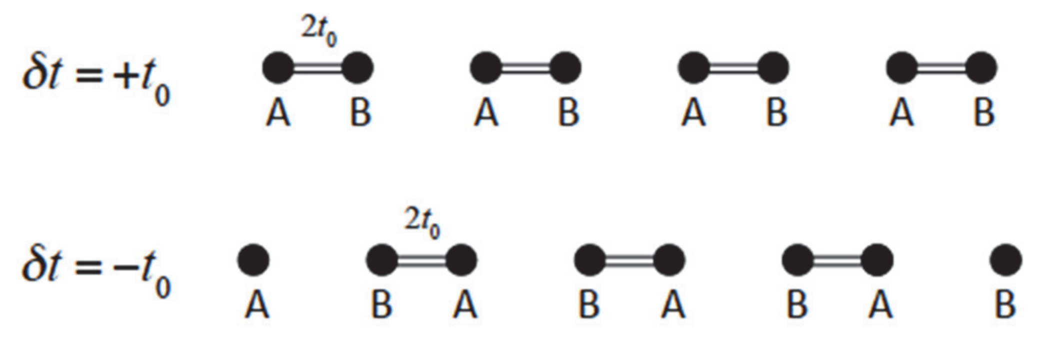
$$a' = -2|\delta t|, d' = (t_0 - |\delta t|)\hat{x} - (t_0 + |\delta t|)\hat{y}$$
$$b' = 2t_0, c' = (t_0 - |\delta t|)\hat{x} + (t_0 + |\delta t|)\hat{y}$$

- Can ask the question : how many times does the vector $\mathbf{d}(k)$ go around the origin as k evolves through the Brillouin zone ($-\pi/a$ to π/a)
- \`Zero\` on left and \`one' on right - depends on sign of δt
- To go from left to right configuration requires δt to go through zero, implies energy gap goes through zero

$$E(k) = \pm\sqrt{2(t+\delta t)^2 + (t-\delta t)^2 \cos ka)} = 0, \text{when } \delta t = 0, ka = \pm\pi$$

- On the left, circle can be shrunk to a point, so Berry phase is zero
- On the right $\mathbf{d}(k)$ completes a circle around the origin when k goes through the BZ, also a circle. So winding number is one - Berry phase of pi
- Two different topological sectors - LHS is a trivial insulator and RHS describes a topological insulator

Edge states in the Su-Schrieffer Heeger model



- Can also explicitly check for edge states in this model - most obvious for the fully dimerised case when $\delta t = \pm t_0$

$$H = \Sigma_i [(t_0 + \delta t) c^\dagger_{A,i} c_{B,i} + (t_0 - \delta t) c^\dagger_{A,i+1} c_{B,i} + h.c.]$$

- Edge states are topologically protected even when $\delta t \neq \pm t$ - they remain at zero energy, although they are not completely localised at the edge

One dimensional topological superconductor

Kitaev model

- Toy model with Majorana modes - one dimensional spinless p-wave superconductor

$$H = -\mu \sum_{x=1}^{N} c_x^\dagger c_x - \frac{1}{2} \sum_{x=1}^{N} (t c_x^\dagger c_x + \Delta c_x c_{x+1} + h.c)$$

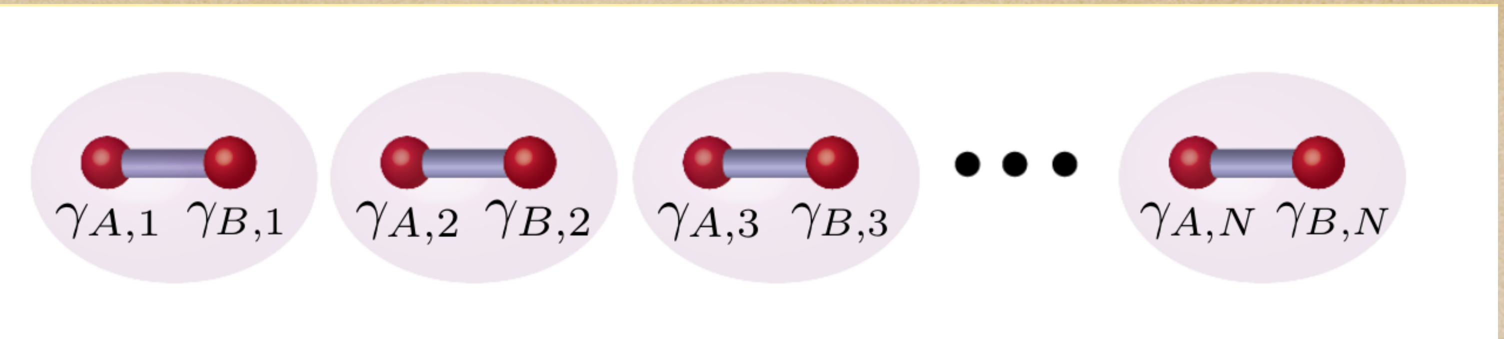
- Here, μ = chemical potential, t = hopping and Δ = pairing term

- We can rewrite the model in terms of Majorana operators

- Can rewrite in terms of Majorana operators

$$c_x = \frac{1}{2}(\gamma_{A,x} + i\gamma_{B,x})$$
$$c_x^\dagger = \frac{1}{2}(\gamma_{A,x} - i\gamma_{B,x})$$

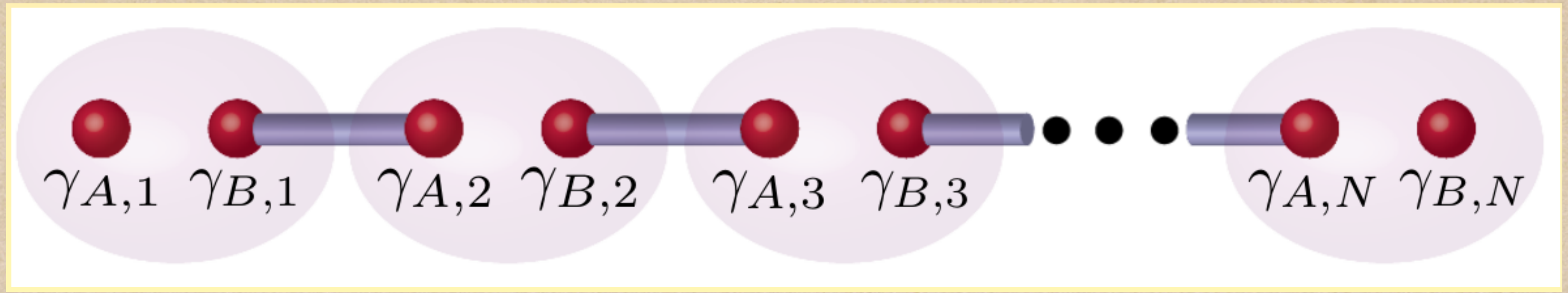
- Model can be easily solved in two limits



- When $\mu < 0, t = \Delta = 0$, topologically trivial phase

$$H = -\frac{\mu}{2} \sum_{x=1}^{N} (1 + i\gamma_{B,x}\gamma_{A,x})$$

- Only bonds between Majoranas at same site x
- Ground state is unique and ends of the chain do not play any unique role



- Second limit : When $\mu = 0, t = \Delta \neq 0$

$$H = -i\frac{t}{2}\sum_{x=1}^{N-1}\gamma_{B,x}\gamma_{A,x+1}$$

- Here bonds between Majoranas on adjacent sites
- But unpaired Majoranas $\gamma_1 \equiv \gamma_{A,1}$ and $\gamma_2 \equiv \gamma_{B,N}$ at the two ends

- The Hamiltonian has no dependence on these two unpaired Majorana modes γ_1 and γ_2
- We can form an ordinary, but non-local fermion from these two Majoranas

$$f = \frac{1}{2}(\gamma_1 + i\gamma_2), f^\dagger = \frac{1}{2}(\gamma_1 - i\gamma_2)$$

- Energy is independent of whether this fermion state is occupied or not
- So non-unique ground state, or rather, ground state here is doubly degenerate

$$|0> \text{ and } |1>= f^\dagger|0>$$

- So the Majorana modes at the two ends define a single quit of information non-locally and can be immune from decoherence
- These excitations can also be shown to obey non-abelian statistics under exchange
- Can be relevant in quantum computation

Current frontiers in the field

Current frontiers in the field

- Many new materials have been found which are topological
- Not only insulators but also what are called semi-metals - Weyl semimetals and Dirac semimetals - essentially generalisations of graphene which has a Dirac cone at the Fermi level, where valence and conduction bands touch
- Higher order topological insulators - 2DTI with corner modes and 3DTI with hinge states as edge states

Floquet topological phases induced by driving

- Recently found that new topological phases and edge states can be obtained by shining light on topologically trivial systems and bands are found to be characterised by other topological invariants besides the Chern number

- Topological phases of periodically driven systems have been characterised using Floquet theory

T.Oka and H. Aoki,prb,2009
N. H.Lindner, G. Refeal and V. Galitsky, Nature,2011

Interplay of interactions and topology

- Know one strongly interacting system which has topological protection - fractional quantum Hall state
- Generalisations of them - fractional Chern insulators or fractional topological insulators?

Quest for Majoranas - several ideas

- Ordinary superconductors in proximity to topological materials
- One dimensional wires with strong spin-orbit coupling and magnetic field proximity coupled to superconductors - effectively topological superconductor
- Majorana modes seem to have been seen!
- Other fractional Majorana fermions or parafermions?

Glimpse of my collaborators

My collaborators

- Senior people from other institutes
- Postdocs and students

- Have explored various aspects of these phases, including quantum Hall effect, graphene, silicene, Weyl semi-metal, Floquet induced phases, Majorana modes, etc

Take-away points

- New class of materials defined by interplay of symmetry and topology
- Insulators, superconductors, metals, now exist in topologically trivial and topologically non-trivial classes
- Even materials in topologically trivial classes can be made interesting (topological) by shining light on the material

Take-away points (cont)

- All kinds of exotic excitations exist in these materials
  relativistic particles like Dirac and Weyl fermions, particles with unusual statistics like anyons and Majorana modes
  other particles like monopoles, dyons and axions
- Exotic particles and exotic effects at low energies!

Topological phases are here to stay!

Thank you all for coming and listening to me!