Towards Understanding Topological Insulators

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Acknowledgement

- S.-Q. Shen (Hong Kong), Lectures at ICTS Topology School
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Goal and Outline

- Goal – Answer the question: What the !@@! is a topological insulator (TI)?

- Where do TIs fit into condensed matter physics?
- Symmetries (revise time reversal)
- Band theory – metals and insulators
- Integer quantum Hall effect
- 2D TIs
- 3D TIs
- Why the fuss? What can you do with TIs?

Prerequisites

- Graduate quantum mechanics (including second quantization)
- Basic solid state physics (@Kittel)
- ...
- A keen desire to understand things and put in the necessary effort

Follow the maxim (source: T. V. Ramakrishnan):

There are no stupid questions, only stupid *answers*!

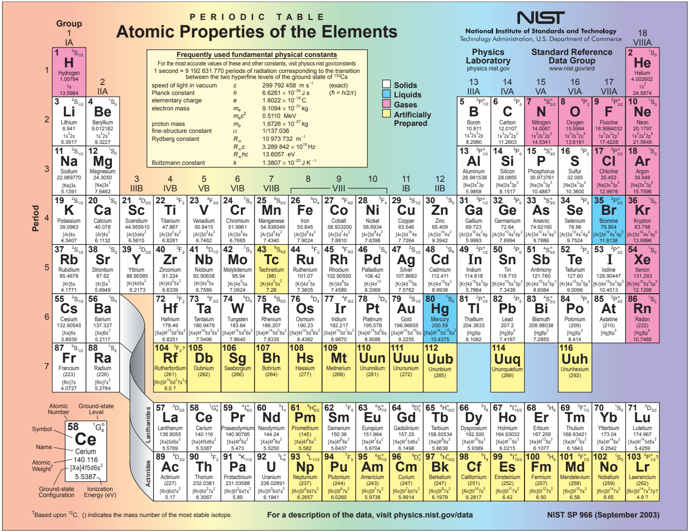
DISCLAIMER: The speaker is *NOT* an expert! Focus is on *elementary concepts*...not on calculations

References

- *RMP* by Hassan and Kane
- *Physics Today* article by Qi and Zhang
- *Annual Reviews of Condensed Matter* by Hassan and Moore
- *PRB* Papers by Rahul Roy

Condensed Matter

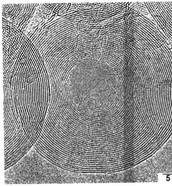
- Operative definition of condensed matter: A collection/aggregate of atoms/ions in the non-relativistic regime
- "Raw materials" for condensed matter



Condensed Matter

- What happens when we aggregate atoms? Many things...
- In fact, the *same atoms* will give you *very* different things if aggregated differently! Eg., carbon atoms give

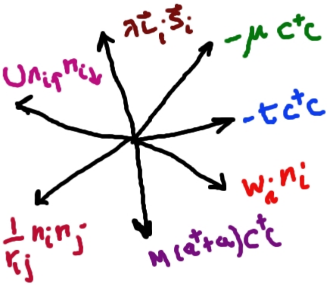




- Different arrangement of atoms leads to very different emergent properties!
- Again: More is different... *Different* mores are more so!
- Natural question: What are all the different "emergent states/things/properties" can we obtain by aggregating atoms?

Quantum Condensed Matter Physics

- We will dwell mainly on electrons in materials
- Electrons in materials experience various things:



...this defines the "space of Hamiltonians" for the electrons

- The ground state (and concomitant excitations) of the electrons depend on *where* in the Hamiltonian space you are! There are many "electronic phases"
- One encounters (quantum) phase transitions as one moves about in the Hamiltonian space!

Electronic Phases

- Electrons in materials can organize themselves in many different ways – "phases/states"...we have
  - Metals
  - Semi-metals
  - Insulators/Semiconductors
  - Topological insulators
  - Superconductors
  - Magnets
  - Charge density wave systems
  - Spin liquids
  - ...
- Each of these have a common set of characteristics...(similar in sprint to: all liquids flow). In this sense each of the above is an "electronic phase"!

Electronic Phases

- The goal of condensed matter research is to discover and understand “all” the phases of electrons!
- Think of a “character table”

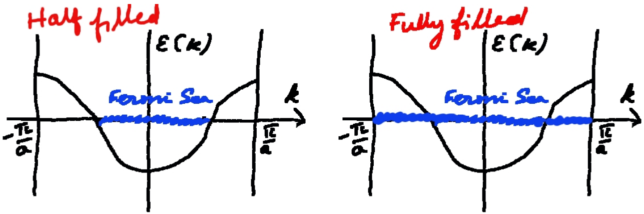
Phase / Prop	Metal	Insult	SC	....
C_v	$\sim T$	e^{-T/E_g}	$e^{-T/\Delta}$	...
χ	c	e^{-T/E_g}	$e^{-T/\Delta}$	....
σ	$\sigma_0 + T^2$	~ 0	∞	....
⋮	⋮	⋮	⋮	⋱

...idea is to tabulate phases and their properties...and *add* to this table!

- This is useful ...and *most interesting!*

Characterization of Phases

- Question: How do we characterize phases?
- Key idea: Symmetry...many electronic phases break the symmetries of the Hamiltonian...e.g., a ferromagnet breaks time reversal and spin rotation symmetry
- Not all phases can be distinguished by symmetry...



...we go from the half filled state to the fully filled state by tuning the chemical potential

- There is *no* symmetry difference, but the states are *very* different!

Characterization of Phases

- Phases with the same symmetry can have very different *responses*
- This is the idea behind classification as "metals" ($\sigma_{DC} > 0$) and "insulators" ($\sigma_{DC} = 0$)
- Abstractly: The phase is characterized by how "test particles behave in the phase (system)"...the "most natural" test particle – light(photon)!
- In somewhat more technical language: ψ – "matter" fields, A^μ gauge fields associated with light

$$\mathcal{S}[\psi, A^\mu] = \int \left(\mathcal{L}(\psi^\star, \psi, A^\mu) - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \right)$$

$$\bigvee$$

$$\text{Integrate out } \psi$$

$$\bigvee$$

$$\mathcal{S}^{\text{eff}}[A^\mu] = \int \mathrm{d}1\, \mathrm{d}2\, A^\mu(1) K_{\mu\nu}(1,2) A^\nu(2) - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

Characterization of Phases

- $K_{\mu\nu}(1,2)$ is the electromagnetic response function which can be calculated by the Kubo formula

$$K_{\mu\nu}(1,2) \sim -\langle T\, j_\mu(1) j_\nu(2) \rangle$$

where j_μ is the current...the mean is taken over the ensemble describing an (equilibrium) state of the fermionic system ☞ **Find out more: Kubo formula is actually just second order perturbation theory.**

- $K_{\mu\nu}(\mathbf{q},\omega)$ (written in Fourier space) *characterizes the system*...A metal has a very different characteristic functional form of $K_{\mu\nu}$ than an insulator or superconductor!
- The DC conductivity of the system is related to $K_{\mu\nu}$

$$\sigma_{DC} \sim \lim_{\omega\to 0,\, \mathbf{q}\to\mathbf{0}} \frac{1}{i\omega} K_{\mu\nu}(\mathbf{q},\omega)$$

- Key point: The nature of the state of electrons *modifies* how an electromagnetic wave propagates in the system...this can be used to *characterize* the phase that the electrons organize themselves in

Insulators

- An insulating state is characterized by $\sigma_{DC} = 0$
- This can arise in many ways
- Non-interacting systems
  - Band insulators
  - Anderson insulators (due to disorder)
- Interacting systems
  - Mott insulators
- These states have $\sigma_{DC} = 0$, but very different $\sigma(\omega)$...electromagnetic response *can distinguish* these phases!

We are interested in *band insulators*...*non-interacting electrons*!
These come in two varieties:

- Ordinary (trivial) insulators (OI)
- Topological insulators (TI)

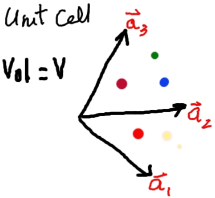
Immediate goal: Look at one-electron physics in crystals

One-Electron Physics in Crystals

- Preliminaries
- Symmetries – mainly time reversal
- Tight binding models
- Metals and insulators
- Example: Graphene
- Example: Insulator (related to graphene)
- Edge states

One-Electron Physics in Crystals: Preliminaries

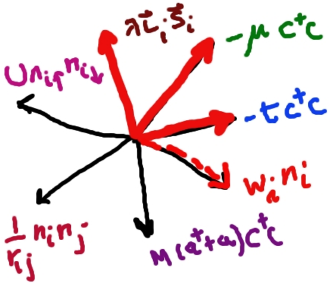
- Unit cell with many atoms (unit cell vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$)



- Hamiltonian

$$\mathcal{H} = T + V + H_{\rm SO}$$

  - $T = \frac{\mathbf{P}^2}{2}$ – kinetic energy
  - V – potential due to ions
  - $H_{\rm SO}$ spin-orbit interaction (keep aside for now)



Subspace of focus in the Hamiltonian space

Symmetries

Symmetry – Quick Revision

- System $\equiv$ A Hilbert space + Hamiltonian $\mathcal{H}$
- A symmetry operation $\mathcal{U}$ on a system is a function on the Hilbert space, such that if $|\tilde{\phi}\rangle = \mathcal{U}(|\phi\rangle)$ and $|\tilde{\psi}\rangle = \mathcal{U}(|\psi\rangle)$, then $|\langle\tilde{\phi}|\tilde{\psi}\rangle| = |\langle\phi|\psi\rangle|$ for all $|\phi\rangle$ and $|\psi\rangle$ ☞Question: What are some symm. ops. on $\mathbb{R}^3$?
- Wigner's theorem: A symmetry operation $\mathcal{U}$ is either a *linear/unitary* or an *anti-linear/unitary* operator ☞Find out more: Look at Gottfried and Yan
- A symmetry operation $\mathcal{U}$ is a symmetry of the system if $\mathcal{U}^{-1}\mathcal{H}\mathcal{U} = \mathcal{H}$, i. e., the Hamiltonian is unchanged by the symmetry operation

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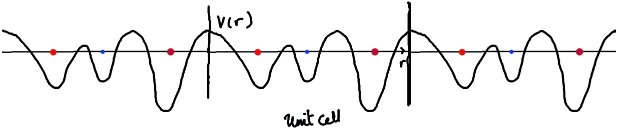
- Hilbert space: space spanned by $\{|\mathbf{r}\sigma\rangle = |\mathbf{r}\rangle \otimes |\sigma\rangle\}$ where $\mathbf{r}$ runs over points in a box of volume $\Omega = N\mathcal{V}$, N number of unit cells, $|\sigma\rangle, \sigma = \uparrow, \downarrow$ span the spin sector
- Hamiltonian: $\mathcal{H} = T + V \equiv \frac{-\boldsymbol{\nabla}^2}{2} + V(\mathbf{r})$
- Symmetries
  - Lattice translation
  - Time reversal
  - Parity (Inversion) – Not always, but in most crystals

Lattice Translations

- Translation operator $\mathcal{T}(\mathbf{a}) = e^{-i\mathbf{a}\cdot\mathbf{P}}$; $\mathcal{T}(\mathbf{a})|\mathbf{r}\rangle = |\mathbf{r}+\mathbf{a}\rangle$
- Every lattice translation $\mathcal{T}(\mathbf{l})$, $\mathbf{l} = \sum_\alpha n^\alpha \mathbf{a}_\alpha$ is a symmetry of our Hamiltonian ☞ **Exercise: Show that $\mathcal{T}(\mathbf{l})$ form a group. Is it a non-Abelian group?**
- Seen by noting that $V(\mathbf{r}+\mathbf{l}) = V(\mathbf{r})$ for all $\mathbf{l}$



- $\mathcal{T}(\mathbf{l})$ has right eigenstates which are labelled by the crystal momentum $\mathbf{k}$ which lives in the 1st Brillouin zone ...this is Bloch theorem

$$\mathcal{T}(\mathbf{l})|\phi_\mathbf{k}\rangle = e^{-i\mathbf{l}\cdot\mathbf{k}}|\phi_\mathbf{k}\rangle, \quad \forall \mathbf{l}$$

Every $|\phi_\mathbf{k}\rangle = \sum_\mathbf{G} \phi_\mathbf{k}(\mathbf{G})|\mathbf{k}+\mathbf{G}\rangle$, where $|\mathbf{k}+\mathbf{G}\rangle$ are plane waves, $\mathbf{G}$s are reciprocal lattice vectors, $\phi_\mathbf{k}(\mathbf{G})$ are c-numbers ☞ **Exercise: Prove this statement**

Lattice Translations

- Since $[\mathcal{T}(\mathbf{l}), \mathcal{H}] = 0, \forall \mathbf{l}$, find simultaneous eigenstates of $\mathcal{H}$ and $\mathcal{T}(\mathbf{l})$

$$\mathcal{T}(\mathbf{l})|\psi_{\mathbf{k}}\rangle = e^{-i\mathbf{l}\cdot\mathbf{k}}|\psi_{\mathbf{k}}\rangle, \quad \forall \mathbf{l} \quad \text{and} \quad \mathcal{H}|\psi_{\mathbf{k}}\rangle = \varepsilon|\psi_{\mathbf{k}}\rangle$$

- Note that $\psi_{\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r}|\psi_{\mathbf{k}}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$ where $u_{\mathbf{k}}(\mathbf{r}+\mathbf{l}) = u_{\mathbf{k}}(\mathbf{r})$...Bloch states are modulated plane waves ☞ **Exercise: Show this**
- $u_{\mathbf{k}}(\mathbf{r})$ satisfies a Schrödinger equation

$$\left[\frac{1}{2}\left(-i\boldsymbol{\nabla} + \mathbf{k}\right)^2 + V(\mathbf{r})\right] u_{\mathbf{k}}(\mathbf{r}) = \varepsilon u_{\mathbf{k}}(\mathbf{r})$$

  which is an eigenvalue problem defined *only on the unit cell $\mathcal{V}$*!
  ☞ **Exercise: Show this**

- For each $\mathbf{k}$, therefore, there is a discrete spectrum $\varepsilon_n(\mathbf{k})$ and associated states $u_{\mathbf{k}n}(\mathbf{r})$; equivalently

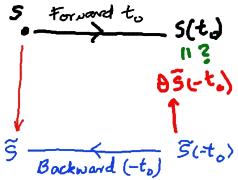
$$\mathcal{H}|\psi_{\mathbf{k}n}\rangle = \varepsilon_{\mathbf{k}n}(\mathbf{k})|\psi_{\mathbf{k}n}\rangle, \quad \langle \mathbf{r}|\psi_{\mathbf{k}n}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}n}(\mathbf{r})$$

  The energy functions $\varepsilon_n(\mathbf{k})$ is the n^{th} band
- Diagonalized Hamiltonian $\mathcal{H} = \sum_{\mathbf{k}n} \varepsilon_n(\mathbf{k})|\mathbf{k}n\sigma\rangle\langle\mathbf{k}n\sigma|$

Time Reversal (TR) Symmetry

- TR symmetry $\mathbf{\Theta}$ requires two things:
  - Idea of a time reversed state
  - Idea of reverse time evolution

  ..understand this first in classical mechanics
- A state $\mathbf{s} = (\mathbf{r}, \mathbf{p})$, $\mathbf{\Theta s} = \tilde{\mathbf{s}} = (\mathbf{r}, -\mathbf{p})$
- Reverse time evolution, integrate Hamilton's equation "backwards", i. e., negative times
- Understand this for a simple classical system
- A system is said to be time reversal invariant if the following diagram commutes



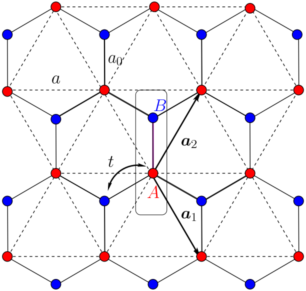
...system is time reversal invariant if $\mathbf{\Theta}(\tilde{\mathbf{s}}(-t_0)) = \mathbf{s}(t_0)$ *for all* $\mathbf{s}$ and t_0

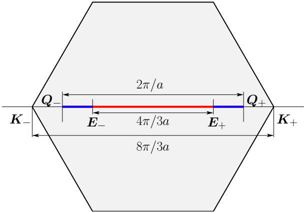
- Examples of systems with and without TR symmetry

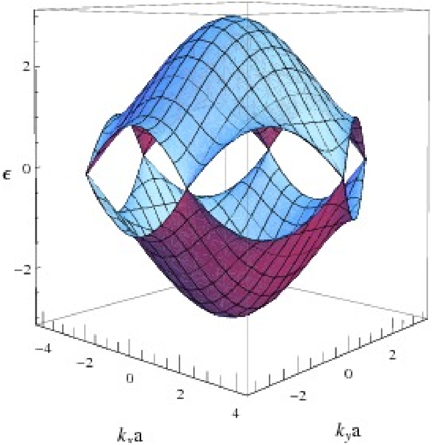
TI Crash Course: Plan of Action

- Complete TR invariance, Kramer's theorem
- Tight binding models, role of TR invariance
- Graphene – massless
- Graphene – massive
- Edge states
- Integer quantum hall effect: landau levels, edge states
- Laughlin's argument
- Quantum Hall effect on a lattice: Hofstadter butterfly
- TKNN formula $\equiv$ Chern number, topological quantization
- Hatsugai's connection between Chern number and edge states
- QHE without magnetic field – Haldane model and edge states
- Introduction of spin-orbit interaction
- Obtaining a TI by gluing two Haldanes – edge states
- General arguments using TR in 2D – Z_2 index
- 3D - brief statements
- Possibilities with TIs
- Topology and geometry in physics

Graphene



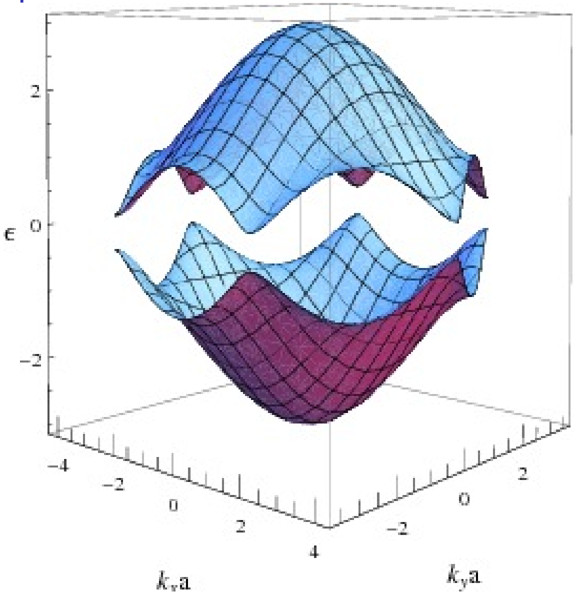




Thanks: J. P. Vyasanakere

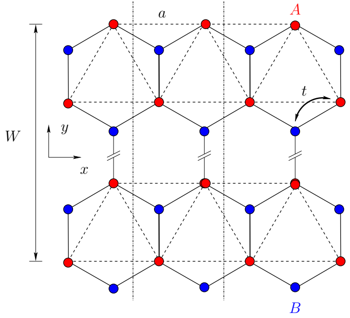
☞ Question: Which are the TR invariant momenta?

Massive Graphene



Thanks: J. P. Vyasanakere

Edge States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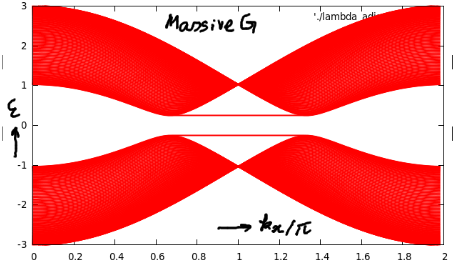
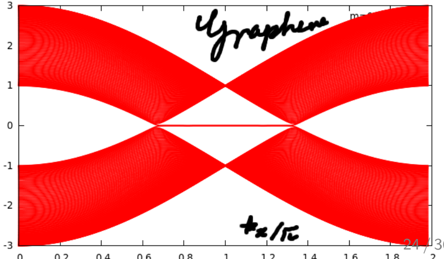
A
t
W
y
x
B


Massive G
ε
kx/π
3
2
1
0
-1
-2
-3
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2


Graphene
kx/π
3
2
1
0
-1
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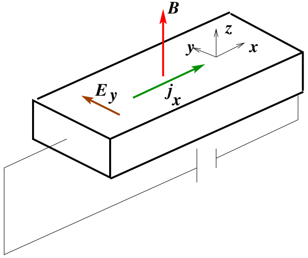
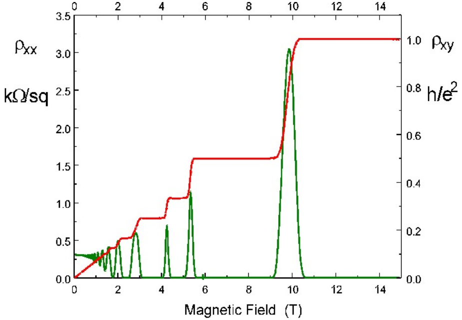
-3

Integer Quantum Hall Effect

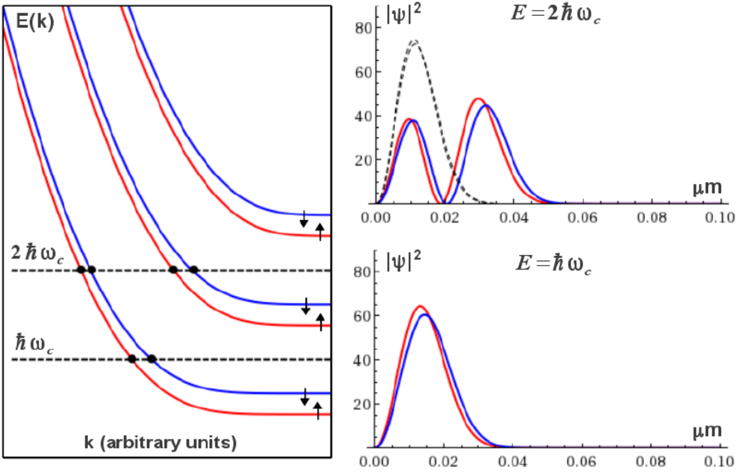




Source: von Klitzing's homepage

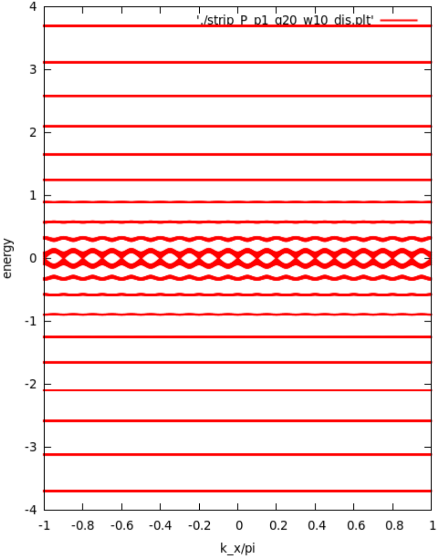
- Puzzle: The plateaus, and why integer?
- We will *not* discuss the resolution of the puzzle in detail... ☞ **Find out more: Look at any standard book on QHE, e. g., by Jain**

Edge States in Integer Quantum Hall

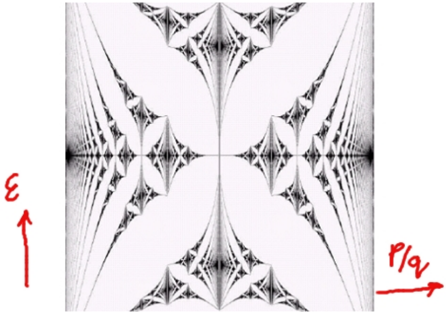


Venturelli, Ph. D. Thesis, SISSA

Hofstadter Spectrum and Butterfly

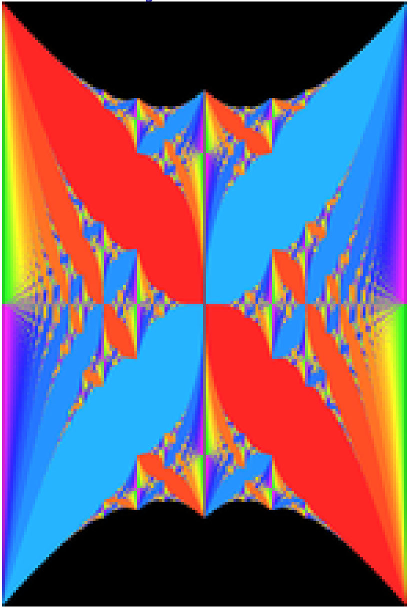


$p/q = 1/20$



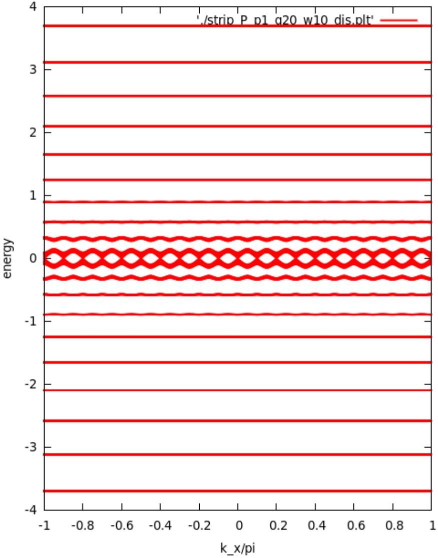
Avron et al.

Hofstadter Chern Butterfly

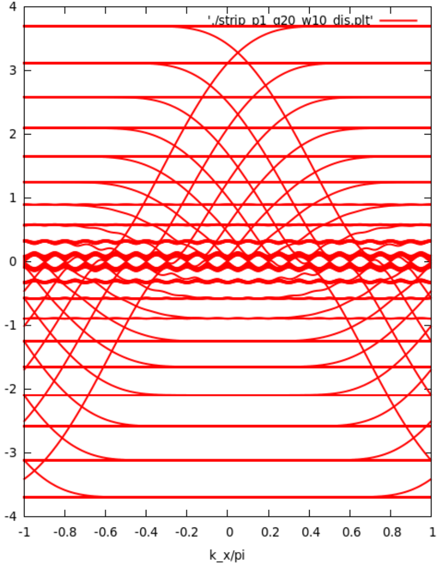


Avron et al.

Hofstadter Model Edge States

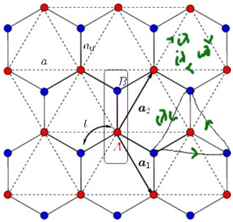


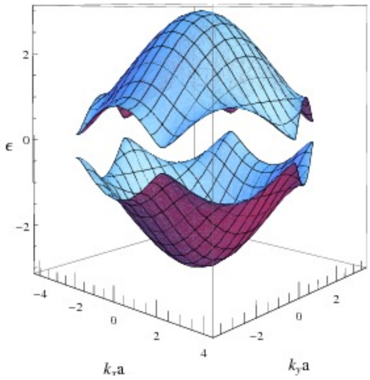
$p/q = 1/20$



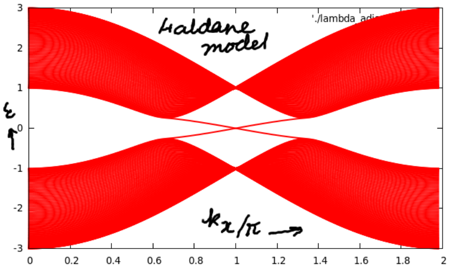
$p/q = 1/20, withedges$

Haldane Model



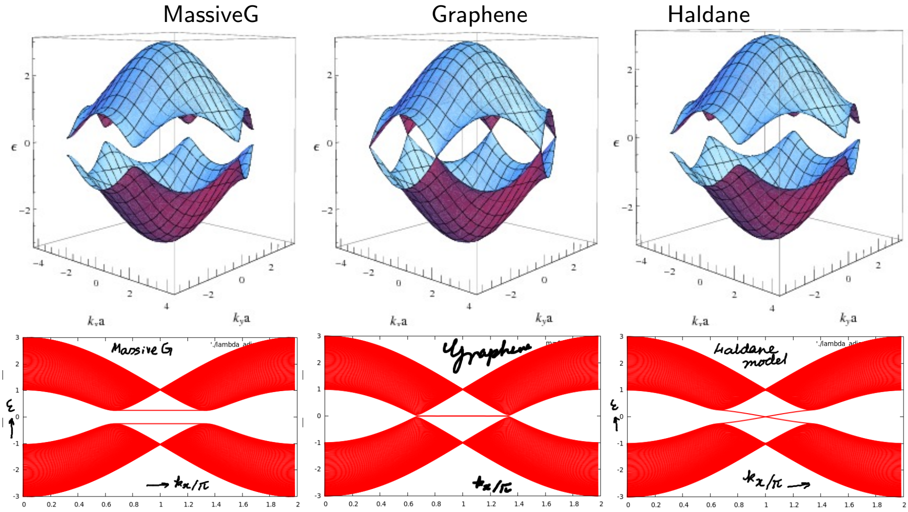


Edge states



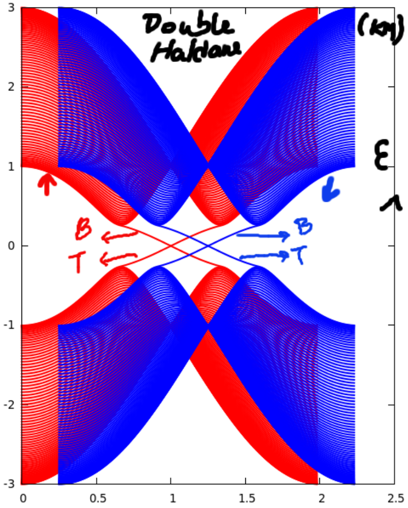
- The states corresponding to the two edge bands are associated with *different* edges!
- Both bands have *non-zero Chern number* – *Chern* bands!
- For one (spinless) fermion per unit cell, bottom band is filled – bulk insulator!
- ...and a *quantum Hall state*!

From MassiveG to Haldane



- Massive graphene and Haldane *differ* at the edge!
- We need to close the bulk gap to go from MassiveG to Haldane, i. e., *via* graphene – need a quantum phase transition

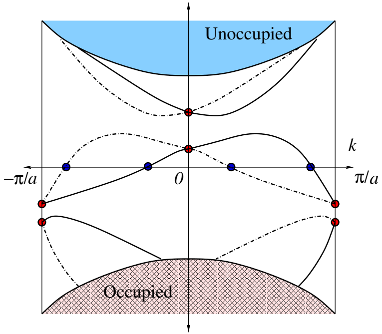
Kane-Mele Double Haldane Model



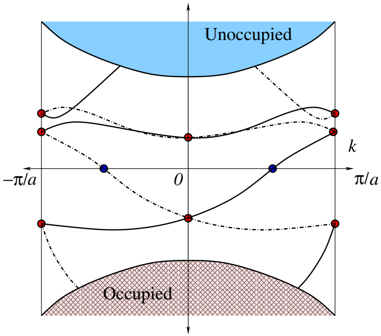
- Two time reversed copies $(\uparrow, \downarrow)$ of the Haldane model glued together
- The Chern number of the $\downarrow$-band is *negative* of that of the $\uparrow$ band, $\sigma_{xy} = 0$...*has* to be since the system is TR invariant...
- But there is a SPIN current on application of the voltage!! This is quantized and related to the number of edge modes! In this example it is e^2/h...and is dissipation less!!
- We get the quantum spin Hall state, with a fully insulating bulk
- This is the simplest realization of a Topological Insulator!
- Robust against TR invariant perturbations

Trivial and Topological Insulator (2D)

Edge State



Ordinary (Trivial) Insulator



Topological Insulator

3D TIs

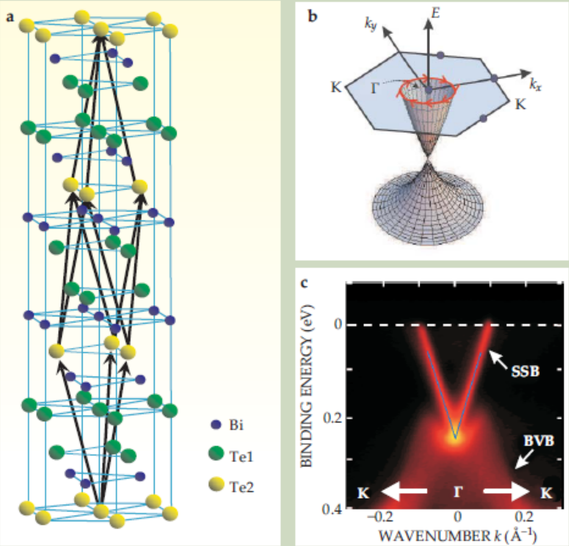


Figure 4. In three-dimensional topological insulators, the linearly dispersing edge states of figure 3b become surface states described by a so-called Dirac cone. **(a)** The crystal structure of the 3D topological insulator Bi_2Te_3 consists of stacked quasi-2D layers of Te-Bi-Te-Bi-Te. The arrows indicate the lattice basis vectors. The surface state is predicted to consist of a single Dirac cone.[6] **(b)** Angle-resolved photoemission spectroscopy maps the energy states in momentum space. Spin-dependent ARPES of the related compound Bi_2Se_3 reveals that the spins (red) of the surface states lie in the surface plane and are perpendicular to the momentum.[7] **(c)** This ARPES plot of energy versus wavenumber in Bi_2Te_3 shows the linearly dispersing surface-state band (SSB) above the bulk valence band (BVB). The dashed white line indicates the Fermi level. The blue lines meet at the tip of the Dirac cone.[8]

Qi and Zhang, *Physics Today* (2010)

TI Possibilities

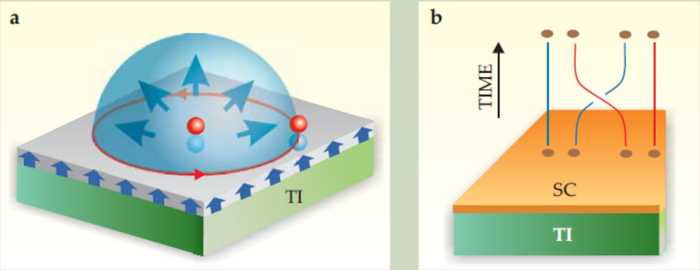


Figure 5. Novel behavior is predicted for topological insulators. **(a)** When a topological insulator (TI, green) is coated by a thin ferromagnetic layer (gray), each electron (red sphere) in the vicinity of the surface induces an image monopole (blue sphere) right beneath it.[12] When one electron winds around another (red circle), it will experience the magnetic flux (arrows in the blue dome) carried by the image monopole of the other, so that the electron–monopole composite, called a dyon, obeys fractional statistics. **(b)** When a TI is coated by an *s*-wave superconductor (SC), the superconducting vortices are Majorana fermions—they are their own antiparticles. Exchanging or braiding Majorana vortices, as sketched here, leads to non-abelian statistics.[17] Such behavior could form the basis for topological quantum computing.

Qi and Zhang, *Physics Today* (2010)

Trivial or Topological?

Trivial or Topological?

Trivial or Topological?