

# Literature Review

Matthew Gebert

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Interfacing topological insulators surface states with ferroics

## 1 Introduction

TO COMPLETE AFTER

## 2 Topological Insulators

### 2.1 Primer on TI materials

In the last two decades there has been a vast discovery of new materials that exhibit phenomenal properties interesting for condensed matter physics research. Usually these materials are stumbled upon experimentally, however in the case of topological materials the setting and expectation was purely theoretical.

Topological insulators (TIs) attract interest because of their unique properties related to electronics. 2D and 3D compounds have edge and surface electronic states respectively, and these states exhibit useful properties such as momentum-spin locking (or localised spin densities) and suppressed back-scattering.

These properties may be used for applications like directing currents that are spinful, ie, exerting magnetic fields or used in spintronics, as well as providing currents that are robust with low resistance due to ensured conductivity.

## 2.2 History through Hall effects

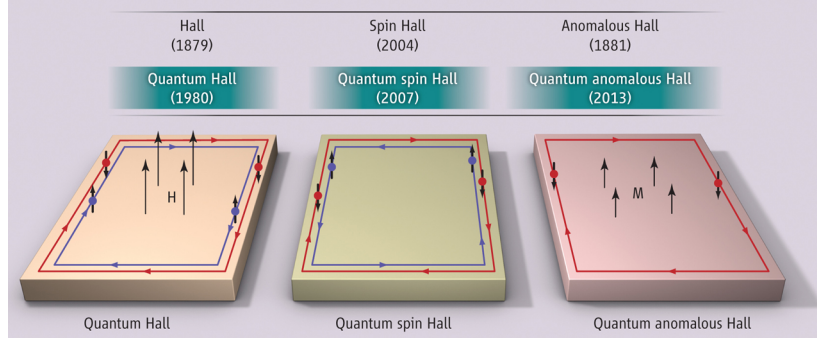


Figure 1: The three QH states discovered thus far<sup>[1]</sup>

### 2.2.1 Quantum Hall Effect

The quantum hall effect (QHE) was first discovered in MOSFET<sup>1</sup> transistors 1980<sup>[2]</sup>, through a 2 dimensional electron gas (2DEG) found at the interface of a bulk semiconductor and the gate oxide.

When introducing a magnetic field to materials, you can produce something called Landau quantisation. You can think of the physical mechanism as the quantisation of cyclotron orbits for charged particles in magnetic fields<sup>2</sup>. This has the effect of creating new bands called "Landau Levels", that each possess large numbers of orbitals. The degeneracy of the level goes as

$$\text{Degeneracy} = \frac{B \times A}{\phi_0} = \frac{B \times A}{h/e} \quad (1)$$

This means for some Fermi energy, that you can choose the magnetic field to appropriate values to fill these Landau levels.

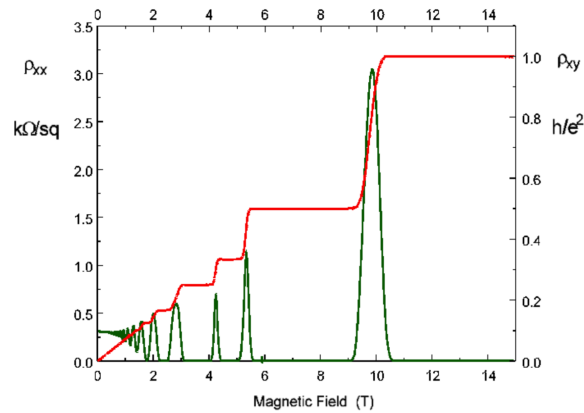


Figure 2: The quantum Hall effect.  
Courtesy of D.R. Leadley, Warwick University 1997.

The QHE looks finely tuned, but because of electrons interacting at the edge there is a confinement of edge states<sup>[3]</sup>. The edge states dominate transport when the Landau levels of the bulk are filled.

<sup>1</sup>Metal-oxide semiconductor field effect transistors

<sup>2</sup>The reason for cyclotron orbits is due to the single valued electron wavefunction, ie  $\oint \vec{P} \cdot d\vec{r} = 2\pi N$

Because they are dissipationless, the resistivity  $\rho_{xx}$  of the system vanishes, before reaching the next Landau level, where scattering between bulk states can occur again. This is the hallmark<sup>3</sup> of topological states, where there exists some states between different phases of matter.

The Hall resistivity  $\rho_{xy}$  exhibits quantized levels however.

$$\sigma_{xy} = \nu \frac{e^2}{h} \quad (2)$$

Thouless (who later received the noble prize in 2016, before passing away in 2019), Kohmoto, Nightingale, and den Nijs (TKNN)<sup>[4]</sup> were interested in gapped bulk systems but with conductive edges and a periodic lattice potential. These systems had been argued for explaining the QHE by Laughlin<sup>[5]</sup> and the integer effects had earlier been demonstrated theoretically by Hofstadter's Butterfly<sup>[6]</sup>. TKNN recognised that  $\mathbf{K}$  space maps to a non-trivial hilbert space for the QHE; the space has a topology. This topology can be specified by the integer  $\nu$  which also corresponds to the hall conductance above in Eq. 2. In particular, their calculations only depended on details of the wavefunctions of the bandstructure.

What makes this fascinating is that the QHE is a clear example of macroscopic quantum phenomena. Other such phenomena include Bose Einstein Condensation, where many atoms condense into the same uniform quantum state, and superconductivity where the pairing of electrons (Cooper pairs) also produce a new phase of macroscopic quantum behaviour.

Show calculation of berry phase of the bloch wave function calculated around the BZ boundary divided by 2 pi

For the QHE to occur, the Landau quantisation opens gaps in the band structure of the material, and the chemical potential is situated within this gap. In a classical picture, the boundaries of the material cannot sustain these cyclotron orbit, because of the phase transition to an ordinary insulator, rather than the QHE insulator, and so edge channels open in a **bulk-boundary correspondence**.

Note that the QHE does not preserve **time reversal (TR) symmetry**, as charge carriers experience different forces due to the magnetic field when their direction is inverted. The magnetic field breaks TR symmetry. You can see this in the two degrees of freedom in the system; For an out of plane magnetic field, charge is separated into two lanes, and those channels move a particular direction, ie forward above for electrons, backward below for holes. Reversing the direction of carriers yields the same channels but switched, forward above for holes, backward below for electrons.

### 2.2.2 Quantum Spin Hall Effect

The spin hall was observed in 2004 by Kato *et al.*<sup>[7]</sup>, where for particular semiconductors a spin density was observed rather than a charge density, like in the regular hall effect. The origins for such an phenomenon are similar to that of the quantum anomalous Hall effect in ferromagnets, sometimes being extrinsic, sometimes intrinsic. Intrinsically, the **Berry curvature** of the electronic valence-band Bloch wave functions result in spin-Hall effect.

The spin Hall insulator was proposed by Zhang's group<sup>[8]</sup>, where the **Berry phase** is finite implying a finite spin Hall conductivity. While this idea did not "generate spin currents due to an absense of any electrons at the Fermi level"<sup>[9]</sup>, it allowed further exploration to find it quantised version, a quantum spin Hall (QSH) insulator<sup>[10;11;12]</sup>.

In a real 1D system with spin, you have a regular four degrees of freedom; Spin can move either direction, and can move forward and backward. This could be separated into two copies of the QH system - spin up moving forward with spin down moving backward at the top, and spin down moving forward with spin up moving backward on the bottom. This is referred to the quantum spin Hall effect (QSHE). But what is the key ingredient that allows this separation of states to occur? In the QHE, it's the magnetic field that breaks time reversal symmetry. For QSH insulators, the essential ingredient is spin orbit coupling (SOC).

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<sup>3</sup>Although unrelated to the Hall effect, get the pun? Haha.

An important step made by Kane and Mele<sup>[11]</sup> was finding a “topological invariant” to characterize the QSH insulator states using an index. This index is called the  $Z_2$  index. Topological invariants have appeared before. In the QHE, the TKNN invariant  $\mu$ , where the quantised conductance is proportional to  $\nu$ . The consequence of the  $Z_2$  index is it maps the parity of the number of times the 1D edge state crosses the Fermi level. An odd parity ensures the existence of an edge state and consequently the phase of a topological insulator. The result is significant in it shows how topological phases exist in band structures of insulators, and do not require external magnetic fields breaking TRS like in the QHE<sup>[9]</sup>.

Whilst Kane and Mele used their SOC model to investigate the bandgap opening of graphene, SOC is very difficult to experimentally detect in graphene due to the low coupling strength, compared to that of heavier species. Bernevig *et al.*<sup>[10]</sup> (Zhang’s group) instead proposed a  $Z_2$  model for the band structure of mercury telluride (HgTe). They predicted a CdTe/HgTe/CdTe quantum well would give rise to the QSH effect, when the HgTe layer reached a certain critical thickness. Experimental observation was confirmed soon thereafter by König<sup>[13]</sup>, who observed a quantized conductivity  $\sigma_{xx}$  of  $2e^2/h$ , due to two conducting edges. They also observed the thickness dependence.

### 2.2.3 Topological insulators

By this time theorists (Moore & Balents<sup>[14]</sup>, Fu, Kane and Mele<sup>[15]</sup>) had already leapt forward and predicted 3D systems that would exhibit quantum spin hall effects. It was at this point that the term “topological insulator” was first coined<sup>[14]</sup>. This is distinct to the 2D QSH insulators, but analogous in a 3D version. For these systems there was no longer one invariant to determine the topology of a system, but rather 4 separate invariants, for 16 classes of materials. Generally they could be separated into two groups - strong and weak 3D TIs.

The first prediction for a 3D TI was by Fu and Kane<sup>[16]</sup>. They predicted that the surface states of bismuth antimony ( $\text{Bi}_{1-x}\text{Sb}_x$ ) could be observed by looking at angle resolved photo emission (ARPES, see 6.2.1). The signature for non-trivial topology was in observing surface states crossing the Fermi energy between two TR-invariant momenta<sup>[16]</sup>. This was observed in the same system by Hsieh *et al.*<sup>[17]</sup>.

### 2.2.4 Quantum Anomalous Hall Effect

<https://science-sciencemag-org.ezproxy.lib.monash.edu.au/content/340/6129/167>

“QHE can also occur in some insulators with TRS, broken by current loops, or magnetic ordering, but without Landau levels or external magnetic fields, where it is considered the QAHE. The first Chern number can give the quantized Hall conductance.” QAHE can occur by the introduction of a ferromagnetic layer.

## 2.3 Relevant theory and phenomena

### 2.3.1 Topological field theory

In 2001 the QHE state was generalized to a 4D TR-invariant state by Zhang and Hu, and was generalized by to field theory by Bernevig *et al.*. It was also shown later by Zhang how the  $Z_2$  topology could be described in this field theory, and be reduced to the 2D and 3D cases.

Practically according to Ando’s review<sup>[9]</sup>, this is useful for describing electromagnetic responses of TIs and predicting magnetoelectric effects.

## 2.4 Topological Invariants

## 2.5 Symmetries

### 2.5.1 Inversion Symmetry

Bulk states are spin-degenerate, because of combination of space-inversion symmetry ( $E(k, \uparrow) = E(-k, \uparrow)$ ) and time-reversal symmetry ( $E(k, \uparrow) = E(-k, \downarrow)$ )<sup>[18]</sup>. At the surface however where inversion symmetry is broken, spin-orbit interaction can lift the spin degeneracy.

### 2.5.2 Kramers Theorem

Kramers theorem requires particular points mapped from the BZ (Broullin zone) to retain spin degeneracy. For  $\text{Bi}_{1-x}\text{Sb}_x$ , spin states split at the surface by spin-orbit interaction must remain spin-degenerate at four special TR invariant momenta;  $\Gamma$ , and three equivalent  $M$  points. Ref in Hsieh *et al.*<sup>[18]</sup>.

## 2.6 Spin-Orbit Coupling

Spin-orbit coupling (SOC) is coupling of both spin and orbital angular momentum properties of particles. Spin provides a magnetic moment, and the motion of the charged electron through its orbital angular momentum also provides a magnetic moment. From the electrons point of view, it can be considered to be the interaction of the electron's spin with the orbital motion of the nucleus.

This coupling causes splitting, similar to Zeeman splitting, of electronic energy levels. For different atoms, the SOC is different, with the trend that heavier atoms have a larger SOC<sup>[19]</sup>.

This type of coupling doesn't break time-reversal symmetry like magnetic field for QHE, but can lead to the QSHE, where electrons differentiated by their spin move in opposite directions.

### 2.6.1 Rashba Effect

### 2.6.2 Dresselhaus Effect

## 2.7 Berry Phase

[?] [20]

## 2.8 Kubo formula

## 2.9 Band inversion

## 2.10 2D Dirac Systems

## 2.11 Materials & Growths

### 2.11.1 Bi<sub>2</sub>Se<sub>3</sub>

### 2.11.2 Bi<sub>2</sub>Te<sub>3</sub>

### 2.11.3

# 3 Magnetic Materials

## 3.1 Classifications

### 3.1.1 Ferromagnetic

### 3.1.2 Rashba-Edelstein Effect in Ferromagnetic Materials

<https://doi-org.ezproxy.lib.monash.edu.au/10.1016https://doi-org.ezproxy.lib.monash.edu.au/10.1038>

### 3.1.3 Anti-ferromagnetic

### 3.1.4 Paramagnetic

### 3.1.5 Diamagnetic

## 3.2 Ferromagnetic Insulators

### 3.2.1 2D FIs

Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub> is a thin ferromagnetic insulator. It consists of quintuple layers, similar to Bi<sub>2</sub>Te<sub>3</sub> or Bi<sub>2</sub>Se<sub>3</sub>, and is also terminated with hexagonal Te planes.

# 4 Experimental Methods

## 4.1 Synthesis, growth and fab tools

## 4.2 Experiments

# 5 TI & FI Heterostructures

## 5.1 Theory

## 5.2 Spin Torque

### 5.2.1 Torque

### 5.2.2 Spin Torque Angle - Spin Torque Efficiency

### 5.2.3 Magnetization

Larmor Equation:

$$\vec{T} = \mu_0 \vec{M} \times \vec{H} \quad (3)$$

Torque:

$$\frac{d\vec{L}}{dt} = \vec{T} \quad (4)$$

Gyromagnetic Ratio

$$\gamma \equiv \frac{\mu}{L} \quad (5)$$

Magnetization Change

$$\frac{d\vec{M}}{dt} = \gamma \vec{T} \quad (6)$$

#### 5.2.4 Critical Current Density

#### 5.2.5 Charge Spin Conversion Efficiency

### 5.3 Experiments

#### 5.4

#### 5.5 MBE

#### 5.6 Rashba-Edelstein Effect

<https://www-nature-com.ezproxy.lib.monash.edu.au/articles/nature13534> <https://advances.sciencemag.org/content/5/8/>  
[https://tms16.sciencesconf.org/data/pages/TI\\_lecture2.pdf](https://tms16.sciencesconf.org/data/pages/TI_lecture2.pdf) <https://arxiv.org/pdf/1401.0848.pdf>

#### 5.7 Non-TI Devices

- (2010) Co layer 0.6nm, with Pt 3nm and AlO<sub>x</sub> layers 2nm, transverse magnetic fields. <https://www-nature-com.ezproxy.lib.monash.edu.au/articles/nmat2613?proof=true> May -  
 Spin orbit coupling Rashba Effect Dresselhaus Effect

## 6 Experimental Methods

### 6.1 Synthesis, Growth and Fabrication

Test

#### 6.1.1 MBE Growths

Test

### 6.2 Spectroscopic Metrological Methods

#### 6.2.1 ARPES

For material characterisation, angle resolved photo-emission spectroscopy (ARPES) is a method of resolving the ejection of electrons from a material by high energy photons. Analysis of the momentum of the incident and emission resolve the electronic band structure.

There now exist a variety of different ARPES methods that can be employed in understanding the electronic structure of materials; these include “soft-X-ray ARPES, time-resolved ARPES, spin-resolved ARPES and spatially resolved ARPES”<sup>[21]</sup>. The progress fo UV and soft-X-ray synchrotron

light sources make it possible to distinguish between bulk and surface states for TI materials. Spin detectors determine the spin state of emitted electrons, allowing insight into spin-textures of surface states. Time-resolved ARPES (using femtosecond pulses) allows observation of “ultrafast electronic dynamics and states above the chemical potential”<sup>[21]</sup>. Finally, spatially resolved ARPES can be used to pinpoint sub-micron scale features, particularly if you want to distinguish between phases, or across material gradients (such as gradient MBE growths).

**Spin Resolved ARPES** The first spin resolved (SR) ARPES that yielded the direct observation of helical spin-polarization was done by Hsieh *et al.*<sup>[18]</sup> at the end of 2008, again in  $\text{Bi}_{1-x}\text{Sb}_x$ , followed with more detailed results by Nishide *et al.*<sup>[22]</sup>.

In these experiments, topological details could be found by studying the surface band-dispersion and their respective spin polarizations. For example, the fact that there are 5 bands implies that an odd number of Fermi-surfaces enclose the spin-degenerate K points. This gives rise to determining the topological quantum number  $\nu_0 = 1$  (0 if even).

### 6.2.2 Spin polarized STS

The first scanning tunnelling spectroscopy (STS) study on  $\text{Bi}_{1-x}\text{Sb}_x$  was published in 2009 by Roushan *et al.*<sup>[23]</sup> who detected the absence of backscattering even with strong system disorder. By taking fourier transforms of the surface state data they take, they can infer scattering information and lattice information. Combining this with spin-resolved ARPES they could determine the spin dependent scattering probability, and match their STS measurements to 95%. Doing the same with spin-independent scattering yields a match of only 80%.

## 6.3 Transport Metrological Methods

Test

### 6.3.1 Quantum Oscillations

Taskin & Ando<sup>[24]</sup> used quantum behaviour reported in Bi and  $\text{Bi}_{1-x}\text{Sb}_x$  to differentiate between coherent electronic transport (edge states) and incoherent transport within an impurity band. The measurements (along with magnetic & resistivity measurements) were implemented using “de Haas-van Alphen (dHvA)” methodology. To do this, you measure the magnetization M across magnetic field strengths B. They also measured for different direction of the sample.

The derivative of the both  $\rho_{xx}$  and  $\rho_{yy}$  with respect to B, plotted against  $1/B$  show Shubnikov-de Haas (SdH) oscillations below 2T field strength. This is a quantum effect, and consequently is argued that it comes from a well-defined Fermi surface, not some impurity band which wouldn’t be stable. The previous measurements of the resistivity with different doping proportions confirmed the insulating nature of the samples.

### 6.3.2 Magnetization

Taskin & Ando<sup>[24]</sup> measured DC magnetization using a SQUID magnetometer.

## 7 Knowledge & Concepts

### 7.1 Symmetry

Symmetry is very important in all physical systems. For example, the order exhibited in crystals can be described through the breaking of the continuous (rotational & translational) symmetry of space.



This is due to the electrostatic interactions that cause a periodic lattice. In Magnets, spin space and time reversal symmetry are broken.

## 7.2 Spintronics

### 7.2.1 Ahn-Hofstadter Bohm Effect

## 7.3 Fine Structure Constant

The fine structure constant, also known as Sommerfeld's constant, is the coupling constant " $\alpha$ " that measures the strength of the EM force interacting with light.

Two methods it has been measured by include the anomalous magnetic moment of the electron,  $a_e$ , as well as appearing in the Quantum Hall Effect (QHE).

It was originally introduced by Sommerfeld as a theoretical correction to the Bohr model, explaining fine structure through elliptical orbits and relativistic mass-velocity.

## 7.4 Hamiltonians of Crystal Lattices

Turns out that you can describe the hamiltonian of the electrons in a crystal lattice. For this, there exists first quantisation, second quantisation hamiltonian.

- First quantisation - The classical particles are assigned wave amplitudes. This is "semi-classical" where only the particles or objects are treated using quantum wavefunctions, but environment is classical.
- Second quantisation (Canonical Quantisation, occupation number representation) - The wave fields are "quantized" to describe the problem in terms of "quanta" or particles. This usually means referring to a wavefunction of a state, described the the vacuum state with a series of creation operators to create the current state. Fields are now treated as field operators, similar to how physical quantities (momentum, position) are thought of as operators in first quantisation.

### 7.4.1 Graphene

## 8 Quotes

*Finally we introduce the parameter of which all the fuss is about.*

R.F. Hofstadter,<sup>[6]</sup>

## 9 Questions to Answer

- SOC - Why only in heavier elements? Explain properly. Also, why think relativistically? Motion of electron means magnetic field observed?
- Spin is in the 2D surface plane of a 3D TI, always perpendicular to that of the momentum - how can I couple a ferromagnetic material if there's no out-of plane?
- ARPES - how can this be used to verify the surface states of TI materials? (and differentiate from the bulk).
- Dirac Cones - why do these only appear in 2D systems.
- Why is spin-polarization called "Helical" spin polarization?

## 10 Glossary

### 10.1 B

- **Berry Connection** is the bra-ket of a Gradient operator of vector  $\vec{R}$  acting on a wavefunction over some path  $\Gamma$  with positions  $\vec{R}$ . Physically it is the mechanism from getting one geometric space point to another, ie the change of parameters.

$$\vec{\mathcal{A}}_n(\vec{R}) = i \langle \psi_n(\vec{R}) | \nabla_{\vec{R}} | \psi_n(\vec{R}) \rangle \quad (7)$$

This object has N parts, for each of the vector components. There's a different connection for every eigenstate, of every point in the space. It's a little more subtle than a vector - it transforms under Gauge transformations. For an example wavefunction to include some additional phase factor (i.e. Gauge transformation)  $|\psi'_n(\vec{R})\rangle = e^{-i\beta(\vec{R})} |\psi_n(\vec{R})\rangle$

$$\vec{\mathcal{A}}'_n(\vec{R}) = \vec{\mathcal{A}}_n(\vec{R}) + \nabla_{\vec{R}}\beta(\vec{R}) \quad (8)$$

So the "connection" is that it transforms with the gradient of a function, like a vector potential.

- **Berry Curvature** is the consequence or result of going from one set of starting parameters to the same set of parameters over some path (also called a **connection**). You could use the Schroedinger equation to provide a connection. It turns out that through evolution the state can pick-up a phase factor, relative to the original starting state. This phase factor is also known as the Berry phase, and has consequences for the quantum mechanical properties of the system.
- **Berry Phase** is the integral

$$\gamma_n(\Gamma) = \int_{\Gamma} \vec{\mathcal{A}}_n(\vec{R}) \cdot d\vec{R} \quad (9)$$

$$\text{Changing gauge: } \gamma'_n(\Gamma) = \int_{\Gamma} \vec{\mathcal{A}}_n(\vec{R}) \cdot d\vec{R} + \int_{\Gamma} \nabla_{\vec{R}}\vec{\beta} \cdot d\vec{R} \quad (10)$$

$$\implies \gamma'_n(\Gamma) = \gamma_n(\Gamma) + \beta(R_f) - \beta(R_i) \quad (11)$$

It's not Gauge invariant, which makes it difficult to be useful for different measurements. However, if you begin **AND** end in the same configuration point (ie, a closed loop) then this value is Gauge invariant!

- Eigenstates have to be imaginary to achieve a non-zero Berry phase.
- If the path is 1D, then the integration cancels out to result in a zero Berry phase, again.
- In 3D, the Berry phase over some path  $\Gamma$  enclosing a surface  $S$ , then Stokes theorem lets you specify the **Berry curvature**

$$\oint_{\Gamma} \vec{\mathcal{A}}_n \cdot d\vec{R} = \oint\!\!\!\oint_S (\nabla \times \vec{\mathcal{A}}) \cdot d\vec{a} \quad (12)$$

$$\vec{D} = \nabla_{\vec{R}} \times \vec{\mathcal{A}}(\vec{R}) \quad (13)$$

## 11 Review Article Notes

### 11.1 J. Moore - The Birth<sup>[25]</sup> [2010]

#### 11.1.1 Lessons from the past

- Quantum Hall Effect can occur in 2D systems (condined) in the presence of a magentic field. It is a consequence of topological properties of the electronic wavefunctions.

- Question - Can this effect arise without a large external magnetic field?
- In the 1980s, Predicted that forces from motion through crystal lattice could provide the same hall state<sup>[26]</sup>
- The mechanism which this recently has occurred through is **spin-orbit coupling** or SOC. Spin and orbital angular momentum degrees of freedom are coupled. This coupling causes electrons to feel a spin dependent force.
- QSHE predicted in 2003. Unclear how to measure or if realistic or not.<sup>[27;8]</sup>
- Kane & Mele in 2005 produced a key theory advance, using realistic models. Showed that QSHE can survive by the use of invariants and could compute if the 2D material has an edge state or not. 2D Insulators that have 1D wires that conduct perfectly at low temps, similar to QHE.<sup>[11]</sup>
- (Hg,Cd)Te quantum wells predicted to have quantized charge conductance<sup>[10]</sup>. These were then picked up in 2007<sup>[13]</sup>.

### 11.1.2 Going 3D

- 2006 gave the revelation that while QHE doesn't go 2D to 3D, the TI does, subtly.<sup>[15;14;28]</sup>
- "Weak 3D TI" given through stacking of multiple 2D TIs. Not stable to disorder. A dislocation will always contain a quantum wire at the edge.
- "Strong 3D TI", connects ordinary insulators and topological insulators by breaking time-reversal symmetry.<sup>[14]</sup> This is the focus result for experimental physics at the moment.
- SOC is also required, but mixes all spins, unlike the 2D case. Spin direction dictates the momentum along the surface. Scattering also occurs, but metallic surface cannot vanish.
- First 3D TI was  $\text{Bi}_x\text{Sb}_{1-x}$ . Surfaces mapped using ARPES experiment. The surface was complex, but launched a search for other TIs.<sup>[17;18]</sup>
- Heavy metal, small bandgap semiconductors are meant to be the best candidates (this sounds like TMDs haha but not implied) for two reasons.
  - SOC is relativistic, and only strong for heavy elements.
  - Large bandgaps, relative to the scale of SOC, will not allow SOC to change the phase. This is because bands either need to invert or be able to cross or change properties by local deformation (I think).
- The discovery of Bismuth Selenide  $\text{Bi}_2\text{Se}_3$  and Bismuth Telluride  $\text{Bi}_2\text{Te}_3$ . They exhibit TI behaviour to higher temperatures, bulk bandgaps of  $> 0.1 \text{ eV}$ <sup>[29;30;31]</sup>.
  - The large bandgap is good for measurement in higher temperature
  - Simple surface states to investigate heterostructures etc.
  - Complication - Distinction between surface and bulk states - residual conductivity resulting from impurities.
- Graphene?  $\text{Bi}_2\text{Se}_3$  looks like Graphene, due to its Dirac nature. The difference for graphene is that a TI has only one Dirac point. Graphene has spin degeneracy with two Dirac points. The difference is major, including applications for quantum computing. This implies that the bandstructure & reciprocal lattice are really important for preserving coherent spin phenomena.

- STMs found interference patterns near steps / defects, showing electrons aren't completely reflected - even when strong disorder occurs<sup>[23;32;33]</sup>.
  - \* Generally, *anderson localization*, the formation of insulating states, is meant to occur in materials with surface states (ie, Noble metals).
  - \* TI surface states are distinguished through this property!
  - \* In some 2D models, it seems to form as a result of some disorder?
  - \* In graphene, apparently smooth potentials might do the same, but it's quite unlikely!
- Femi level is located **at** the Dirac point for graphene! This is very advantageous, because of the tunability of the material. However, when it comes to other materials, it will not be as easy to tune the DOS around some point of interest like in graphene, without some form of doping. It was demonstrated recently in Bi<sub>2</sub>Se<sub>3</sub> that you could tune to the Dirac point as well<sup>[34]</sup>. The chemical potential is really important to be able to control for purposes like this.

### 11.1.3 Materials Challenges

- Two important experiments:
  - Aharonov-Bohm Effect observed in nano-ribbons
  - MBE grow thin films of Bi<sub>2</sub>Se<sub>3</sub> controlling thickness.
- Items to characterize:
  - Transport & optical properties on the metallic surface to measure the spin state and conductivity.
  - Improved materials with reduced bulk conductivity may be required!

### 11.1.4 A Nascent Field

- Particle physics in the 1980s predicted a particle who coupled to ordinary EM fields.
- Cond.Mat Physics seek phases of matter to respond to influence.
  - Solid in response to sheer force
  - Superconductor in response to Meissner effect
  - T.I. in response to axion electrodynamics, ie in response to a scalar product **E.B**. (1980s)
    - \* Two coefficients correspond to OIs (ordinary) and TIs.
- Just like insulators modify dielectric constant, coefficient of **E**<sup>2</sup> in Lagrangian, TI's generate non-zero coefficient of **E.B**
- Applications are in electronics and magnetic memeory, not due to speed, but rather due to reproducability and no fatigue, as a result purely from the electrons.
- Apparently, you can determine if a material is topological or not, purely from a polarizing magnetic field measurement.
- The magnetoelectric effect can also create an electric field from a magnetic source, and vice versa.
- Some work also done to find similar phases, in materials with differing symmetries. Cooper pairs in superfluids (<sup>3</sup>He) are closely connected to the quasiparticles/electrons in topological insulators. Direct experimental signatures would be awesome.

- Moore goes on to talk about new phenomena, particularly at the interface of a superconductor and a topological insulator:
  - Creation of emergent particles
  - New particle statistics could be useful for 'topological' quantum computing which would protect from errors.
  - Fractional QHE also indicate new quasiparticle and statistics in materials.
  - TI surface becomes superconducting — Proximity effect
    - \* Vortex line from SC into the TI, a 0-energy Majorana fermion is trapped.
    - \* Majorana fermions have different quantum numbers to that of a regular electron.
    - \* Is roughly 'half' of an electron, and it's own antiparticle.
  - Direct observation of Majorana fermions is a long sought goal
  - New particle statistics for other quasiparticles and systems.

## 11.2 The Quantum Spin Hall Effect & Topological Insulators<sup>[35]</sup> - Physics Today (2010)

### 11.2.1 Intro

- Phases & phenomena defined by symmetry
  - Translation = Crystal Solids
  - Rotational = Magnets
  - Gauge = Superconductors
- QHE first example of non-spontaneously broken symmetry.
  - Topologically defined, not geometrically!
- SQHE states are distinct again.
  - Immune to impurities or geometric perturbations (momentum spin locking, scattering is suppressed)
  - Maxwells equations altered by an additional 'topological' term, with remarkable effects.
- QHE differs to QSH
  - QHE External magnetic field required, TR symmetry broken
  - QSHE TR symmetric.

### 11.2.2 QH to QSH

- Traffic control separating out lanes of movement provides much less resistance. Same for QSH.
- QHE Magnetic field pushes electrons to side lanes.
  - there are only two degrees of freedom in the system (forward above and back below)
  - There is no way for electrons to turn around
  - limited by external Magnetic Field requirement
- In a real 1D system, you have four channels - spin up and down, moving forward and backward

- These were predicted to be able to split into 2 separate channels on two sides of the material.
- The backscattering suppression is quantum mechanical.
  - Electrons in edge states can be thought to circle around the edge of the impurity and scatter backwards.
  - Depending on which way they rotate, they pick up a phase of  $\pi$  or  $-\pi$  (imagine a vector rotating around a circle).
  - This induces a  $2\pi$  phase difference between the two bodies.
  - In QM, this corresponds to a negative sign. This means their amplitudes destructively interfere, leading to perfect transmission instead.
  - If the impurity is magnetic, TR symmetry is broken, and there is no longer destructive interference.
  - In an unseparated system (two movers back and forward) then spin doesn't need to change phase and regular scattering can take place.
  - The consequence then is, that there needs to be an "odd" number of forward and backward movers.
  - This is the heart of the  $Z_2$  topological quantum number, and why a QSH insulator is also referred to as a topological insulator.
- Requirements for 2D TIs
  - Heavy elements produce coupling of spin and orbital motion, relativistic.
- Bernevig, Hughes and Zhang proposed a mechanism for finding TIs, nanoscopic layers sandwiched between other materials, become TIs after a critical thickness  $d_c$ <sup>[10]</sup>. This must be a pretty cool model, to achieve such a simple analytic result.
  - Mechanism is "band inversion", where general ordering of valence and conduction band is inverted by SOC.
  - Generally,  $s$  orbitals contribute to conduction band, and valence is from the  $p$  band.
  - In Hg and Te, SOC pushes S band above, and P band below.
  - Sandwiched between with Cadmium Telluride (similar lattice constant, but VERY different SOC).
  - Changing the thickness parameter changes the overall SOC of the quantum well.
- Discovered less than a year later<sup>[13]</sup>. Clear difference from conduction quantum edge states at  $2\frac{e^2}{h}$  to massive resistance (10M-Ohms) below that thickness.

### 11.2.3 2D to 3D

- 2D insulator has a pair of 1D edge states crossing at momentum  $k=0$ . Linear dispersion here. Dispersion in QFT from the Dirac Equation for a massless relativistic fermion in 1D, the equation is consequently used to describe the QSH state.
- This can be generalised to a 3D system, with a 2D surface. Linear crossing becomes a Dirac cone. Crossing point is also at a TR-invariant point, such as at  $k=0$ . Degeneracy is protected by TR symmetry, if you break TR then you break the degeneracy.
- Liang Fu and Kane predicted  $\text{Bi}_{1-x}\text{Sb}_x$  to be a 3D TI<sup>[15]</sup>, observed by Hasan's group<sup>[17]</sup> using ARPES to measure the surface states. The authors of this review, Qi and Zhang<sup>[35]</sup>, predicted the states existent in  $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Te}_3$  and  $\text{Sb}_2\text{Te}_3$  (note that  $\text{Sb}_2\text{Se}_3$  is not)<sup>[30]</sup>.

- In  $\text{Bi}_2\text{Te}_3$  family, topology is again a result of band inversion between two orbitals, resulting from strong spin-orbit coupling of Bi and Te. By similarity, the family can also be described by a 3D version of the HgTe model which is awesome!
- First principle calculations show the Dirac cone.
- Note that  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  are both excellent thermoelectric materials as well.
- The spin resolved measurements of Hasan's group with samples prepped by Robert Cava and co-workers managed to make this happen, showing spin lies in plane of surface, always perpendicular to the momentum
- Unfortunately the experiments also observed bulk carriers co-existing with surface states.
- A pure TI phase without bulk carriers was observed in  $\text{Bi}_2\text{Te}_3$ , by Chen and Shen's group at Stanford<sup>[31]</sup>, with materials prepped by Ian Fisher.

- Models of TIs

- Models are formed for QSHE by a Hamiltonian that is a Taylor expansion in the wavevector  $\mathbf{k}$  of interactions between highest and lowest conduction bands.

\* HeTe (Mercury Telluride)

$$H(\mathbf{k}) = \epsilon(k)\mathbb{1} + \begin{pmatrix} M(k) & A(k_x + ik_y) & 0 & 0 \\ A(k_x + ik_y) & -M(k) & 0 & 0 \\ 0 & 0 & M(k) & -A(k_x + ik_y) \\ 0 & 0 & -A(k_x + ik_y) & -M(k) \end{pmatrix} \quad (14)$$

with

$$\epsilon(k) = C + Dk^2, M(k) = M - Bk^2 \quad (15)$$

- The upper 2x2 block describes the spin-up electrons in the s-like E1 conduction and p-like H1 valence bands. The lower 2x2 block describes the spin-down electrons in those same bands.
- $\epsilon$  is the unimportant bending of all bands, where  $\mathbb{1}$  is the identity matrix.
- Energy gap between the bands is  $2M$ , and  $B$  describes the curvature of the bands.
- $A$  incorporates the inter-band coupling at lowest order.
- $M/B \gg 0$  has eigenstates of a trivial insulator.
- $M/B \lesssim 0$ ,  $M$  becomes negative, and solution yields edge states of QSHE.
- Can also practise doing this with a 2D TI honeycomb lattice to gain explicit understanding.<sup>[12;11]</sup>

\*  $\text{Bi}_2\text{Te}_3$  (Bismuth Telluride)

$$H(\mathbf{k}) = \epsilon(k)\mathbb{1} + \begin{pmatrix} M(\mathbf{k}) & A(k_x + ik_y) & 0 & A_1k_z \\ A(k_x + ik_y) & -M(\mathbf{k}) & A_1k_z & 0 \\ 0 & A_1k_z & M(\mathbf{k}) & -A(k_x + ik_y) \\ A_1k_z & 0 & -A(k_x + ik_y) & -M(\mathbf{k}) \end{pmatrix} \quad (16)$$

with

$$\epsilon(k) = C + D_1k_z^2 + D_2k_\perp^2, M(k) = M - B_1k_z^2 - B_2k_\perp^2 \quad (17)$$

- This follows a similar model, in the context of bonding and anti-bonding  $p_z$  orbitals with both spins.  $B_1$  and  $B_2$  have the same sign, and as before, depending on the sign of  $M$ , the bands undergo inversion.
- It is essential to be in 3D to be able to construct a single Dirac cone for a 2D surface - the degeneracy of graphene with six Dirac cones makes it clear. The 2D HgTe quantum well at the crossover point  $d = d_c$  also has two Dirac cones.

#### 11.2.4 TI Classification

- Mathematicians group objects into broad classes. Topological invariants also created to classify.
- For materials, Topological invariants can be found in topological field theories (TFT).
  - First classification: insulators that observe TR symmetry or not.
    - \* QH State breaks TR symmetry
    - \* QHS state does not break TR symmetry
  - Thouless et al. showed that physically measured QH conductance is given by an invariant, called **the first Chern number**. See Physics TODAY- Aug2003, p38, Avron, Osadchy, Seiler
  - Topological properties can be described by effective TFT, based on Chern-Simons theory.
- Originally believes that 2D and TR breaking required for topological effects.
  - 2001 first model of TR-invariant TI, in 4D.
  - Later reduced to 3D and 2D.
  - Theory developed for SHE and SOC identified as the missing ingredient for materials.
  - Theory extended to TR invariant TIs.
  - 2D TR-Invariant QSH insulators shown to fall into two topological classes, through the  $Z_2$  classification.
  - "Beautiful topological band theory" extended to 3D hahah
- Now there are two precise definitions for TR-invariant TIs
  - Non-interacting topological band theory
    - \* Non interacting electrons filling a certain number of bands can calculate a binary value,  $Z_2$ .
  - Topological field theory
    - \* If with inversion symmetry, algorithm for electronic structure calculations can numerically evaluate the topological band invariant.
- It's important to have a definition for TIs that is valid for interacting systems (as insulators are interacting), whilst still being experimentally measurable. Turns out that topological field theory solves this.
- This can be explained by elementary concepts in undergraduate electromagnetism:
  - Inside insulators,  $\mathbf{E}$  and  $\mathbf{B}$  are both well defined.
  - Can describe the electromagnetic response by an effective action.
  - This action is not topological, as it depends on a spatial geometry. This is seen in the fact that  $\epsilon\mathbf{E}^2 - 1/\mu\mathbf{B}^2$  can be represented in the electromagnetic tensor form with indices. The summation over indices implies use of the metric tensor, which depends on the geometry (this leads to gravitational lensing of light?).
  - A different possible term is possible though, the spin-orbit coupling term  $\mathbf{E}\cdot\mathbf{B}$ . It turns out that this term is independent of the metric and IS a topological term, because it only depends on the topology of the underlying space.

$$S_\theta = \frac{\theta\alpha}{4\pi^2} \int d^3x dt \mathbf{E}\cdot\mathbf{B} \equiv \frac{\theta\alpha}{32\pi^2} \int d^3x dt \epsilon_{\mu\nu\rho\tau} F^{\mu\nu} F^{\rho\tau} \quad (18)$$

$$= \frac{\theta}{2\pi} \frac{\alpha}{4\pi} \int d^3x dt \partial^\mu (\epsilon_{\mu\nu\rho\tau} A^\nu \partial^\rho A^\tau) \quad (19)$$



- \* This value would naively break TR symmetry due to B, however in the periodic system, there are only two values of  $\theta$ , 0 or  $\pi$ . Phase doesn't change for these values, as if we were considering special values of flux, maintaining TR symmetry.
- \* Introducing a ferromagnetic layer on the boundary will also open up a bandgap under this theory, breaking TR on the surface but not in the bulk.
- \* The last term in the equation above shows the bulk topological term is actually a total derivative expressed in a surface term in the parenthesis.
  - Specifies the hall conductance.  $\theta = \pi$  translates to a half hall conductance  $\frac{1}{2}e^2/h$ .
  - As additions can only change the quantum conductance by an interger multiple of  $e^2/h$ , the system is topologically robust, because this term can never be reduced to zero.

### 11.2.5 Outlook

- Interesting experiments:
  - Nanoribbons
  - Non-local measurements in HgTe devices to confirm QSH edge states.
- Interesting theory:
  - Exotic excitations resulting from solving Maxwell's equations.
  - 2D QSH insulator predicted to have fractional charge at edge, spin-charge separation in bulk.
  - A point charge above a material was expected to induce an image charge below. For a TI, this changes to also induce a magnetic monopole. This composite of electric and magnetic charges would be called a dyon, and would behave like an 'anyon', rather than obeying Bose or Fermi statistics.
  - A secondary system is expected to arise in the coupling of a SC system with a TI system, in the interface. The arrival of Majorana fermions.
  - It sounds like the magnetic monopoles are the methodology to be able to write magnetic memory, check out the citing article. (X.-L. Qi, Hughes, Zhang, Phys Rev. B, 195424, 2008, and ... Qi, science, 323, 11184 (2009))

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