

Topological Insulators and Superconductors

Tejas Deshpande

Xiao-Liang Qi and Shou-Cheng Zhang. “Topological insulators and superconductors.” *Reviews of Modern Physics* **83**, no. 4 (2011): 1057.

I. Introduction

- “Fundamental” science: **reductionism**
 - Greeks: Concept of the atom



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- “Fundamental” science: **reductionism**
 - Greeks: Concept of the atom
 - 19th century:
 - Periodic table of elements



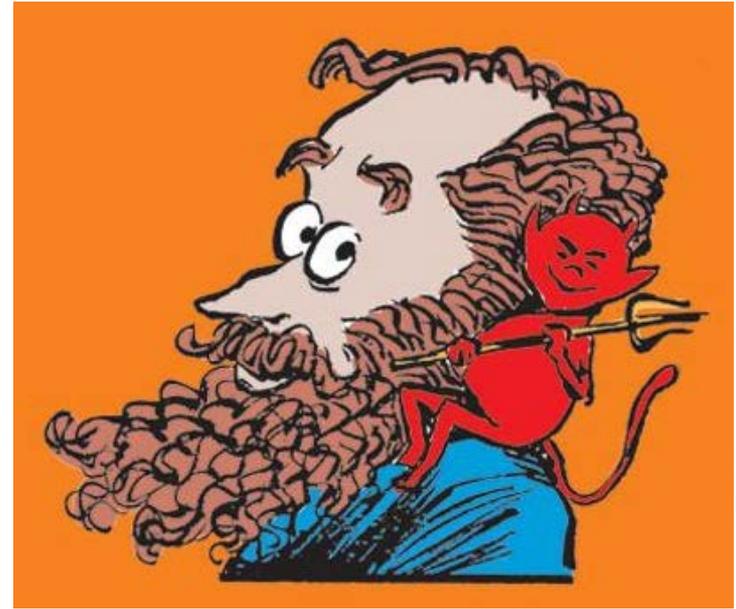
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 - Statistical mechanics
 - Electrodynamics
- 20th century:
 - Quantum mechanics + Relativity
 - Subatomic (elementary) particles

Three generations of matter (fermions)

	I	II	III		
mass	2.4 MeV/c ²	1.27 GeV/c ²	171.2 GeV/c ²	0	125 GeV/c ²
charge	2/3	2/3	2/3	0	0
spin	1/2	1/2	1/2	1	0
name	u up	c charm	t top	γ photon	H Higgs boson
	4.8 MeV/c ²	104 MeV/c ²	4.2 GeV/c ²	0	
	-1/3	-1/3	-1/3	0	
	1/2	1/2	1/2	1	
Quarks	d down	s strange	b bottom	g gluon	
	<2.2 eV/c ²	<0.17 MeV/c ²	<15.5 MeV/c ²	91.2 GeV/c ²	
	0	0	0	0	
	1/2	1/2	1/2	1	
	ν_e electron neutrino	ν_μ muon neutrino	ν_τ tau neutrino	Z⁰ Z boson	
	0.511 MeV/c ²	105.7 MeV/c ²	1.777 GeV/c ²	80.4 GeV/c ²	
	-1	-1	-1	±1	
	1/2	1/2	1/2	1	
Leptons	e electron	μ muon	τ tau	W[±] W boson	Gauge bosons

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4 August 1972, Volume 177, Number 4047

- Condensed Matter Physics: **emergence**
 - Anderson: “More is different”



SCIENCE

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson

The reductionist hypothesis may still be a topic for controversy among philosophers, but among the great majority of active scientists I think it is accepted

planation of phenomena in terms of known fundamental laws. As always, distinctions of this kind are not unambiguous, but they are clear in most cases. Solid state physics, plasma physics, and perhaps

less relevance they seem to have to the very real problems of the rest of science, much less to those of society.

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other. That is, it seems to me that one may array the sciences roughly linearly in a hierarchy, according to the idea: The elementary entities of science X obey the laws of science Y.

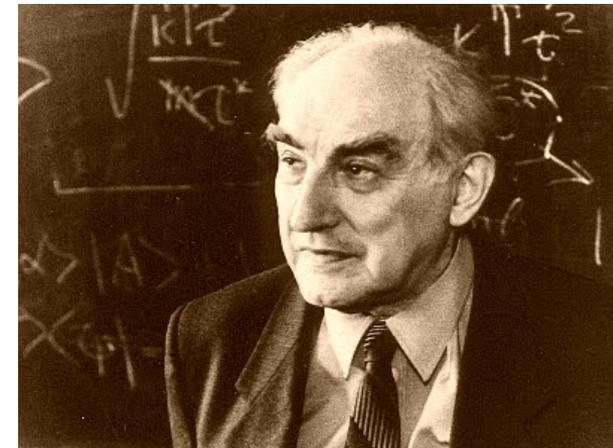
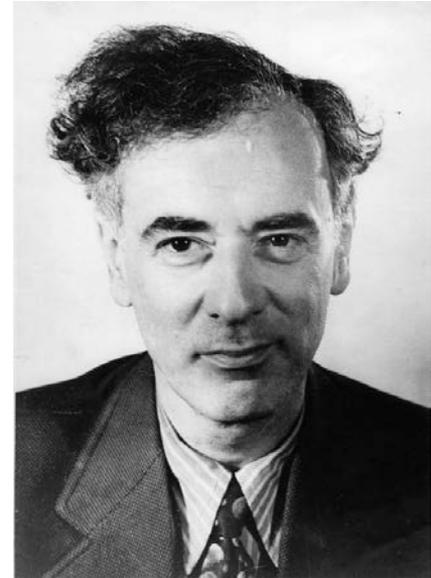
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 - Spontaneous symmetry breaking in high energy physics: Yoichiro Nambu (inspiration: superconductivity)



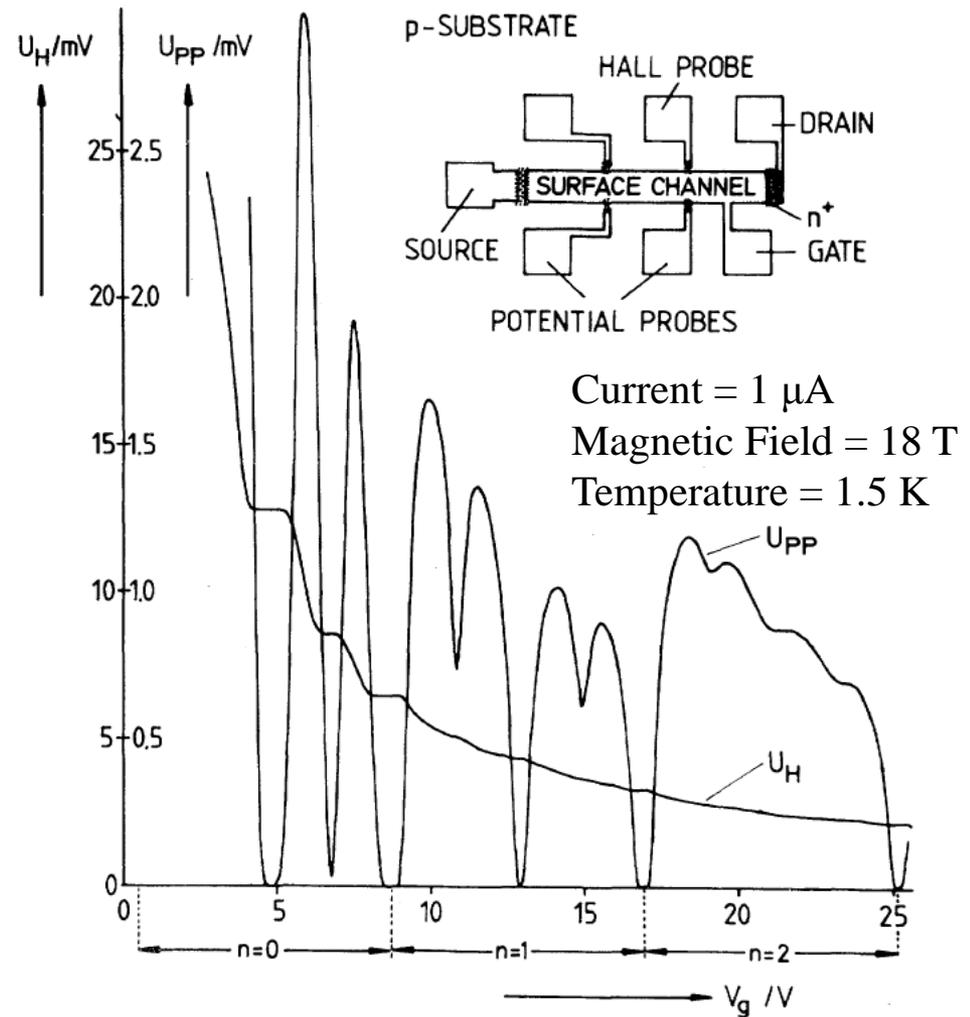
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 - Lev Landau: Classification of phases by symmetry breaking
 - Vitaly Ginzburg: **Local** order parameter
 - Success of Landau-Ginzburg: crystalline solids, magnets and superconductors



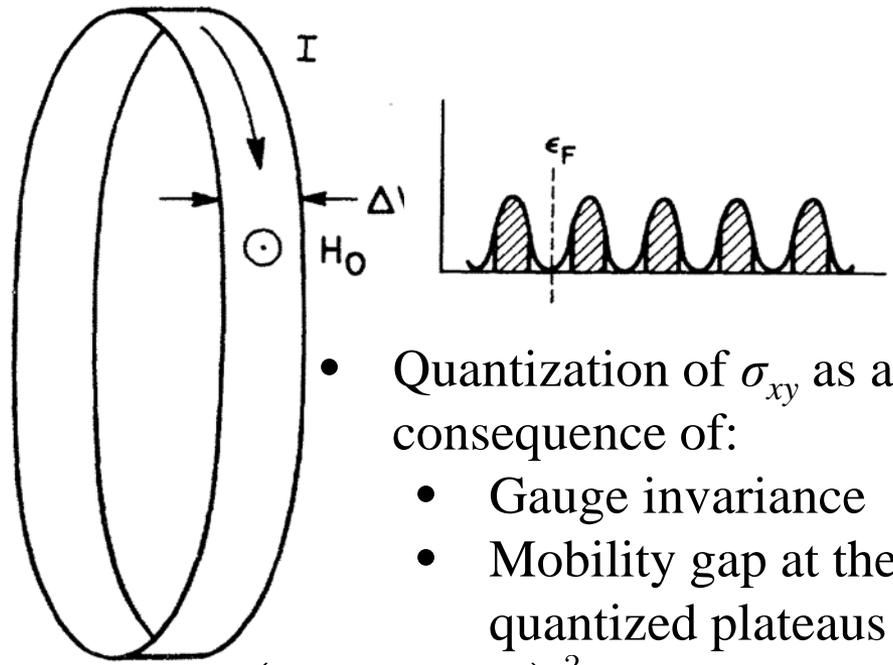
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- Topological Phases of Matter
 - von Klitzing's discovery of the Integer Quantum Hall (QH) Effect (IQHE) in 1980
 - Topological invariant \rightarrow Hall conductance *quantized* in units of e^2/h



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- Topological Phases of Matter
 - von Klitzing's discovery of the Integer Quantum Hall (QH) Effect (IQHE) in 1980
 - Topological invariant \rightarrow Hall conductance *quantized* in units of e^2/h
 - Laughlin's argument of the "quantum pump"
 - Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) \rightarrow Analytically showed quantization of Hall conductance
 - Quantization of σ_{xy} was shown by brute force evaluation of Kubo formula



- Quantization of σ_{xy} as a consequence of:
 - Gauge invariance
 - Mobility gap at the quantized plateaus

$$\hat{H}(k_1, k_2) = \frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial x} + \hbar k_1 \right)^2 + \frac{1}{2m} \left(-i\hbar \frac{\partial}{\partial y} + \hbar k_2 - eBx \right)^2 + U(x, y)$$

$$\sigma_H = \frac{ie^2}{A_0 \hbar} \sum_{\epsilon_\alpha < E_F} \sum_{\epsilon_\beta > E_F} \frac{1}{(\epsilon_\alpha - \epsilon_\beta)^2} \left[\begin{aligned} & \left(\frac{\partial \hat{H}}{\partial k_1} \right)_{\alpha\beta} \left(\frac{\partial \hat{H}}{\partial k_2} \right)_{\beta\alpha} \\ & - \left(\frac{\partial \hat{H}}{\partial k_2} \right)_{\alpha\beta} \left(\frac{\partial \hat{H}}{\partial k_1} \right)_{\beta\alpha} \end{aligned} \right]$$

Note: *the TKNN paper was before Michael Berry's seminal paper on Berry phase*

I. Introduction

- Topology in mathematics
 - Notion of topological invariance → classification of different geometrical objects into *equivalence classes*
Example: classification of 2D surfaces → number of holes (or genus)



- Topology in physics
 - In physics, consider Hamiltonians of many-particle systems with an energy gap or vacuum of a theory with gapped excitations
 - Examples of real systems: Hamiltonians of insulators and superconductors with a **full** energy gap
 - **NOT**: metals, doped semiconductors, or nodal superconductors
 - “Smooth deformation” → Tuning parameters in the Hamiltonian without closing the bulk gap
 - Topological invariant → extra label in addition to Landau-Ginzburg order parameter

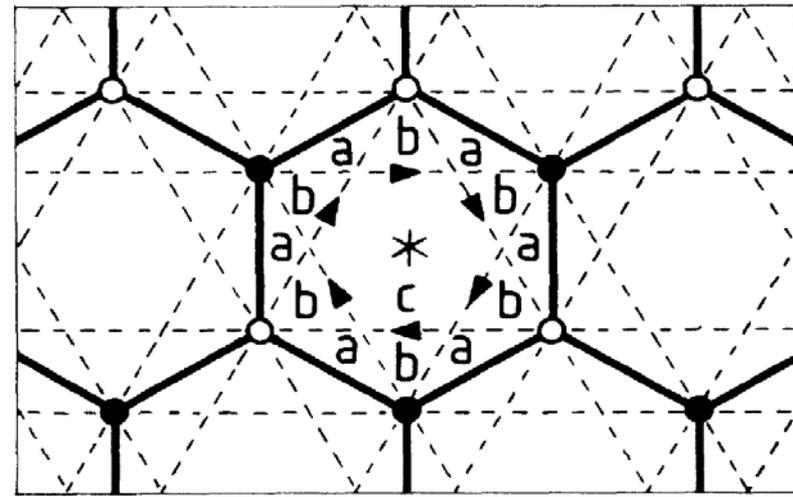
I. Introduction

- Overview of important developments in topological materials
 - Quantum Hall states belong to a topological class which explicitly breaks time-reversal symmetry (TRS)
 - Recently, new topological class of materials theoretically predicted and experimentally observed: Symmetry Protected Topological (SPT) phases preserving TRS in 2D and 3D

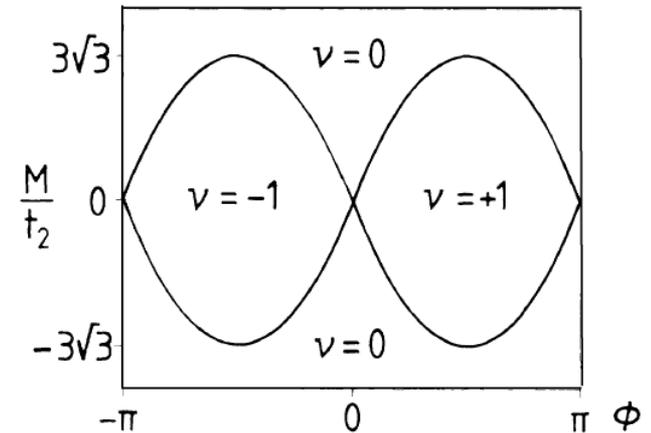
Discovery	Theoretical	Experimental
Quantum spin Hall insulator state in HgTe quantum wells	Bernevig <i>et al.</i> , Science 314, 5806 (2006), pp. 1757-1761	König <i>et al.</i> , Science 318, 5851 (2007), pp. 766-770.
Topological insulators (TIs) in three dimensions: theory and prediction in $\text{Bi}_x\text{Sb}_{1-x}$	(Theory) Fu <i>et al.</i> , PRL 98, 10 (2007), pp. 106803	Hsieh <i>et al.</i> , Nature 452, 7190 (2008), pp. 970-974
	$(\text{Bi}_x\text{Sb}_{1-x})$ Fu <i>et al.</i> , PRB 76, 4 (2007), pp. 045302	
Second generation of 3D topological insulators: Bi_2Se_3 , Bi_2Te_3 , and Sb_2Te_3	Zhang <i>et al.</i> , Nature Physics 5, 6 (2009), pp. 438-442	(Bi_2Se_3) Xia <i>et al.</i> , Nature Physics 5, 6 (2009), pp. 398-402
		(Bi_2Te_3) Chen <i>et al.</i> , Science 325, 5937 (2009), pp. 178-181

I. “Real” Introduction

- The (twisted) Road to Topological Insulators
 - IQHE without external gauge field (Haldane, 1988)
 - Topological Field Theory (TFT) of the QH effect based on Chern-Simons (CS) term (Zhang *et. al*, 1992)
 - Microscopic model for QH Effect (QHE) in 4D (Zhang *et. al*, 2001)
 - 2D and 3D TIs result from dimensional reduction of 4D QHE

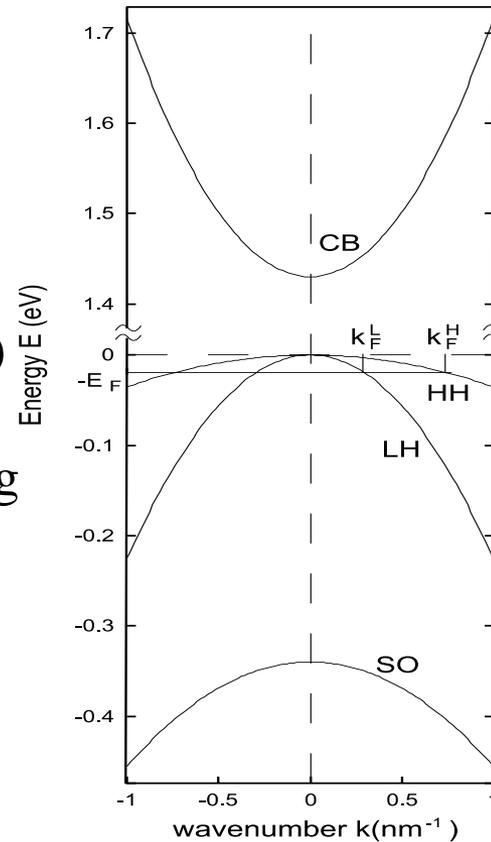


$$\begin{aligned}
 H(\mathbf{k}) = & 2t_2 \cos(\phi) \left(\sum_i \cos(\mathbf{k} \cdot \mathbf{b}_i) \right) I_{2 \times 2} \\
 & + t_1 \left(\sum_i [\cos(\mathbf{k} \cdot \mathbf{a}_i) \sigma^1 + \sin(\mathbf{k} \cdot \mathbf{a}_i) \sigma^2] \right) \\
 & + \left[M - 2t_2 \sin(\phi) \left(\sum_i \sin(\mathbf{k} \cdot \mathbf{b}_i) \right) \right] \sigma^3
 \end{aligned}$$



I. “Real” Introduction

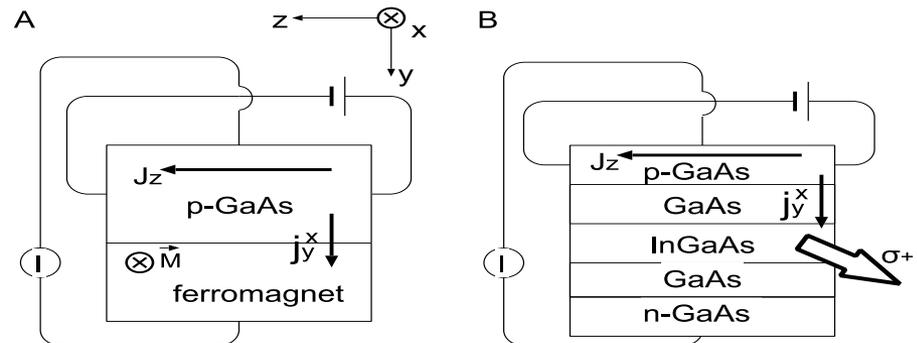
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 - 2D and 3D TIs result from dimensional reduction of 4D QHE
 - Intrinsic spin Hall effect (Murakami *et. al.*, 2003)
 - Dissipationless Spin Hall Insulator (SHI) (Murakami *et. al.*, 2003)



Spin conductance

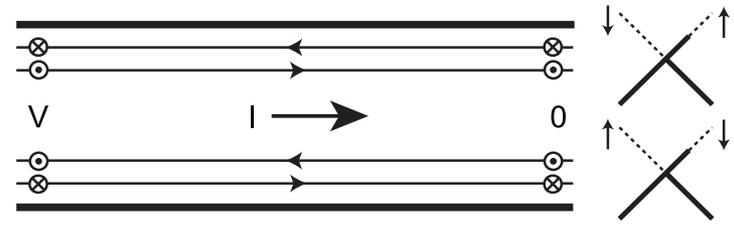
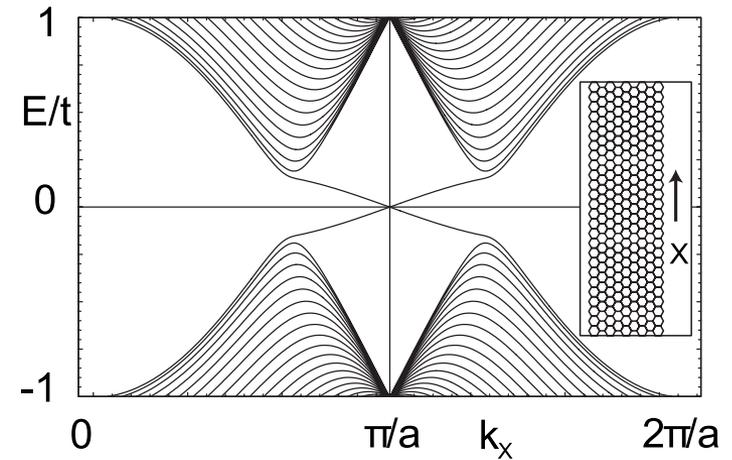
$$\sigma_{\text{spin}} \propto n_{\text{LH}}(\mathbf{k}) - n_{\text{HH}}(\mathbf{k})$$

Occupations of Light-Hole (LH) and Heavy-Hole (HH) bands



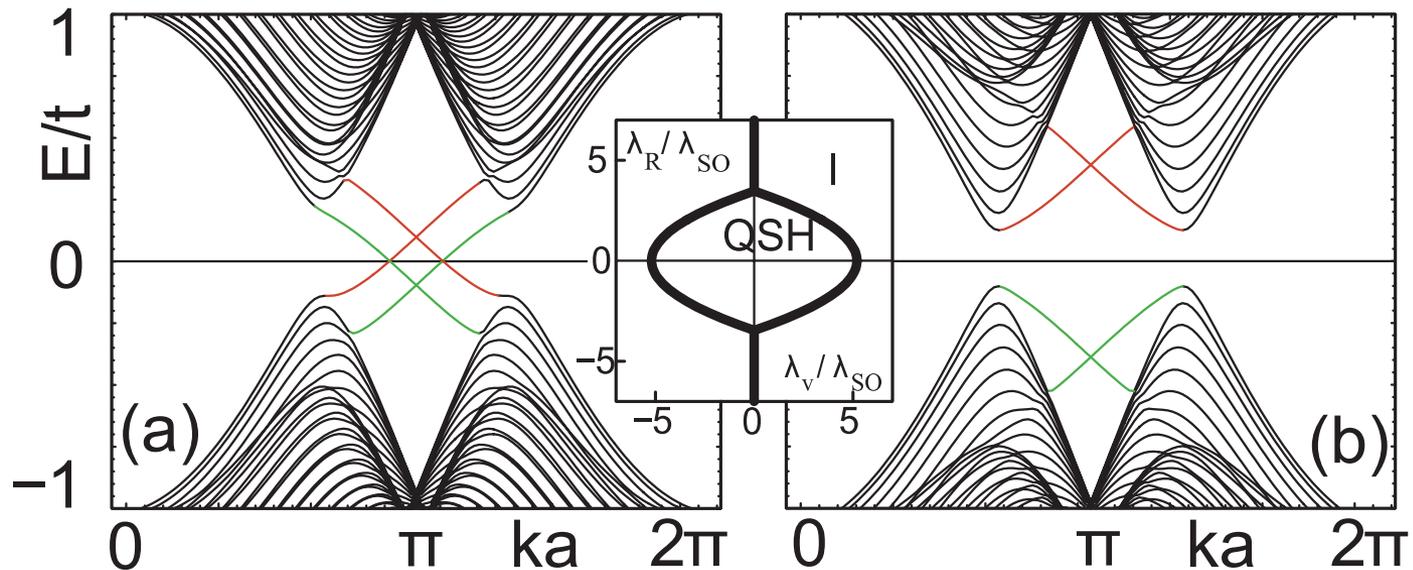
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 - QSHE in strained semiconductors (Bernevig *et. al*, 2006)



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- **Important Note:** Z_2 classification of TRI insulators \rightarrow “protected” edge states in QSHE (Kane *et. al.*, 2005b)



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- **Important Note:** Z_2 classification of TRI insulators → “protected” edge states in QSHE (Kane *et. al.*, 2005b)
- Edge states due to band inversion of HgTe relative to CdTe known back in 1986 by Volkov and Pankratov!

Solid State Communications, Vol. 61, No. 2, pp. 93–96, 1987.
Printed in Great Britain.

0038/1098/87 \$3.00 + .00
Pergamon Journals Ltd.

SUPERSYMMETRY IN HETEROJUNCTIONS: BAND-INVERTING CONTACT ON THE BASIS OF $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$
AND $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$

O.A. Pankratov, S.V. Pakhomov and B.A. Volkov

P.N. Lebedev Physical Institute, USSR Academy of Sciences, 117924, Moscow, Leninsky Prospect 53, USSR

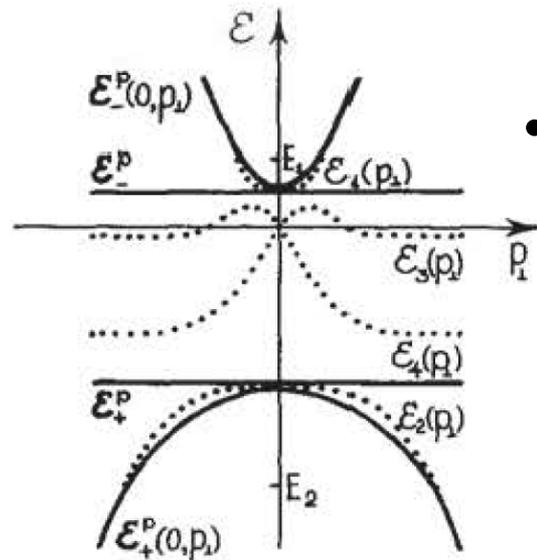
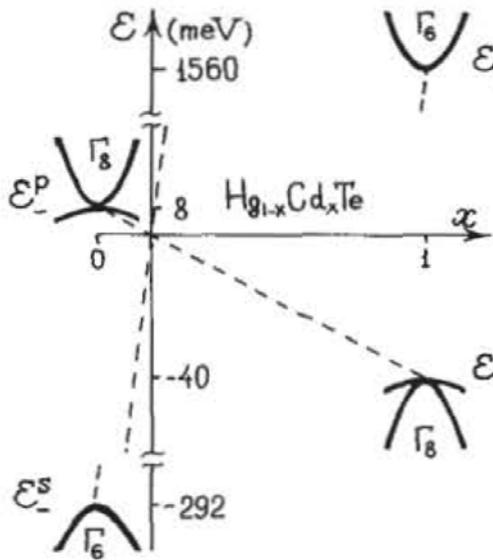
(Received 18 August 1986 by V.M. Agranovich)

In the inhomogeneous structure, which is the contact of two semiconductors with mutually inverted bands, two-dimensional non-degenerate electron states exist. These states appear due to the supersymmetry of an effective Hamiltonian and do not depend on the specific form of the transition region. When the energy increases the supersymmetry is broken and therefore the interface states exist only in a definite energy interval.

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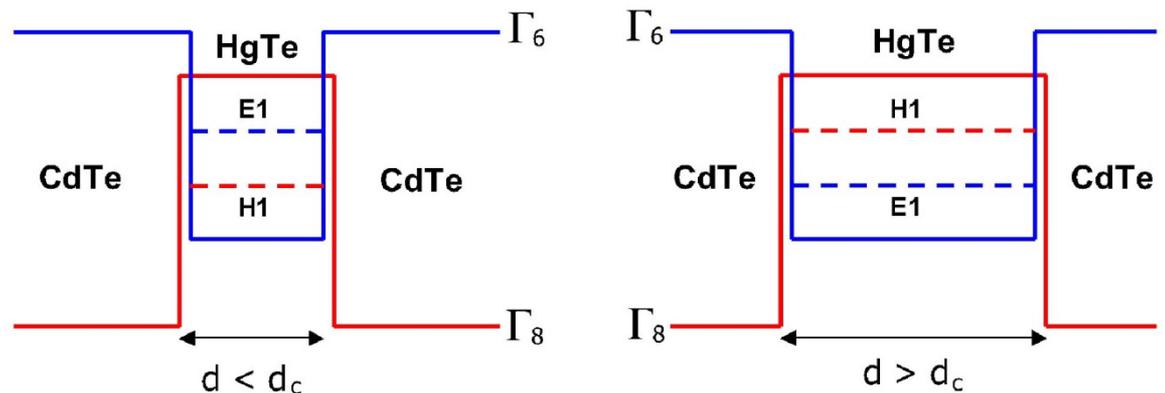
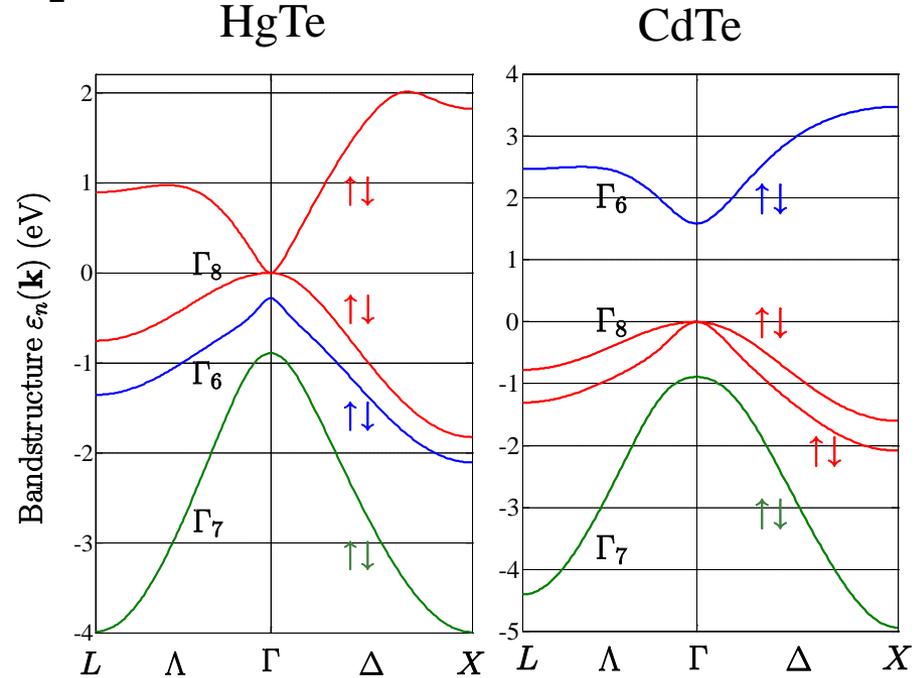
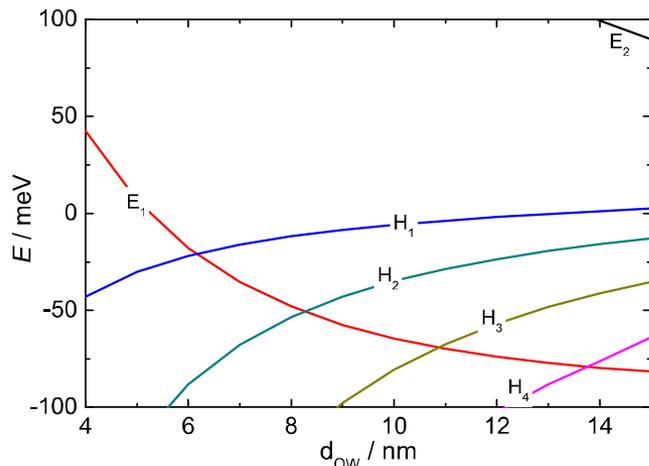
- **Important Note:** Z_2 classification of TRI insulators \rightarrow “protected” edge states in QSHE (Kane *et. al.*, 2005b)
- Edge states due to band inversion of HgTe relative to CdTe known back in 1986 by Volkov and Pankratov!
- Volkov and Pankratov did not make the connection to topology or protection of edge states
- TFT for topological insulators using dimensional reduction of 4D QHE (Qi *et. al.*, 2008)



II. Two-Dimensional Topological Insulators

A. Effective model of the two-dimensional time-reversal invariant topological insulator in HgTe/CdTe quantum wells

- Inversion of the Γ_6 and Γ_8 bands in HgTe relative to CdTe
- HgTe can be a 3D topological insulator
- HgTe has no gap!
- Quantum confinement provides subbands with gaps
- For well thickness (d_{QW}) $>$ 6.3 nm phase transition occurs
- Bands get “inverted”



II. Two-Dimensional Topological Insulators

B. Explicit solution of the helical edge states

Divide the model Hamiltonian into two

$$\hat{H} = \tilde{H}_0 + \tilde{H}_1$$

parts:

$$\tilde{H}_0 = \tilde{\epsilon}(k_x) + \begin{pmatrix} \tilde{M}(k_x) & Ak_x & 0 & 0 \\ Ak_x & -\tilde{M}(k_x) & 0 & 0 \\ 0 & 0 & \tilde{M}(k_x) & -Ak_x \\ 0 & 0 & -Ak_x & -\tilde{M}(k_x) \end{pmatrix}$$

$$\tilde{H}_1 = -Dk_y^2 + \begin{pmatrix} -Bk_y^2 & iAk_y & 0 & 0 \\ -iAk_y & Bk_y^2 & 0 & 0 \\ 0 & 0 & -Bk_y^2 & iAk_y \\ 0 & 0 & -iAk_y & Bk_y^2 \end{pmatrix} \quad \begin{aligned} \tilde{M}(k_x) &= M - Bk_x^2 \\ \tilde{\epsilon}(k_x) &= C - Dk_x^2 \end{aligned}$$

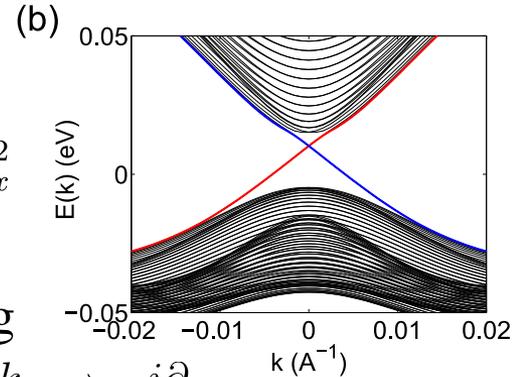
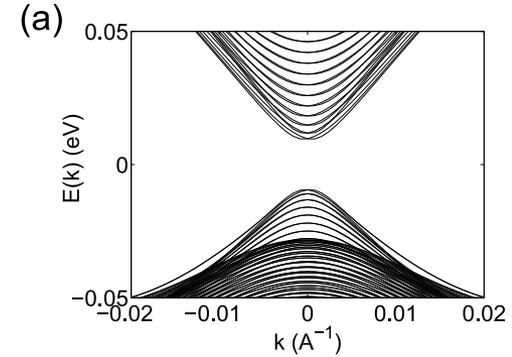
- The model is defined (say) for the region $x > 0$. By breaking translational symmetry in this direction we need to replace: $k_x \rightarrow -i\partial_x$
- The edge energy spectrum (if it exists) belongs to a family of eigen spectra of the *full* Hamiltonian with $k_y = 0$

$$\tilde{H}_0(k_x \rightarrow -i\partial_x) \Psi(x) = E\Psi(x)$$

- Above Hamiltonian is block diagonal \rightarrow solutions take the form

$$\Psi_{\uparrow}(x) = \begin{pmatrix} \psi_0(x) \\ \mathbf{0} \end{pmatrix} \quad \Psi_{\downarrow}(x) = \begin{pmatrix} \mathbf{0} \\ \psi_0(x) \end{pmatrix}$$

The above eigenstates are related by time-reversal



II. Two-Dimensional Topological Insulators

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$$\tilde{H}_0 = \tilde{\epsilon}(k_x) + \begin{pmatrix} \tilde{M}(k_x) & Ak_x & 0 & 0 \\ Ak_x & -\tilde{M}(k_x) & 0 & 0 \\ 0 & 0 & \tilde{M}(k_x) & -Ak_x \\ 0 & 0 & -Ak_x & -\tilde{M}(k_x) \end{pmatrix} \quad \begin{aligned} \tilde{\epsilon}(k_x) &= C - Dk_x^2 \\ \tilde{M}(k_x) &= M - Bk_x^2 \end{aligned}$$

$$\tilde{H}_0(k_x \rightarrow -i\partial_x) \Psi(x) = E\Psi(x) \quad \Psi_{\uparrow}(x) = \begin{pmatrix} \psi_0(x) \\ \mathbf{0} \end{pmatrix} \quad \Psi_{\downarrow}(x) = \begin{pmatrix} \mathbf{0} \\ \psi_0(x) \end{pmatrix}$$

- For $C = D = 0$ (i.e. assuming particle-hole symmetry) and $E = 0$ we get

$$\begin{pmatrix} M + B\partial_x^2 & -iA\partial_x \\ -iA\partial_x & -M - B\partial_x^2 \end{pmatrix} \psi_0(x) = 0$$

- With the ansatz: $\psi_0(x) = \phi e^{\lambda x}$

$$\begin{pmatrix} M + B\lambda^2 & -iA\lambda \\ -iA\lambda & -M - B\lambda^2 \end{pmatrix} \phi = 0 \quad \lambda_{\pm, \pm} = -\frac{1}{2} \left(\pm \frac{A}{B} \right) \pm \sqrt{\frac{1}{4} \left(\pm \frac{A}{B} \right)^2 - \frac{M}{B}}$$

$$(M + B\lambda^2) \tau_z \phi = iA\lambda \tau_x \phi \quad \psi_0(x) = (ae^{\lambda_1 x} + be^{\lambda_2 x}) \phi_+ + (ce^{-\lambda_1 x} + de^{-\lambda_2 x}) \phi_-$$

$$(M + B\lambda^2) (-i\tau_x \tau_z) \phi = A\lambda \phi \quad \lambda_{-, \pm} \equiv \lambda_{1/2}$$

$$\tau_y \phi = \left(\frac{-A\lambda}{M + B\lambda^2} \right) \phi \quad \psi_0(x) = \begin{cases} a (e^{\lambda_1 x} - e^{\lambda_2 x}) \phi_+, & A/B < 0 \\ c (e^{-\lambda_1 x} - e^{-\lambda_2 x}) \phi_-, & A/B > 0 \end{cases}$$

$$\tau_y \phi_{\pm} = (\pm 1) \phi_{\pm}$$

$$\lambda_{\pm, \pm}^2 \pm \frac{A}{B} \lambda_{\pm, \pm} + \frac{M}{B} = 0 \quad H_{\text{edge}}^{\alpha\beta}(k_y) = \langle \Psi_{\alpha} | (\tilde{H}_0 + \tilde{H}_1) | \Psi_{\beta} \rangle$$

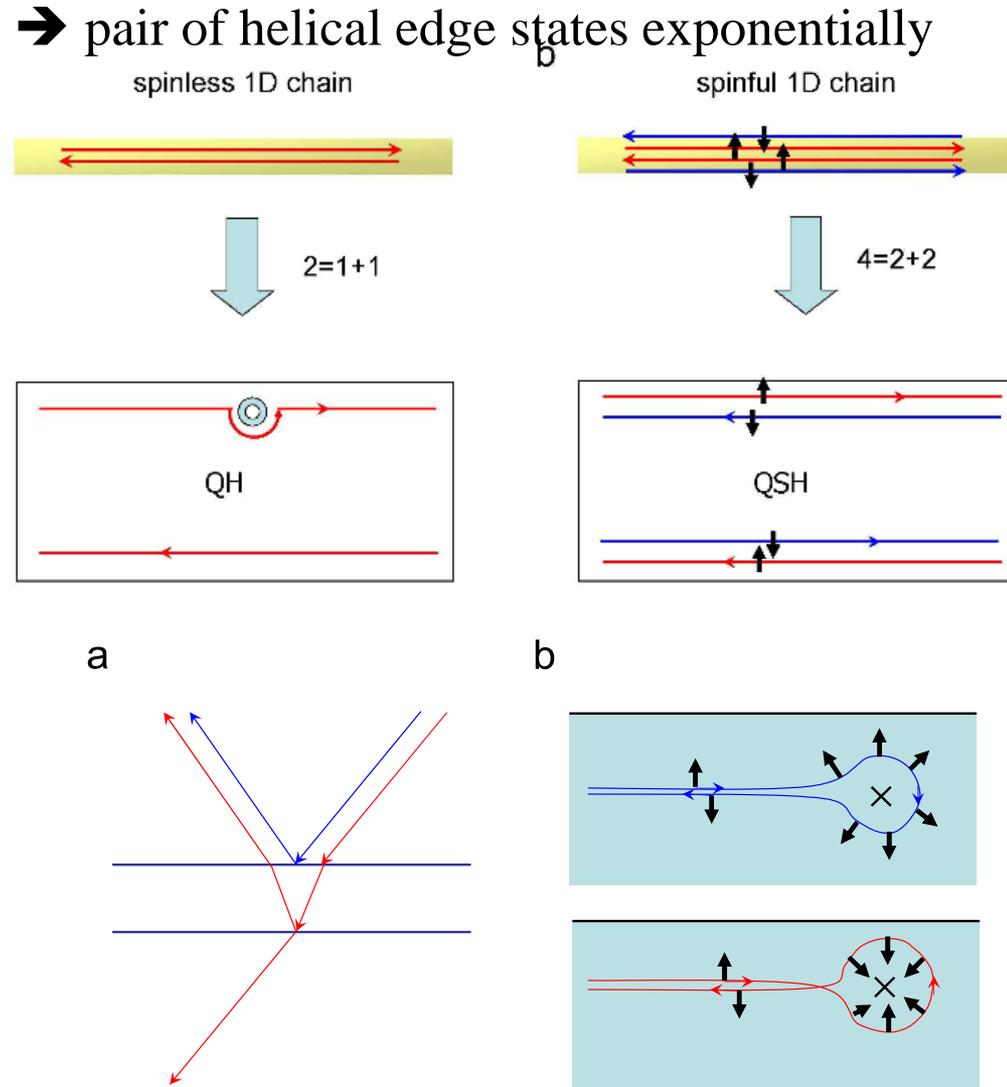
$$\approx Ak_y \sigma_z^{\alpha\beta}$$

II. Two-Dimensional Topological Insulators

C. Physical properties of the helical edge states

1. Topological protection of the helical edge states

- Explicit solution of the BHZ model \rightarrow pair of helical edge states exponentially localized at the edge
- The concept of “helical” edge state \rightarrow states with opposite spin counter-propagate at a given edge
- QH protected by “chiral” edge states; QSH edge states protected due to destructive interference between all possible backscattering paths
- SOC provides spin-momentum locking
- Clockwise and anticlockwise rotation of spin pick up $\pm\pi$ phase leading to destructive interference

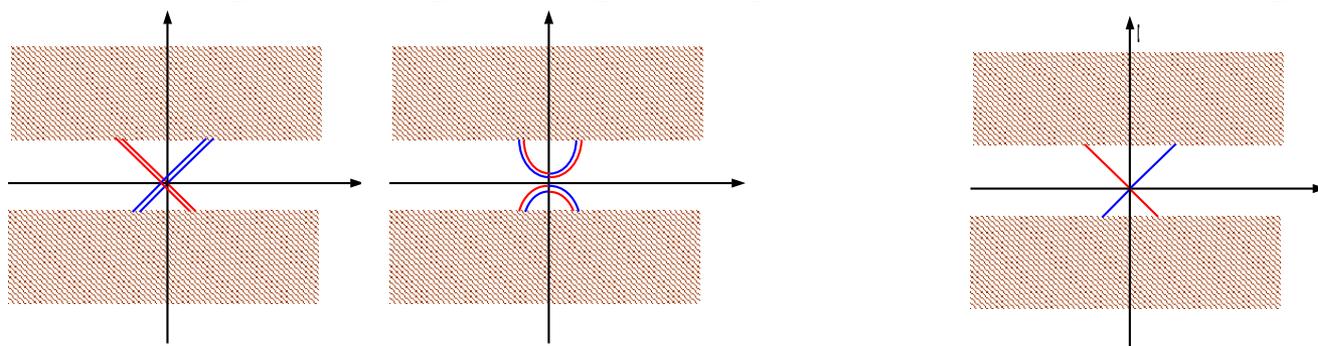


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1. Topological protection of the helical edge states

- The physical description of edge state protection works only for *single* pair of edge states
- With (say) two forward-movers and two backward-movers backscattering is possible without spin flip
- In other words, TRS perturbations can destroy edge states in pairs
- Robust or non-dissipative edge transport requires **odd** number of edge states



- If TR symmetry is not present $H_{\text{mass}} = m \int \frac{dk}{2\pi} \left(\psi_{k+}^\dagger \psi_{k-} + \text{h.c.} \right)$
- Electron operators: $T\psi_{k+}T^{-1} = \psi_{-k,-}$, $T\psi_{k-}T^{-1} = -\psi_{-k,+}$ $TH_{\text{mass}}T^{-1} = -H_{\text{mass}}$
- Define the “chirality” operator $C = N_+ - N_- = \int \frac{dk}{2\pi} \left(\psi_{k+}^\dagger \psi_{k+} - \psi_{k-}^\dagger \psi_{k-} \right)$
- Any operator that changes C by $2(2n-1)$ is odd under TR

II. Two-Dimensional Topological Insulators

C. Physical properties of the helical edge states

2. Interactions and quenched disorder

Only two TR invariant non-chiral interactions can be added

$$H_f = g \int dx \psi_+^\dagger \psi_+ \psi_-^\dagger \psi_- \leftarrow \text{forward scattering term}$$

$$H_u = g_u \int dx e^{-i4k_F x} \psi_+^\dagger(x) \psi_+^\dagger(x+a) \psi_-(x+a) \psi_-(x) + \text{h.c.}$$

Two-particle backscattering or “Umklapp” term

- We can “bosonize” the Hamiltonian

$$H = \frac{v_F}{2} \int dx \left\{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right\}$$

- Boson to fermion field operators

$$\psi_R(x) \sim \frac{1}{2\pi a} e^{ik_F x} e^{i\phi_R(x)}$$

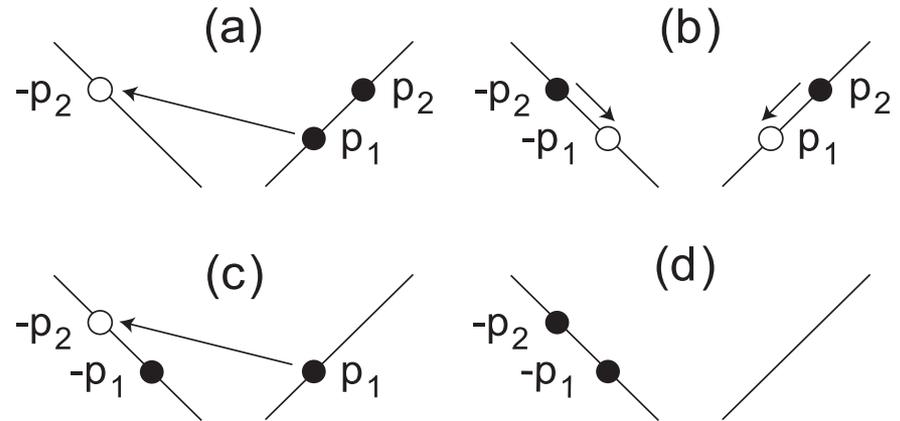
$$\psi_L(x) \sim \frac{1}{2\pi a} e^{-ik_F x} e^{i\phi_L(x)}$$

- The forward scattering term simply renormalizes the parameters K and v_F

$$K = \left(\frac{v_F - g}{v_F + g} \right)^{1/2} \quad v = \sqrt{v_F^2 - g^2}$$

Combined with Umklapp term we get (opens a gap at $k_F = \pi/2$)

$$H = \int dx \frac{v}{2} \left\{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right\} + \frac{g_u (\cos \sqrt{16\pi} \phi)}{2(\pi a)^2}$$



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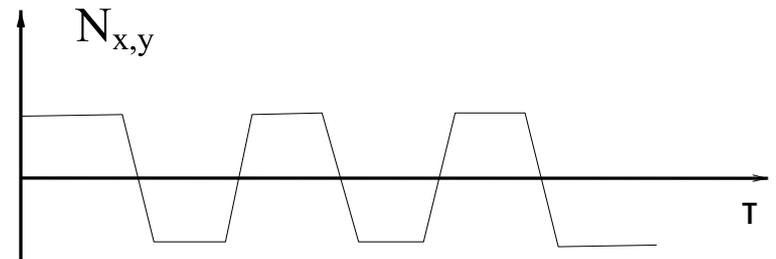
- Total Hamiltonian

$$H = \int dx \frac{v}{2} \left\{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right\} + \frac{g_u (\cos \sqrt{16\pi} \phi)}{2(\pi a)^2}$$

Umklapp term

- Interactions **can** spontaneously break time-reversal symmetry
- TR odd single-particle backscattering: $N_x = \psi_{R\uparrow}^\dagger \psi_{L\downarrow} + \text{h.c.}$ $N_y = i(\psi_{R\uparrow}^\dagger \psi_{L\downarrow} - \text{h.c.})$
- RG analysis \rightarrow Umklapp term relevant for $K < 1/2$ with a gap: $\Delta \approx a^{-1} (g_u)^{\frac{1}{2-4K}}$
- Bosonize N_x and N_y . For $g_u < 0$ fixed points at $\phi = 0, \sqrt{\pi}/2$

	$g_u < 0$	$g_u > 0$
$N_x = \frac{i\eta_R\eta_L}{2\pi a} \sin(\sqrt{4\pi}\phi)$	0	± 1
$N_y = \frac{i\eta_R\eta_L}{2\pi a} \cos(\sqrt{4\pi}\phi)$	± 1	0



- For $g_u < 0$, N_y is the (Ising-like) ordered quantity at $T = 0$
- Due to thermal fluctuations TRS is restored for $T > 0$
- For $0 < T \ll \Delta$ mass order parameter N_y is disordered + TR is preserved with a gap

II. Two-Dimensional Topological Insulators

C. Physical properties of the helical edge states

2. Interactions and quenched disorder

- Total Hamiltonian

$$H = \int dx \frac{v}{2} \left\{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right\} + \frac{g_u (\cos \sqrt{16\pi} \phi)}{2(\pi a)^2}$$

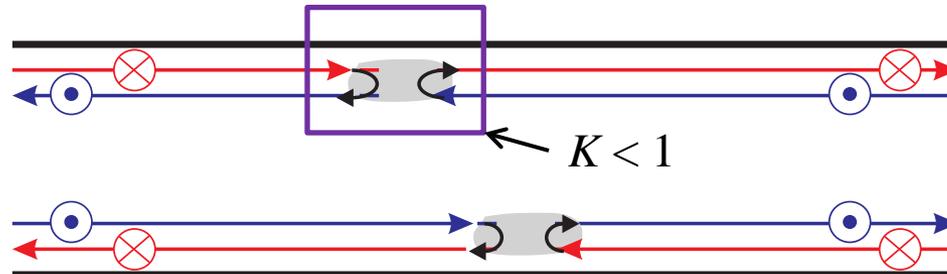
Umklapp term

- Two-particle backscattering due to quenched disorder

$$H_{\text{dis}} = \int dx \frac{g_u(x)}{2(\pi a)^2} \cos \left[\sqrt{16\pi} (\phi(x, \tau) + \alpha(x)) \right]$$

Gaussian random variables

- The “replica trick” in disordered systems shows disorder relevant for $K < 3/8$
- N_x and N_y show glassy behavior at $T = 0$ with TRS breaking; TRS again restored at $T > 0$
- Where would all these interactions come from? locally doped regions? Band bending?
- But edge states are immune to electrostatic potential scattering
- Potential inhomogeneities can trap bulk electrons which may then interact with the edge electrons



II. Two-Dimensional Topological Insulators

C. Physical properties of the helical edge states

2. Interactions and quenched disorder

Static magnetic impurity breaks local TRS and opens a gap

Quantum impurity \rightarrow Kondo

effect: $H = H_0 + H_K + H_u$

$$H_0 = \frac{v_F}{2} \int dx \left\{ \frac{1}{K} (\partial_x \phi)^2 + K (\partial_x \theta)^2 \right\}$$

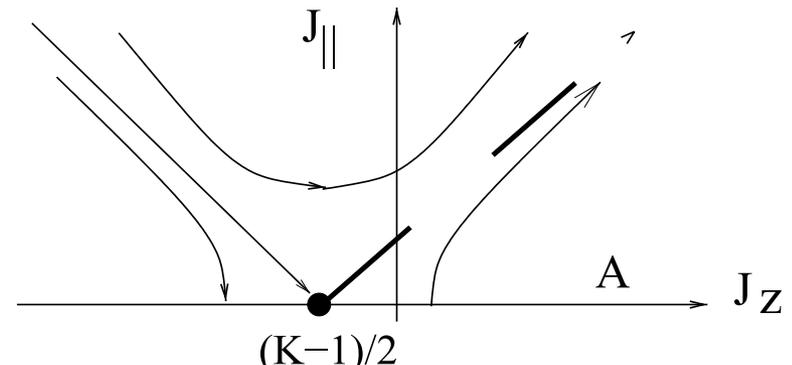
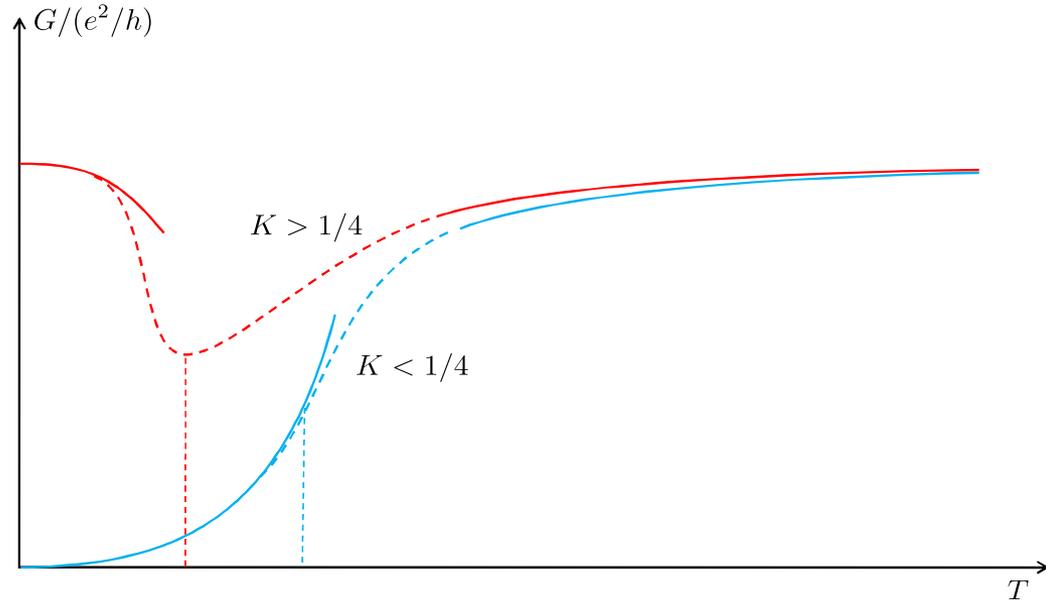
$$H_u = \frac{g_u (\cos \sqrt{16\pi} \phi)}{2(\pi a)^2}$$

$$H_K = \int dx \delta(x) \left\{ \frac{J_{\parallel}}{2} (\sigma_- \psi_R^\dagger \psi_L + \sigma_+ \psi_L^\dagger \psi_R) + J_z \sigma_z (\psi_R^\dagger \psi_R - \psi_L^\dagger \psi_L) \right\}$$

$$H_K = \frac{J_{\parallel} a}{2\pi\xi} (\sigma_- : e^{-i2\sqrt{\pi}\phi(0)} : + \text{h.c.}) - \frac{J_z a}{\sqrt{\pi}} \sigma_z \partial_x \theta(0)$$

- Doing the “standard” RG procedure we get flow equations

$$\frac{dJ_{\parallel}}{d \log(L/a)} = (1 - K + 2J_z) J_{\parallel} \quad \frac{dJ_z}{d \log(L/a)} = 2J_{\parallel}^2$$



II. Two-Dimensional Topological Insulators

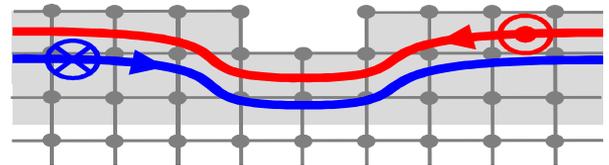
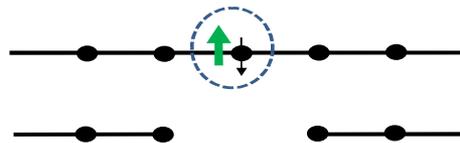
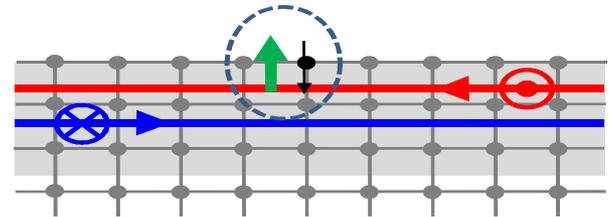
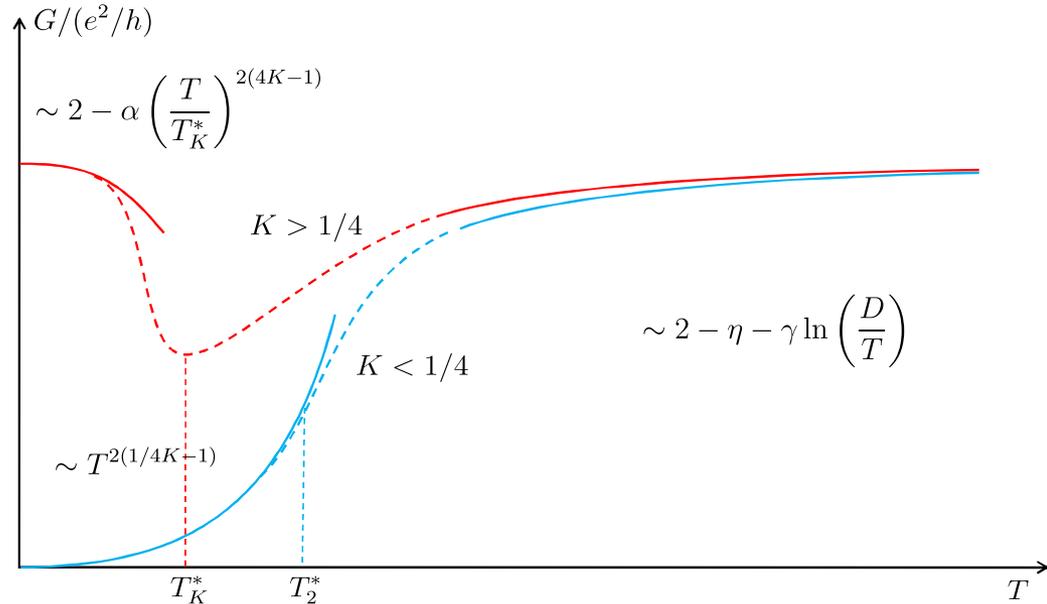
C. Physical properties of the helical edge states

2. Interactions and quenched disorder

- Static magnetic impurity breaks local TRS and opens a gap
- Quantum impurity \rightarrow Kondo effect

effect

1. At high temperature (T) conductance (G) is log
2. For *weak* Coulomb interaction ($K > 1/4$) conductance back to $2e^2/h$. At intermediate T the $G \sim T^{2(4K-1)}$ due to Umklapp term



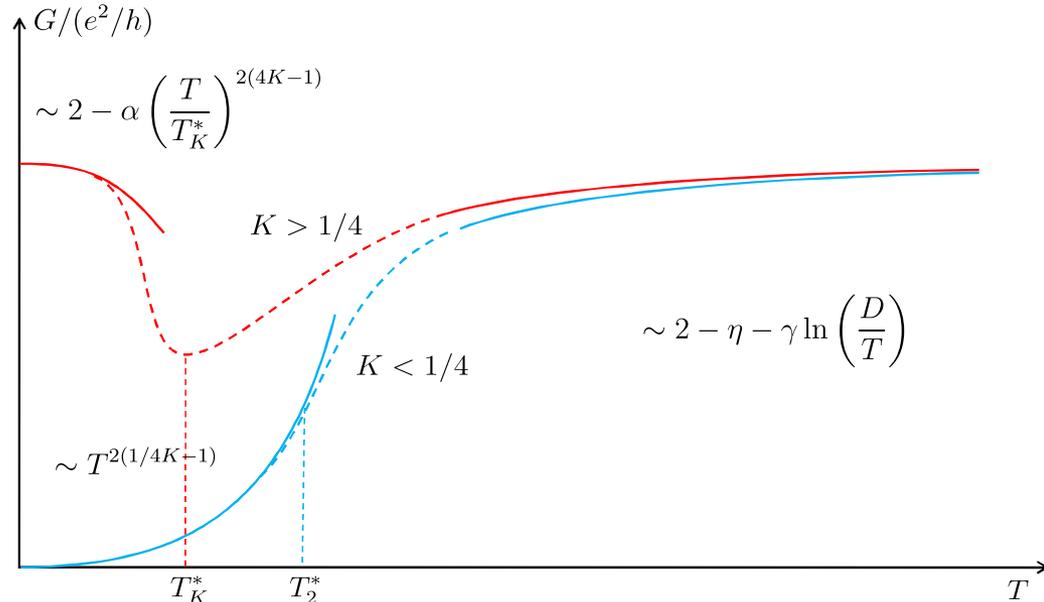
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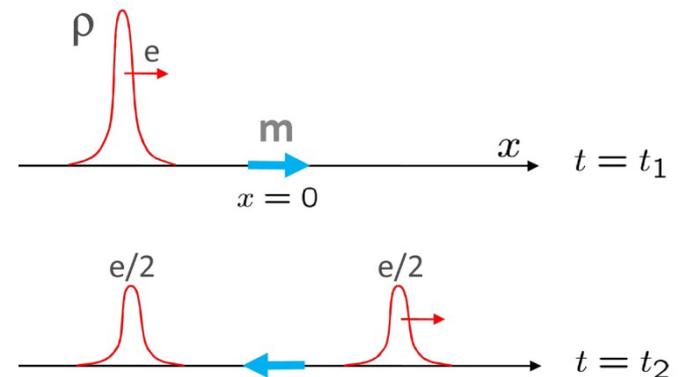
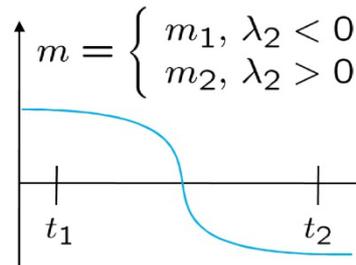
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2. For *weak* Coulomb interaction ($K > 1/4$) conductance back to $2e^2/h$. At intermediate T the $G \sim T^{2(4K-1)}$ due to Umklapp term



3. For *strong* Coulomb interaction ($K < 1/4$) $G = 0$ at $T = 0$ due to Umklapp. At intermediate T the $G \sim T^{2(1/4K-1)}$ due to tunneling of $e/2$ charge

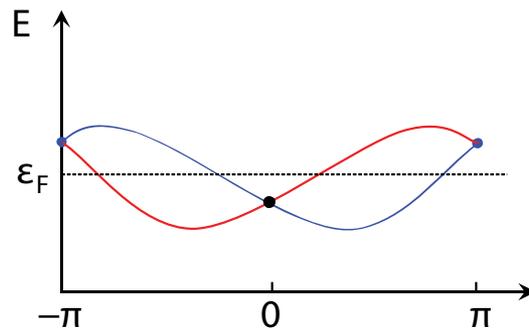


II. Two-Dimensional Topological Insulators

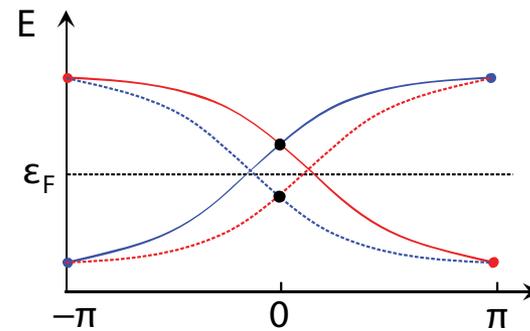
C. Physical properties of the helical edge states

3. Helical edge states and the holographic principle

- The physical description of edge state protection works only for *single* pair of edge states
- With (say) two forward-movers and two backward-movers backscattering is possible without spin flip
- In other words, TRS perturbations can destroy edge states in pairs
- Robust or non-dissipative edge transport requires **odd** number of edge states
- Fermion doubling theorem



(a)



(b)

II. Two-Dimensional Topological Insulators

C. Physical properties of the helical edge states

4. Transport theory of the helical edge states

- Using Landauer-Büttiker formalism for an n -terminal device

$$I_i = \frac{e^2}{h} \sum_{j=1}^n (T_{ji} V_i - T_{ij} V_j)$$

- For the helical edge channels we expect

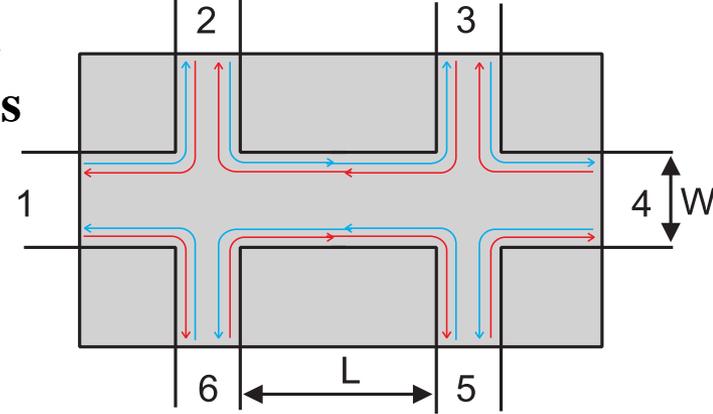
$$T(\text{QSH})_{i+1,i} = T(\text{QSH})_{i,i+1} = 1$$

- For a 2-point transport measurement between terminals 1 and 4

$$\frac{e}{h} \begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 1 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & 1 & -2 & 1 \\ 1 & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ 0 \\ \mu_5 \\ \mu_6 \end{pmatrix} = I_{14} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_5 \\ \mu_6 \end{pmatrix} = \frac{I_{14} h}{e} \begin{pmatrix} -3/2 \\ -1 \\ -1/2 \\ -1/2 \\ -1 \end{pmatrix}$$

$$\begin{aligned} V_{14} &= \frac{1}{(-e)} (\mu_1 - \mu_4) \\ &= \frac{1}{(-e)} \left(-\frac{3I_{14}h}{2e} - 0 \right) \\ &= \left(\frac{3h}{2e^2} \right) I_{14} \end{aligned}$$

$$\begin{aligned} V_{23} &= \frac{1}{(-e)} (\mu_2 - \mu_3) \\ &= \frac{1}{(-e)} \left(-\frac{I_{14}h}{e} - \left(-\frac{I_{14}h}{2e} \right) \right) \\ &= \left(\frac{h}{2e^2} \right) I_{14} \end{aligned}$$

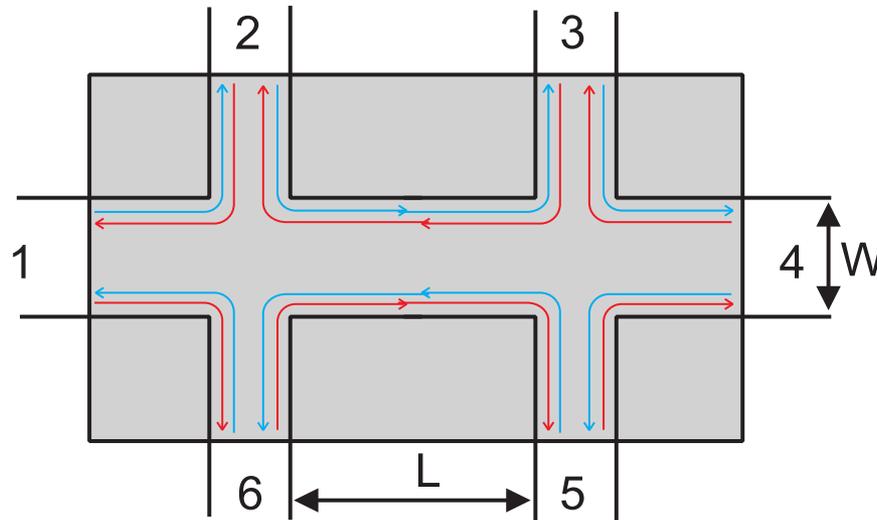
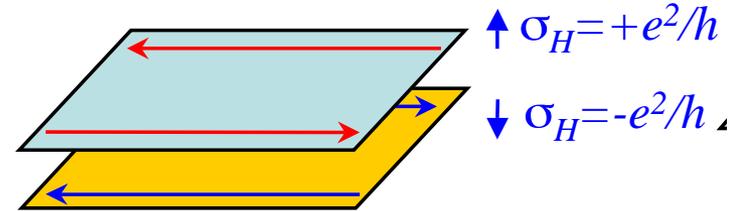


II. Two-Dimensional Topological Insulators

C. Physical properties of the helical edge states

4. Transport theory of the helical edge states

- If the transport is dissipationless where is the resistance coming from?
- In QSHE don't we have spin currents of $e^2/h + e^2/h = 2e^2/h$ and charge currents of $e^2/h - e^2/h = 0$?
- Answer 1: dissipation comes from the contacts. Note that transport is dissipationless only **inside** the HgTe QW
- Answer 2: We do measure charge conductance! The existence of helical edge channels is *inferred* from charge transport measurements



II. Two-Dimensional Topological Insulators

D. Topological excitations

1. Fractional charge on the edge

- Quantized charge at the edge of domain wall
 - Jackiw-Rebbi (1976)
 - Su-Schrieffer-Heeger (1979)
- Helical liquid has half DOF as normal liquid $\rightarrow e/2$ charge at domain walls
- Mass term \propto Pauli matrices \rightarrow external TRS breaking field
- Mass term to leading order

$$H_M = \int dx \Psi^\dagger \sum_{a=1,2,3} m_a(x,t) \sigma^a \Psi = \int dx \Psi^\dagger \sum_{a,i} t_{ai} B_i(x,t) \sigma^a \Psi \quad \Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$$

- Current due to the mass field

$$j_\mu = \frac{1}{2\pi} \frac{1}{\sqrt{m_\alpha m^\alpha}} \epsilon^{\mu\nu} \epsilon^{\alpha\beta} m_\alpha \partial_\nu m_\beta, \quad \alpha, \beta = 1, 2$$

- For $m_1 = m \cos(\theta)$, $m_2 = m \sin(\theta)$, and $m_3 = 0$

$$\rho = \frac{1}{2\pi} \partial_x \theta(x,t), \quad j = -\frac{1}{2\pi} \partial_t \theta(x,t)$$

- Topological response \rightarrow net charge Q in a region $[x_1, x_2]$ at time $t =$ difference in $\theta(x,t)$ at the boundaries $Q = \frac{1}{2\pi} [\theta(x_2, t) - \theta(x_1, t)]$

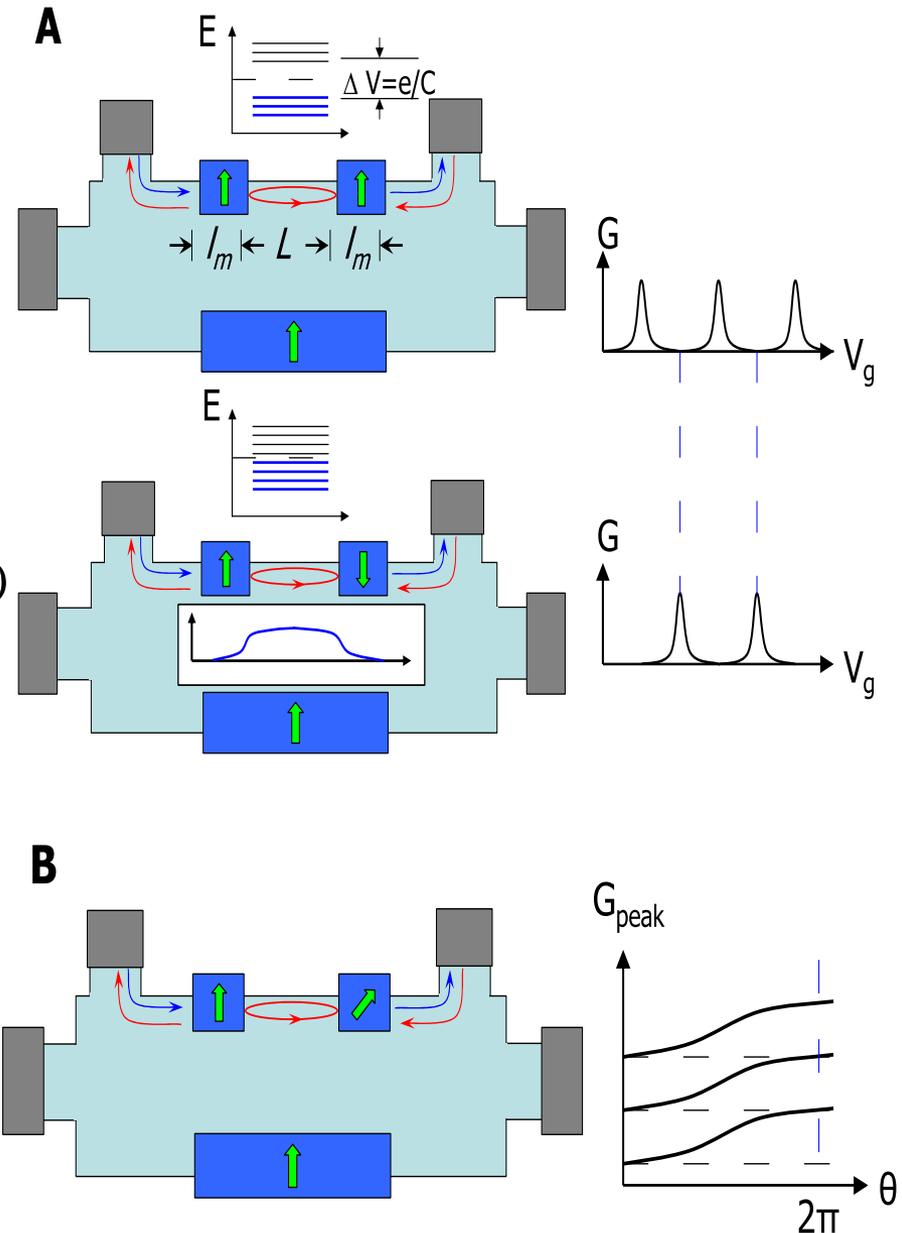
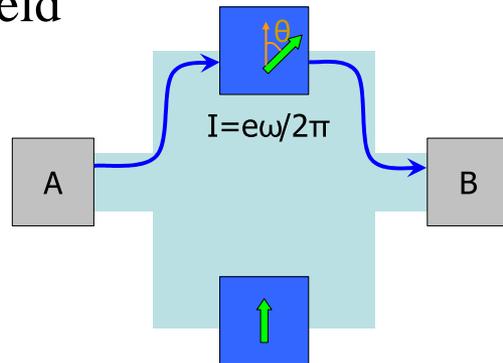
- Charge pumped in the time interval $[t_1, t_2]$ $\Delta Q_{\text{pump}}|_{t_1}^{t_2} = \frac{1}{2\pi} [\theta(t_2) - \theta(t_1)]$

II. Two-Dimensional Topological Insulators

D. Topological excitations

1. Fractional charge on the edge

- Two magnetic islands trap the electrons between them *like* a quantum wire between potential barriers
- Conductance oscillations can be observed as in usual Coulomb blockade measurements
- Background charge in the confined region Q (total charge) = Q_c (nuclei, etc.) + Q_e (lowest subband)
Flip relative magnetization \rightarrow pump $e/2$ charge
- Continuous shift of peaks with $\theta(\mathbf{B})$
- AC magnetic field drives current

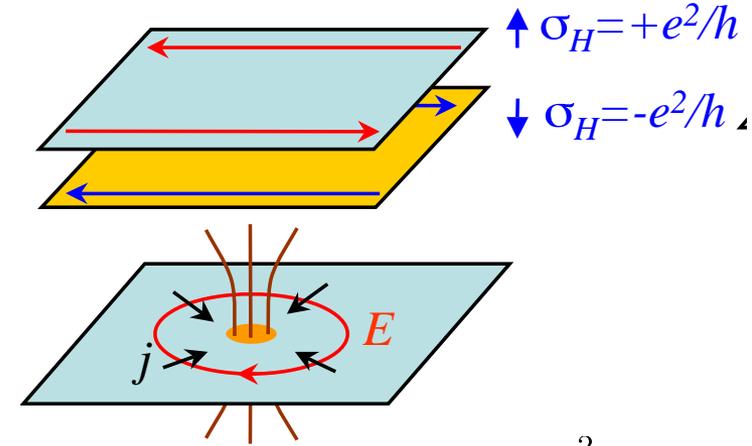


II. Two-Dimensional Topological Insulators

D. Topological excitations

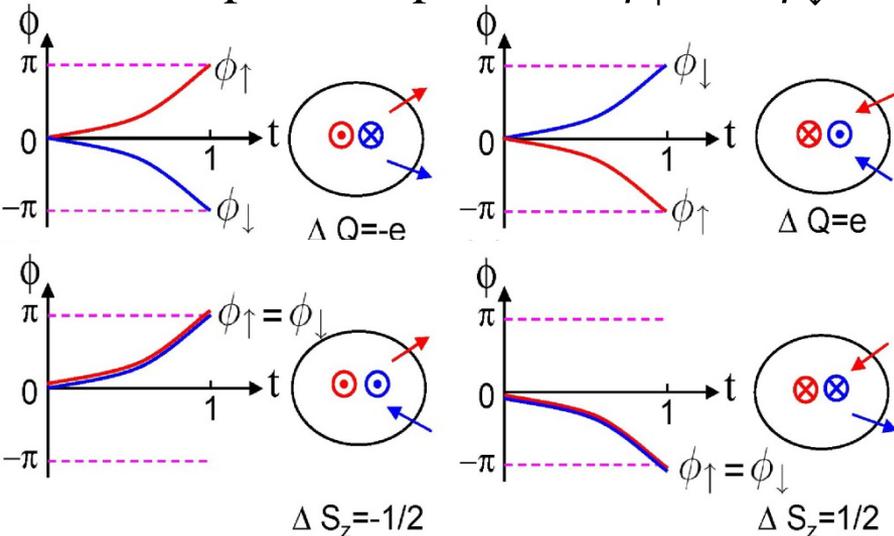
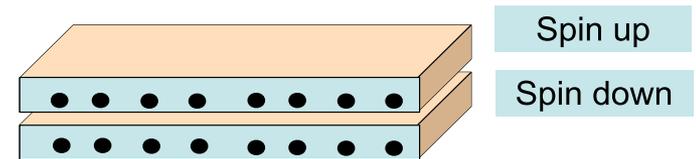
2. Spin-charge separation in the bulk

- Simplified analysis:
 - Assume S_z is preserved
 - QSHE as two copies of QHE
- Thread a π (units of $\hbar = c = e = 1$) flux ϕ
- TRS preserved at $\phi = 0$ and π ; also, $\pi = -\pi$
- Four possible paths for ϕ_\uparrow and ϕ_\downarrow :



- Current density from \mathbf{E}_\parallel : $\mathbf{j}_\uparrow = \frac{e^2}{h} \hat{\mathbf{z}} \times \mathbf{E}_\uparrow$
- Net charge flow:

$$\begin{aligned} \Delta Q_\uparrow &= - \int_0^1 dt \int d\mathbf{n} \cdot \mathbf{j}_\uparrow = - \frac{e^2}{h} \int_0^1 dt \int d\mathbf{l} \cdot \mathbf{E}_\uparrow \\ &= - \frac{e^2}{hc} \int_0^1 dt \frac{\partial \phi}{\partial t} = - \frac{e^2 hc}{hc 2e} = - \frac{e}{2} \end{aligned}$$



$$\Delta Q = \Delta Q_\uparrow + \Delta Q_\downarrow = -e$$

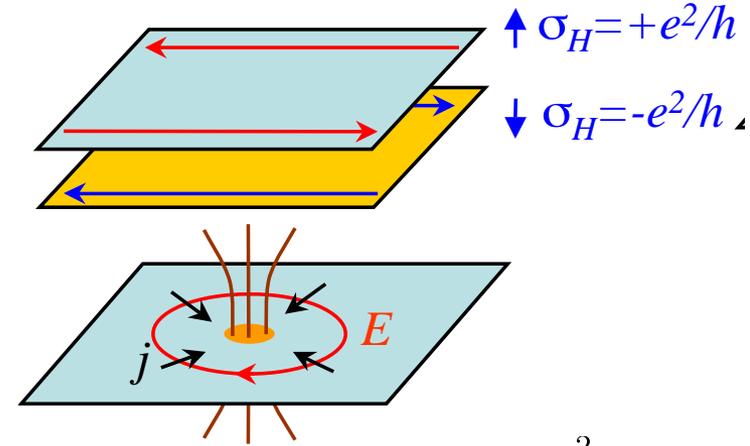
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II. Two-Dimensional Topological Insulators

D. Topological excitations

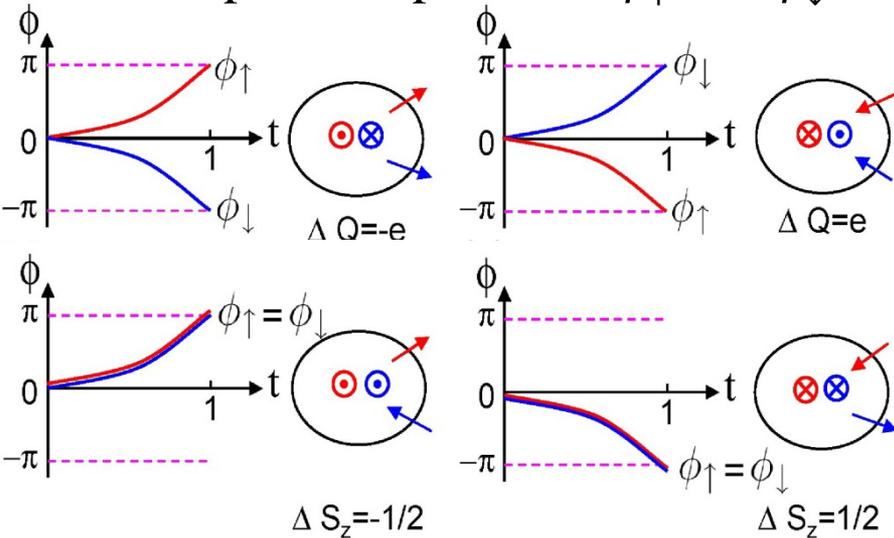
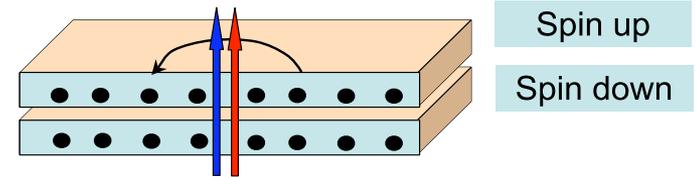
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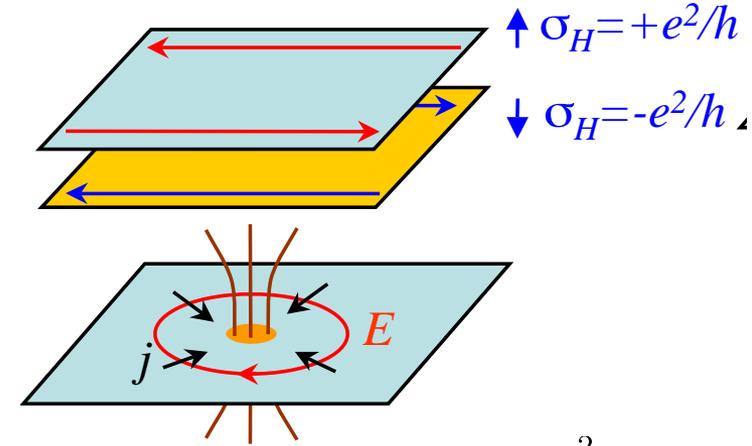
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II. Two-Dimensional Topological Insulators

D. Topological excitations

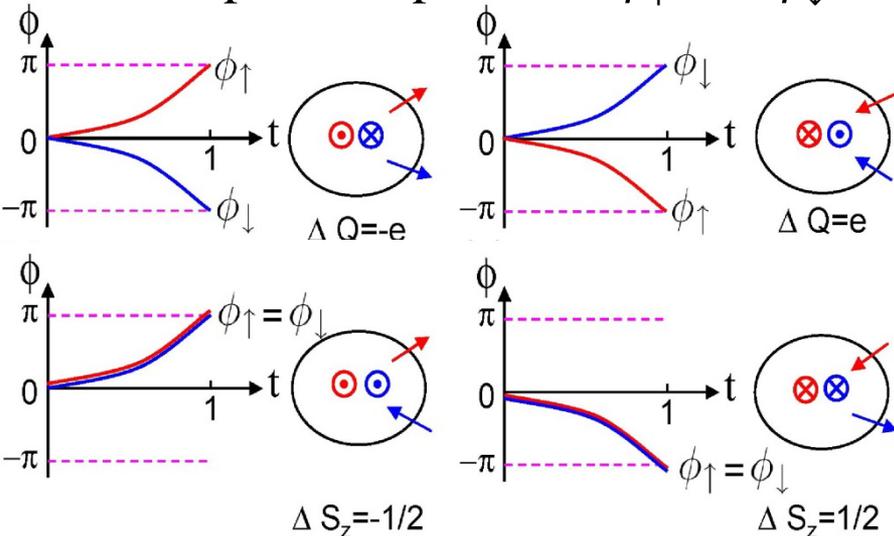
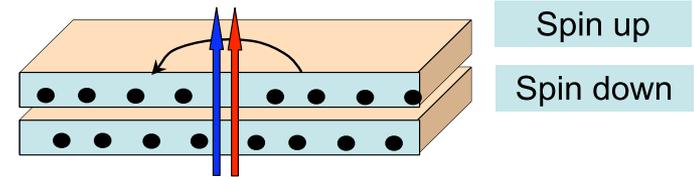
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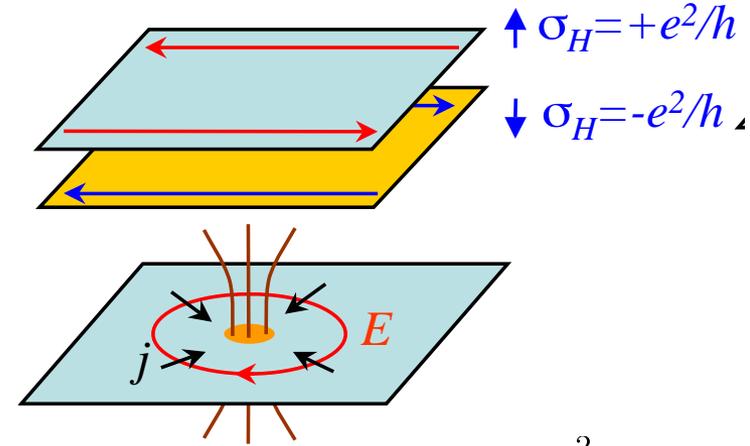
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II. Two-Dimensional Topological Insulators

D. Topological excitations

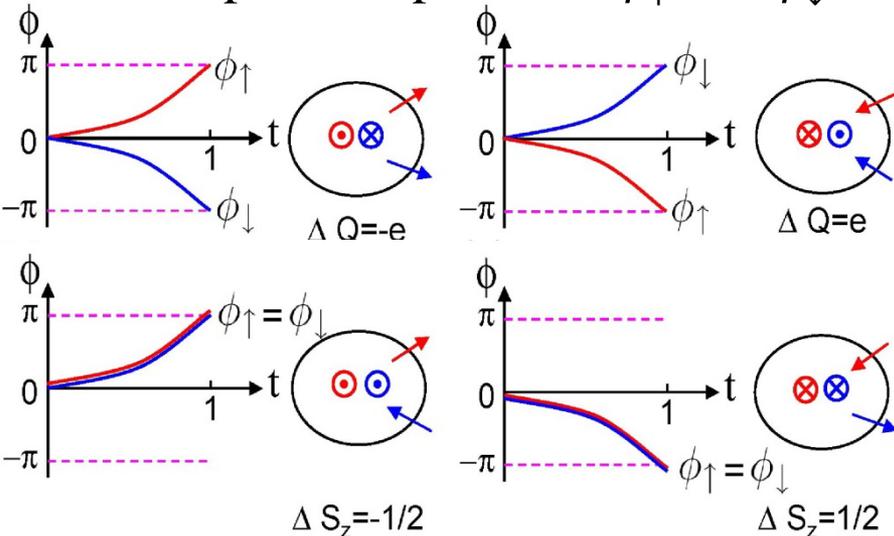
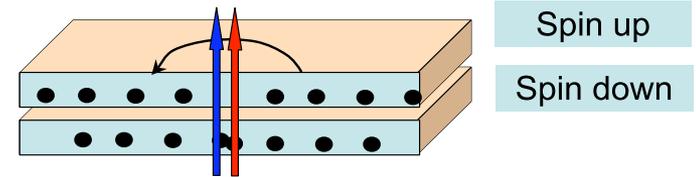
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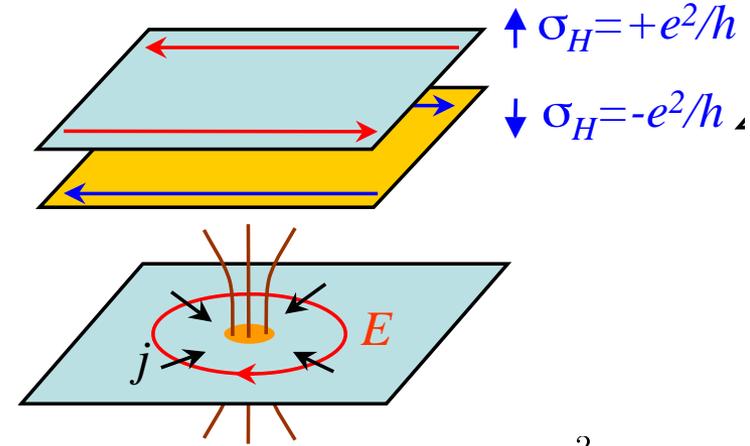
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II. Two-Dimensional Topological Insulators

D. Topological excitations

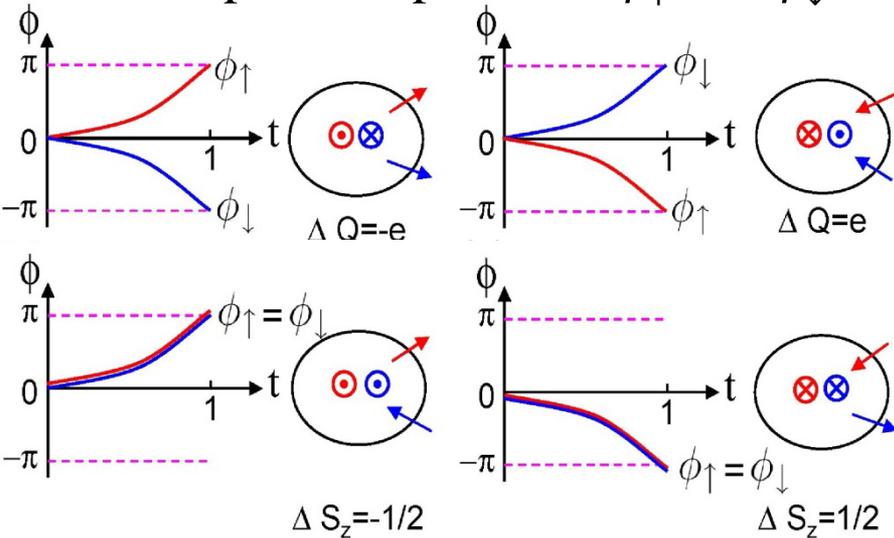
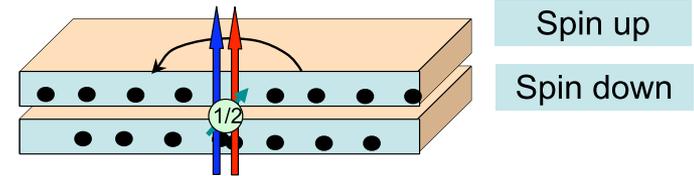
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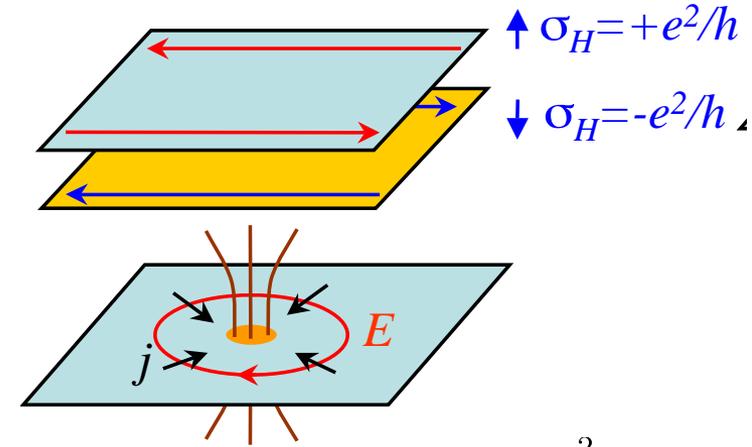
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II. Two-Dimensional Topological Insulators

D. Topological excitations

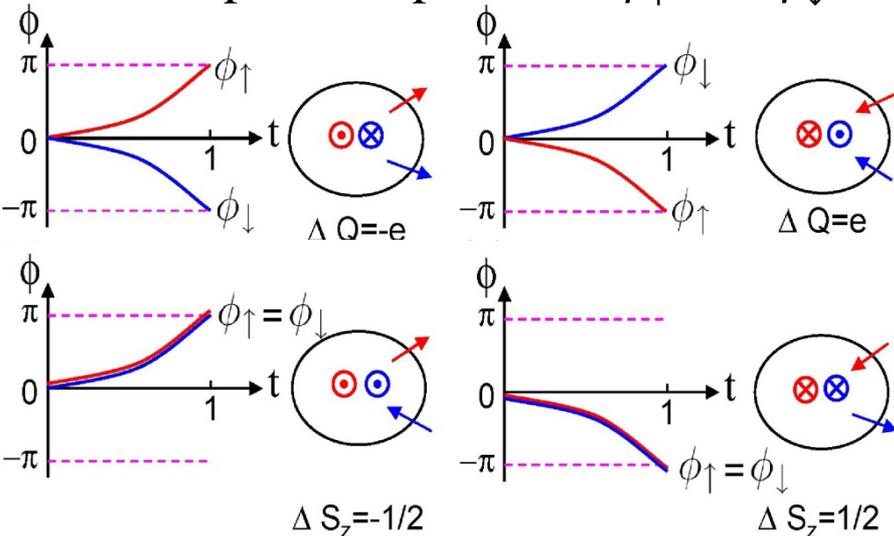
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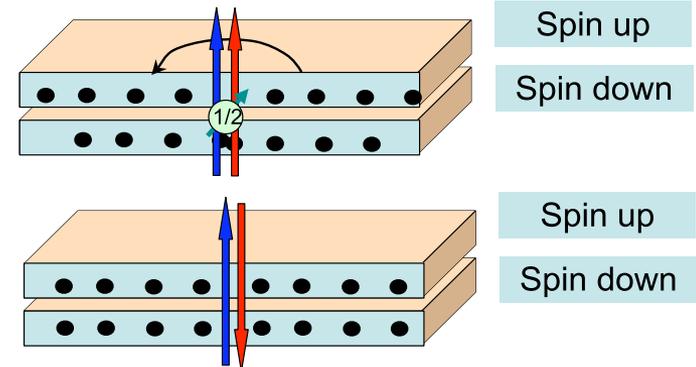
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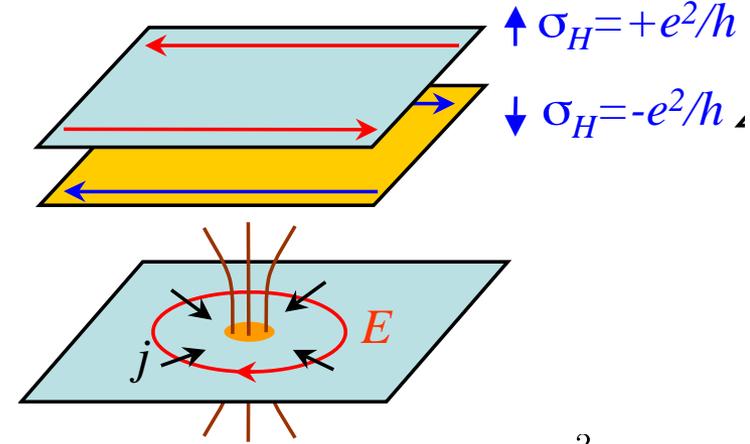


II. Two-Dimensional Topological Insulators

D. Topological excitations

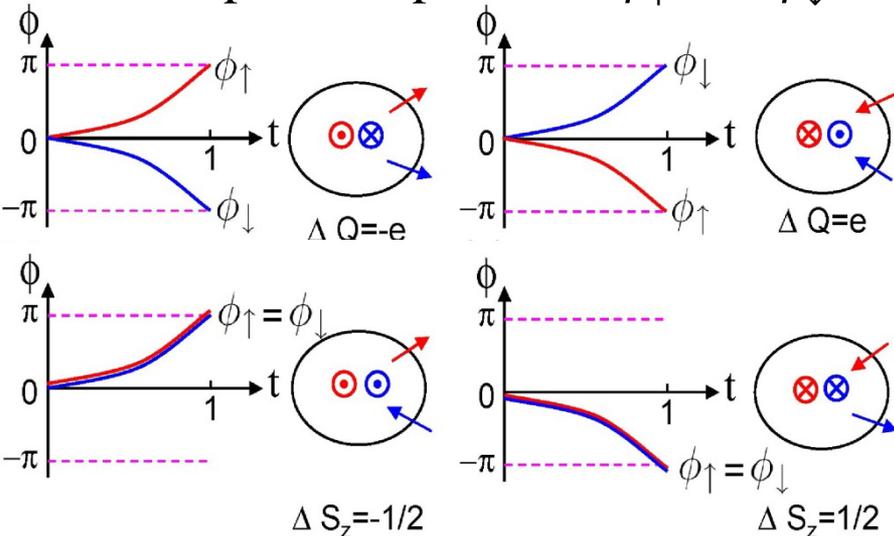
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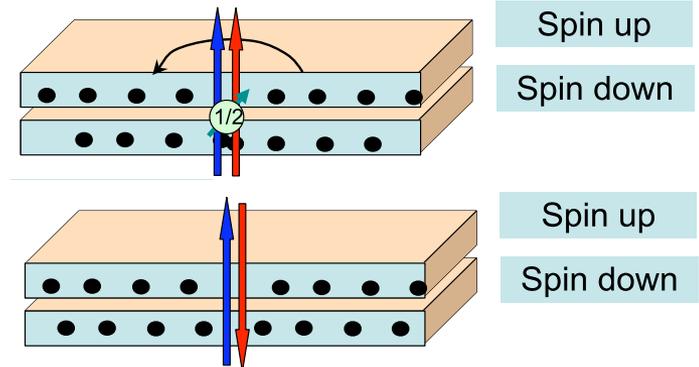
- Current density from \mathbf{E}_\parallel : $\mathbf{j}_\uparrow = \frac{e^2}{h} \hat{\mathbf{z}} \times \mathbf{E}_\uparrow$
- Net charge flow:

$$\begin{aligned} \Delta Q_\uparrow &= - \int_0^1 dt \int d\mathbf{n} \cdot \mathbf{j}_\uparrow = - \frac{e^2}{h} \int_0^1 dt \int d\mathbf{l} \cdot \mathbf{E}_\uparrow \\ &= - \frac{e^2}{hc} \int_0^1 dt \frac{\partial \phi}{\partial t} = - \frac{e^2 hc}{hc 2e} = - \frac{e}{2} \end{aligned}$$



$$\Delta Q = \Delta Q_\uparrow + \Delta Q_\downarrow = -e$$

$$\Delta S_z = \Delta Q_\uparrow - \Delta Q_\downarrow = 0$$

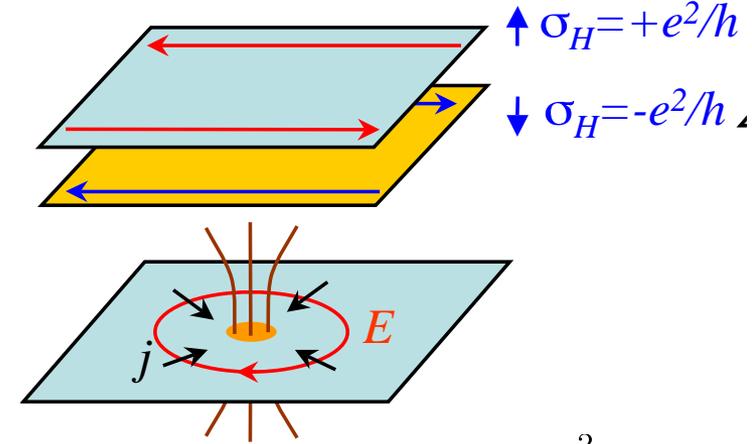


II. Two-Dimensional Topological Insulators

D. Topological excitations

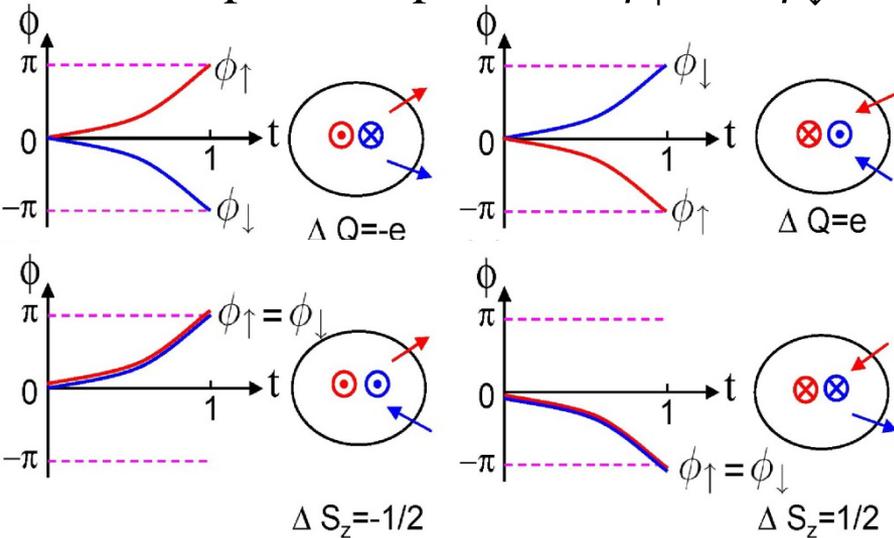
2. Spin-charge separation in the bulk

- Simplified analysis:
 - Assume S_z is preserved
 - QSHE as two copies of QHE
- Thread a π (units of $\hbar = c = e = 1$) flux ϕ
- TRS preserved at $\phi = 0$ and π ; also, $\pi = -\pi$
- Four possible paths for ϕ_\uparrow and ϕ_\downarrow :



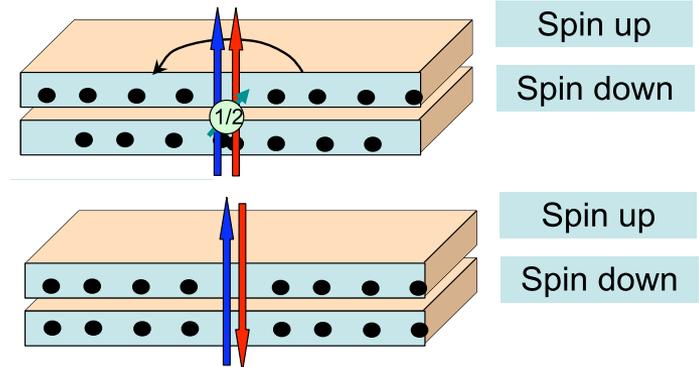
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$$\Delta Q = \Delta Q_\uparrow + \Delta Q_\downarrow = -e$$

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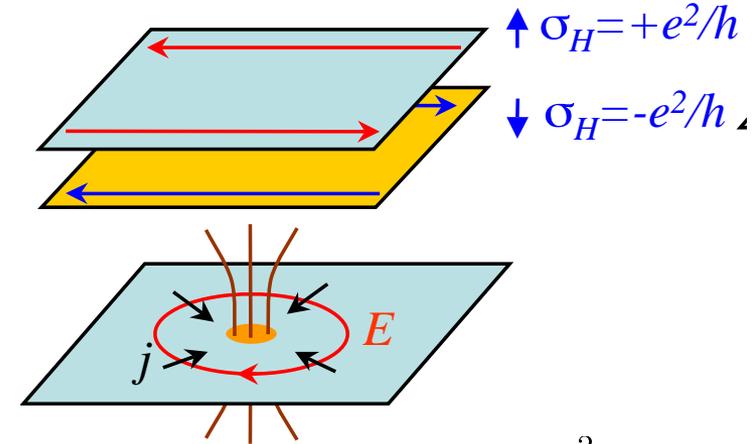


II. Two-Dimensional Topological Insulators

D. Topological excitations

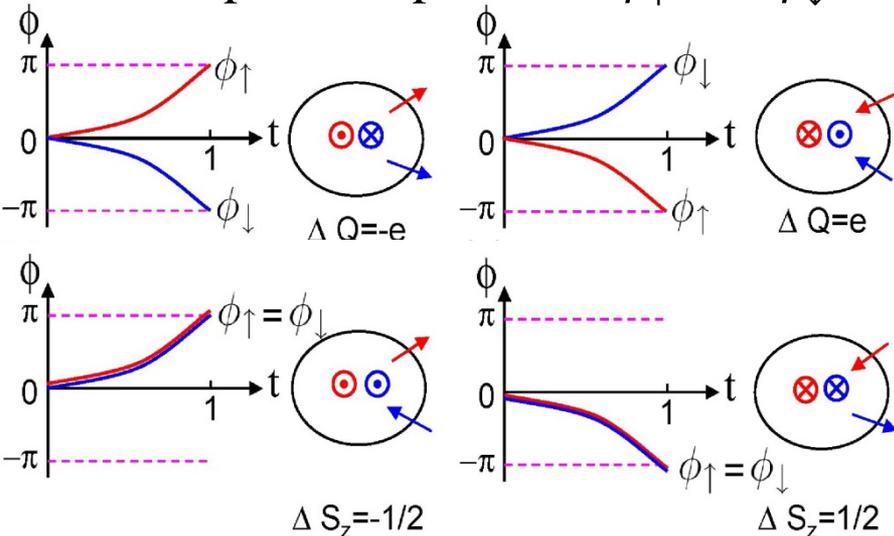
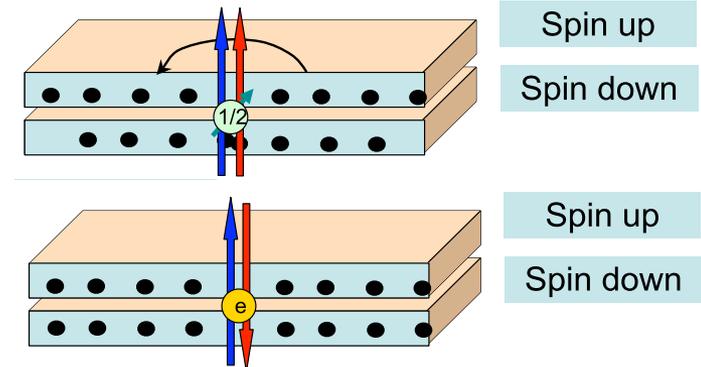
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- Current density from \mathbf{E}_\parallel : $\mathbf{j}_\uparrow = \frac{e^2}{h} \hat{\mathbf{z}} \times \mathbf{E}_\uparrow$
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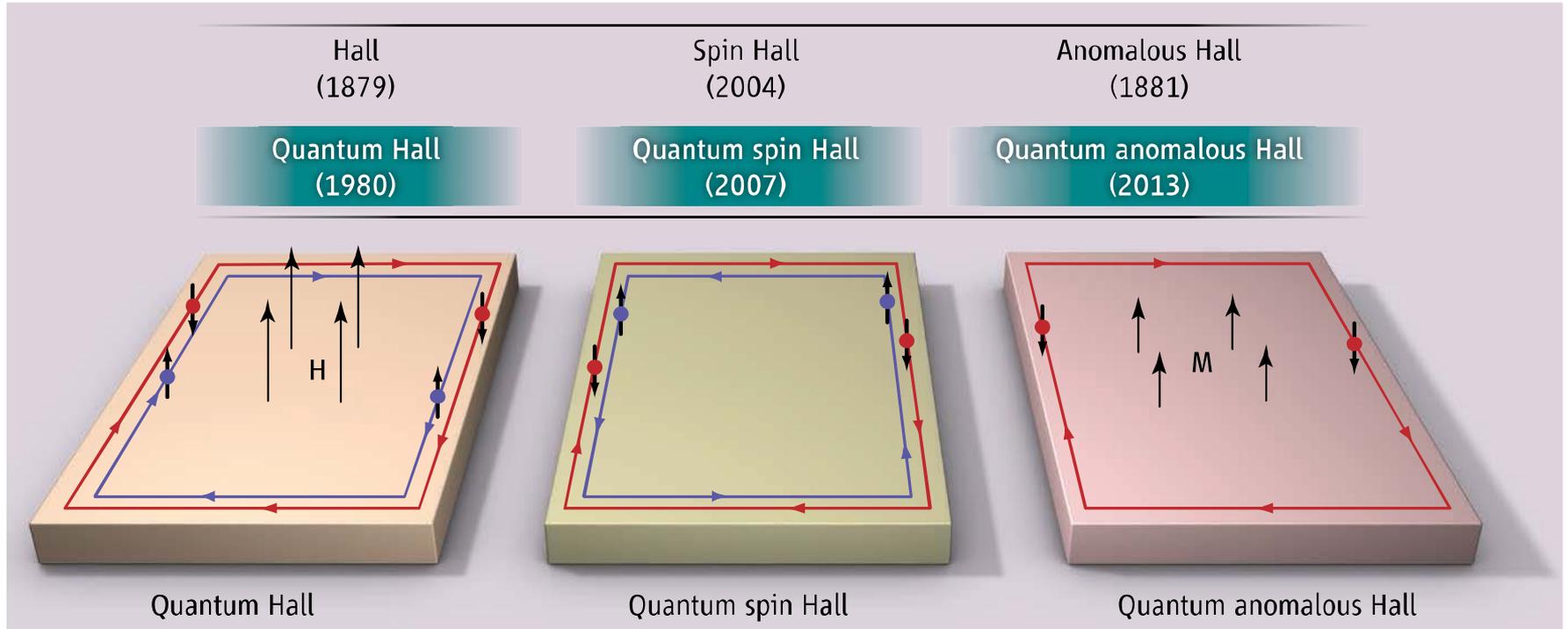
$$\Delta Q = \Delta Q_\uparrow + \Delta Q_\downarrow = -e$$

$$\Delta S_z = \Delta Q_\uparrow - \Delta Q_\downarrow = 0$$

II. Two-Dimensional Topological Insulators

E. Quantum anomalous Hall insulator

- The trio is finally complete!



Ordinary Hall Effect with external magnetic field (H)	Pure Spin Hall Effect	Anomalous Hall Effect with magnetization (M)
Hall voltage but no spin accumulation	Spin accumulation but no Hall voltage	Hall voltage and spin accumulation

II. Two-Dimensional Topological Insulators

E. Quantum anomalous Hall insulator

- Quantum Anomalous Hall Effect (QAHE) described by upper 2×2 block of the QSHE, i.e. 2-band model with explicit TRS breaking

$$h(\mathbf{k}) = \epsilon(\mathbf{k})\mathbb{I}_{2 \times 2} + d_a(\mathbf{k})\sigma^a$$

- The quantized Hall conductance is determined by

$$\sigma_H = \frac{e^2}{h} \frac{1}{4\pi} \int dk_x \int dk_y \hat{\mathbf{d}} \cdot \left(\frac{\partial \hat{\mathbf{d}}}{\partial k_x} \times \frac{\partial \hat{\mathbf{d}}}{\partial k_y} \right)$$

- With TRS breaking charge Hall conductance of counter propagating states do **not** cancel perfectly
- For system doped with magnetic impurities, splitting term added:

$$H_s = \begin{pmatrix} G_E & 0 & 0 & 0 \\ 0 & G_H & 0 & 0 \\ 0 & 0 & -G_E & 0 \\ 0 & 0 & 0 & -G_H \end{pmatrix}$$

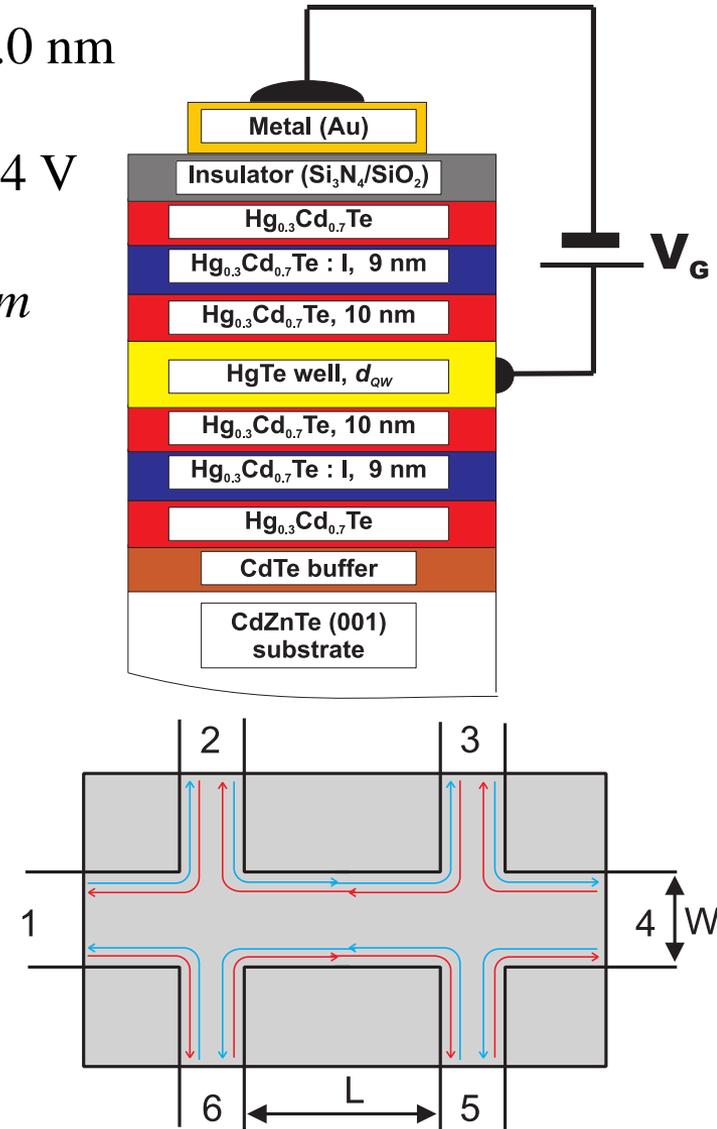
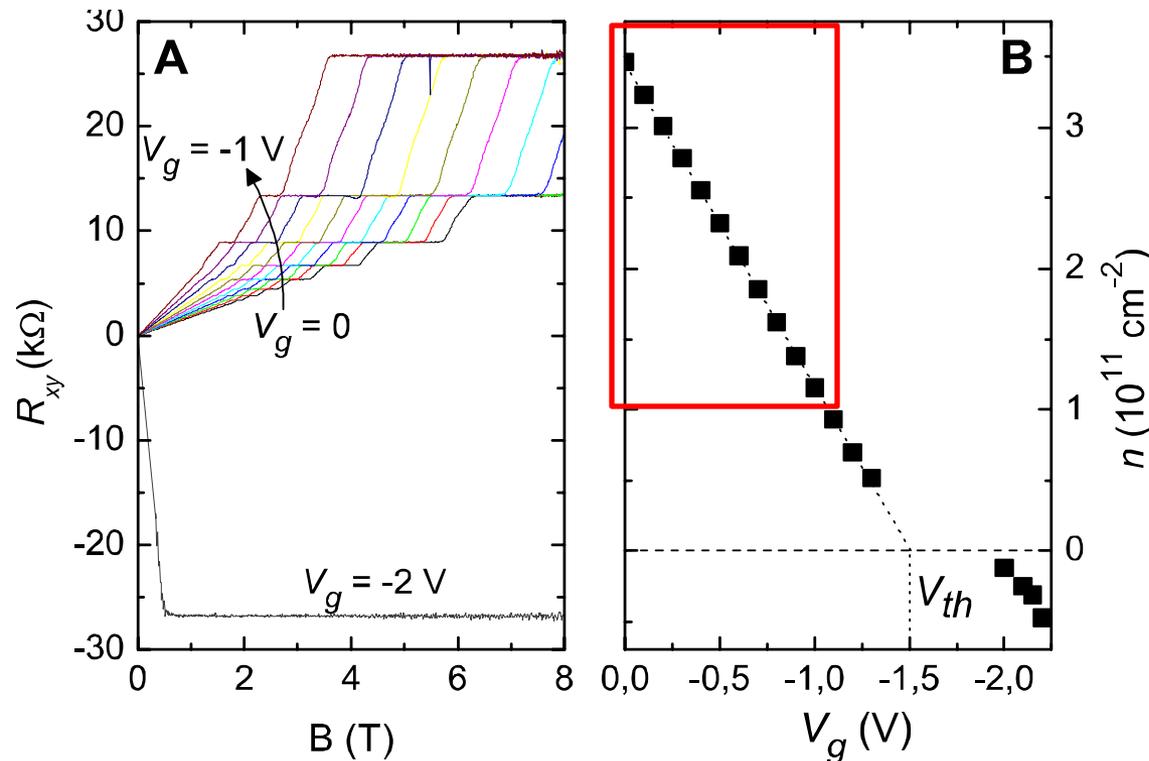
- Upper and lower blocks have masses $M + (G_E - G_H)/2$ and $M + (G_E + G_H)/2$
- QAHE is given by $G_E G_H < 0$
- Mn-doped HgTe QWs or Cr- or Fe-doped Bi_2Se_3 and Bi_2Te_3 thin films satisfy above condition for **different** physical reasons
- In HgTe the 2 bands have opposite signed exchange coupling, i.e. s - d and p - d
- In Bi_2Se_3 and Bi_2Te_3 sign of the spin different in the two blocks

II. Two-Dimensional Topological Insulators

F. Experimental Results

1. Quantum well growth and the band inversion transition

- HgTe width (d_{QW}) in the range from 4.5 nm to 12.0 nm were grown with phase transition at 6.3 nm
- Ranges: $V_g \geq -1.0$ V (n -doped), -1.9 V $< V_g < -1.4$ V (insulating), and $V_g < -2.0$ V (p -doped)
- Hall resistance R_{xy} for $L = 600$ μm and $W = 200$ μm

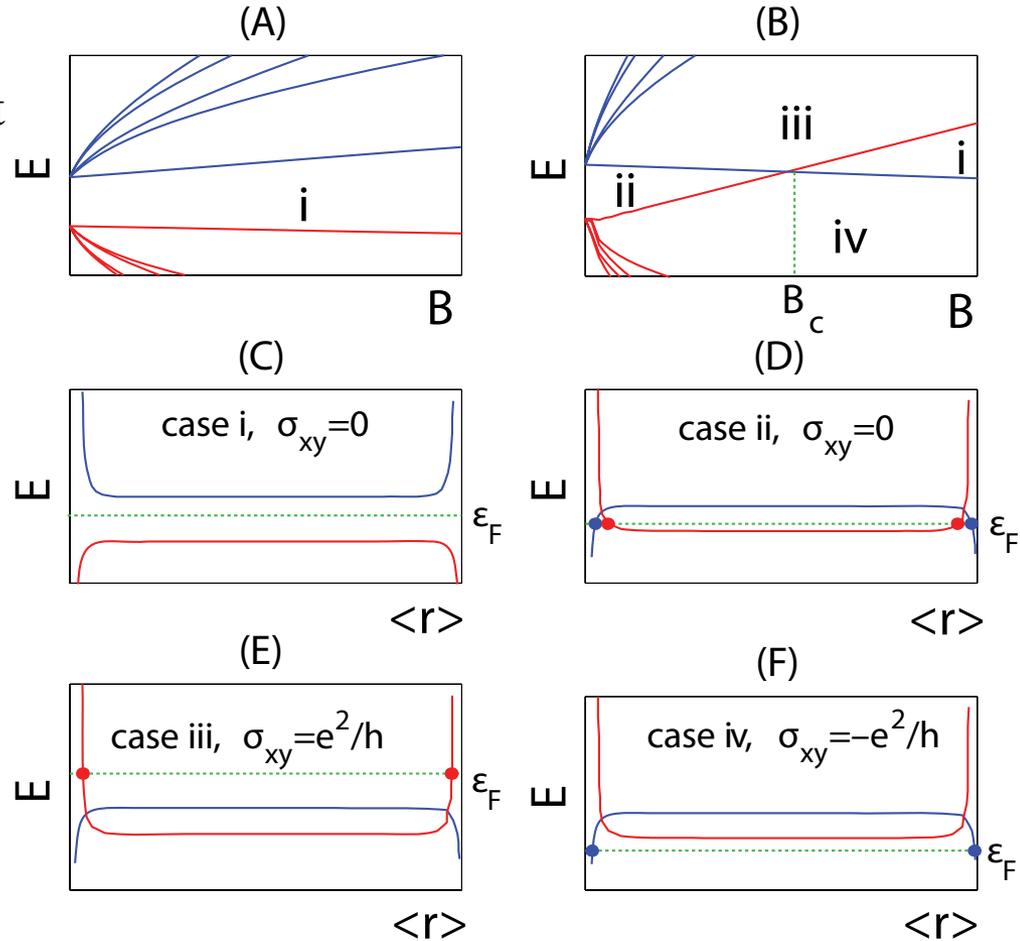


II. Two-Dimensional Topological Insulators

F. Experimental Results

1. Quantum well growth and the band inversion transition

- For normal ordering of bands the Landau levels will get further apart as B increases
- For inverted bandstructures Landau levels will cross at a certain B
- Only inverted bandstructures will reeneter the quantum Hall states when B field increases

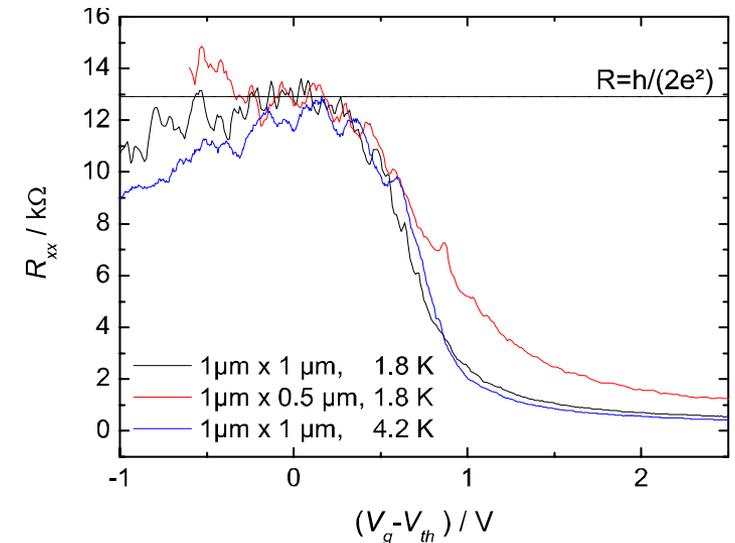
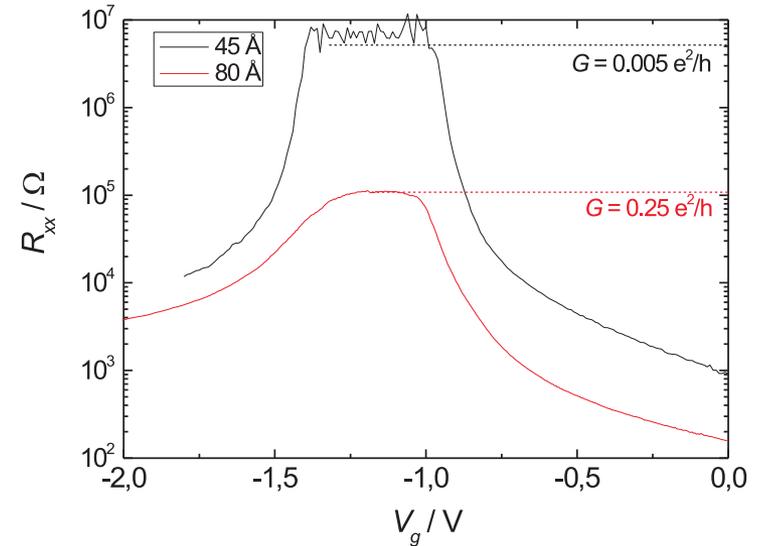


II. Two-Dimensional Topological Insulators

F. Experimental Results

2. Longitudinal conductance in the quantum spin Hall state

- For $d_{\text{QW}} < 6.3$ nm resistance is in the M Ω , i.e. insulating
For $d_{\text{QW}} > 6.3$ nm resistance is 100 k Ω
- 100 k $\Omega \gg h/2e^2$ (12.8 k Ω)
- The extra resistance may come from inelastic scattering
- Estimate inelastic mean free path ~ 1 μm
- Experiments on device with $L = 1$ μm
- 4-point measurements give $R_{xx} = h/2e^2$ as expected
- Changing width between $W = 1$ μm and 0.5 μm gives same result \rightarrow there is no parasitic bulk conduction

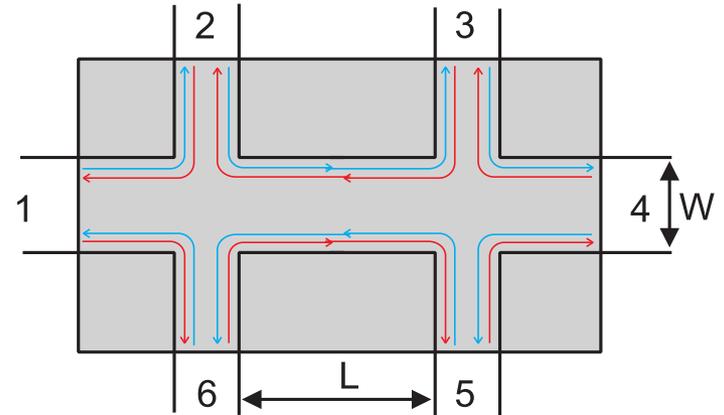
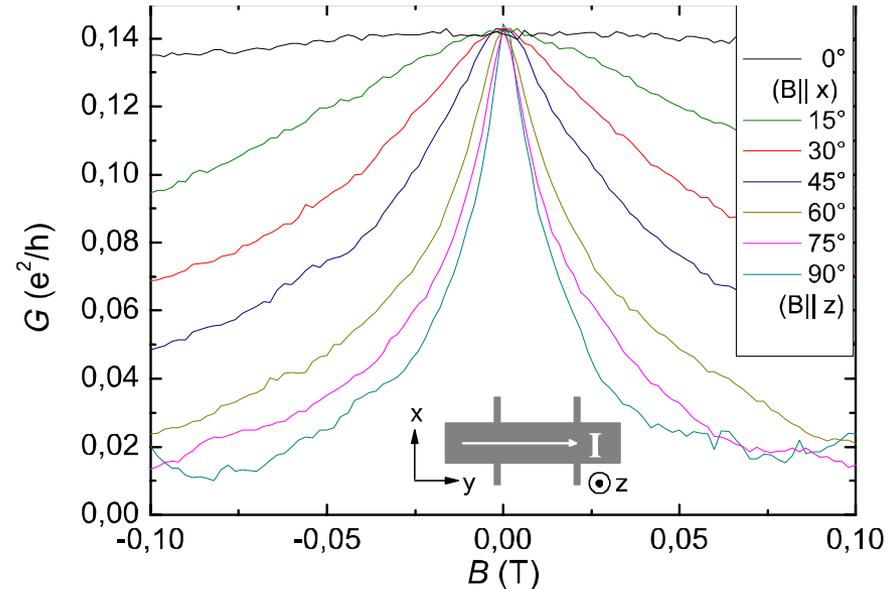


II. Two-Dimensional Topological Insulators

F. Experimental Results

3. Magnetoconductance in the quantum spin Hall state

- There is a large anisotropy in magnetoconductance for magnetic fields pointing in-plane or perpendicular to the plane

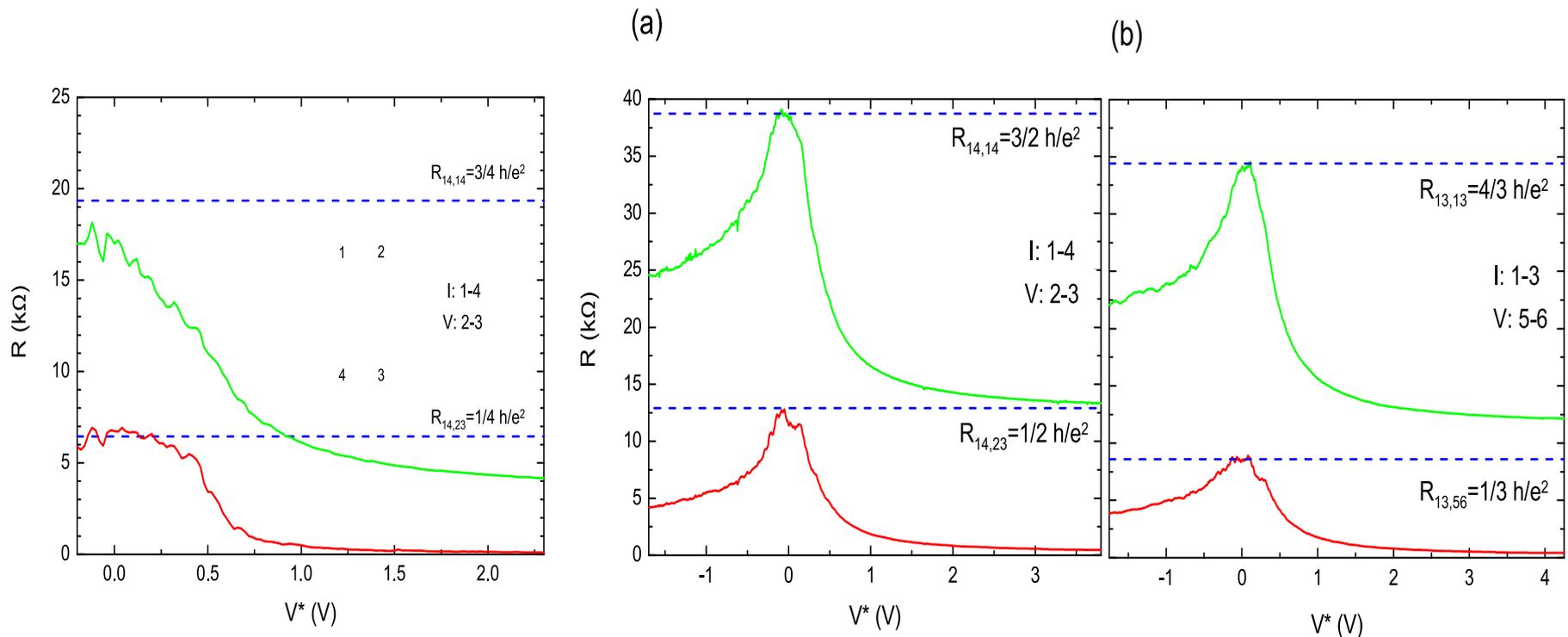


II. Two-Dimensional Topological Insulators

F. Experimental Results

4. Nonlocal conductance

- Using the Landauer-Buttiker formulas we can compute resistance among different terminals
- This type of “nonlocal” conductance was measured and found to match with theory
- This was unambiguous proof that these are helical edge states

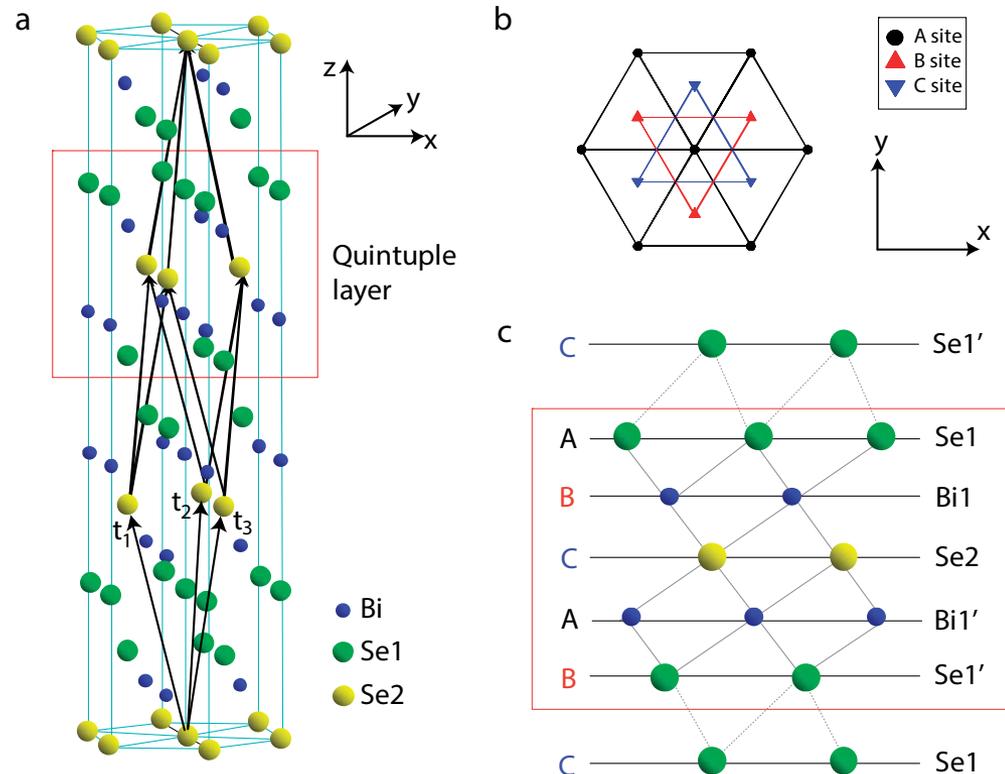


II. Three-Dimensional Topological Insulators

- Simple model Hamiltonian for Bi_2Se_3 , Bi_2Te_3 , Sb_2Te_3 a natural extension of HgTe
- SOC drives band inversion at the Γ point
- Full bulk gap with 2D massless “helical” and “holographic” Dirac surface spectrum
- TR breaking perturbation opens a gap in the surface spectrum \rightarrow Topological Magnetoelectric Effect

A. Effective model of the three-dimensional topological insulator

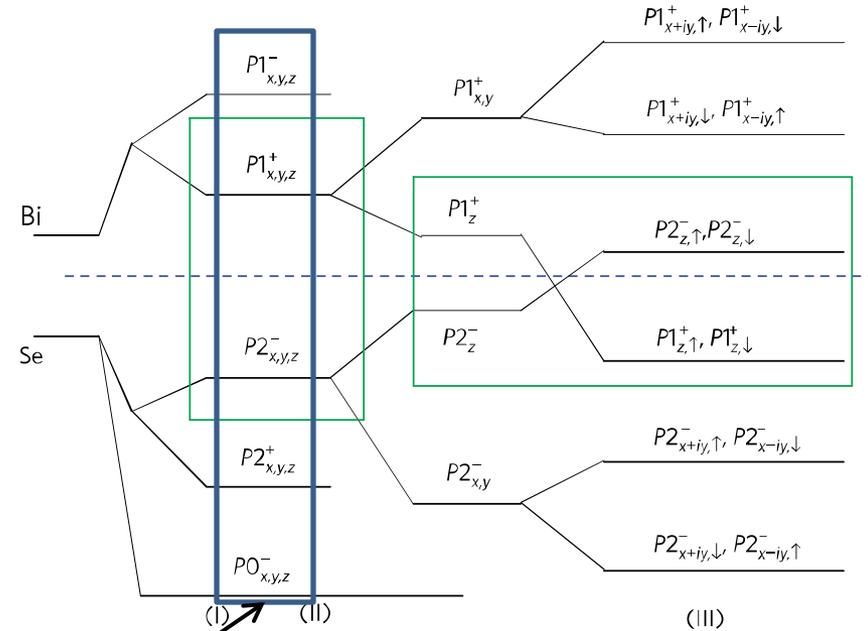
- Rhombohedral crystal structure with space group: $D_{3d}^5 (R\bar{3}m)$
- Each “quintuple layer” consists of five atoms per unit cell
- Each quintuple layer is ~ 1 nm thick
- The primitive lattice vectors are $\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3$
- Under inversion the primed atoms transform into the unprimed atoms



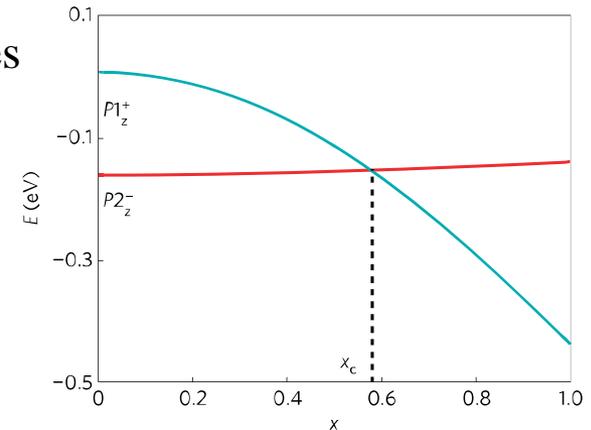
II. Three-Dimensional Topological Insulators

A. Effective model of the three-dimensional topological insulator

- Consider the example Bi ($6s^26p^3$) and Se ($4s^24p^4$)
- Recombine the orbitals in a single unit cell according to their parity
- In step I we have 3 states (2 odd, 1 even) from each Se p -orbital and 2 states (1 odd, 1 even) from each Bi p -orbital
- In step II crystal field splits p_z into p_x and p_y
- In step III we turn on the **L.S** spin-orbit splitting term
- $|P1_z^+\rangle$ and $|P2_z^-\rangle$ as a function of spin-orbit strength λ
- $\lambda(\text{Bi/Se}) = x\lambda_0(\text{Bi/Se})$ with $\lambda_0(\text{Bi}) = 1.25$ eV and $\lambda_0(\text{Se}) = 0.22$ eV
- Phase transition occurs *before* the real values of spin-orbit strength
- Band inversion of opposite parity states at odd TRIM \rightarrow topologically nontrivial



Hybridized states



II. Three-Dimensional Topological Insulators

A. Effective model of the three-dimensional topological insulator

- Similar to HgTe we can define a model Hamiltonian respecting symmetries

$$T = i\sigma^y \mathcal{K} \otimes \mathbb{I}_{2 \times 2}, \quad I = \mathbb{I}_{2 \times 2} \otimes \tau_3, \quad C_3 = \exp\left(i\frac{\pi}{3}\sigma^z \otimes \mathbb{I}_{2 \times 2}\right)$$

- The 4 closest states can be chosen as our basis

$$\begin{pmatrix} |P1_z^+, \uparrow\rangle \\ |P2_z^-, \uparrow\rangle \\ |P1_z^+, \downarrow\rangle \\ |P2_z^-, \downarrow\rangle \end{pmatrix}$$

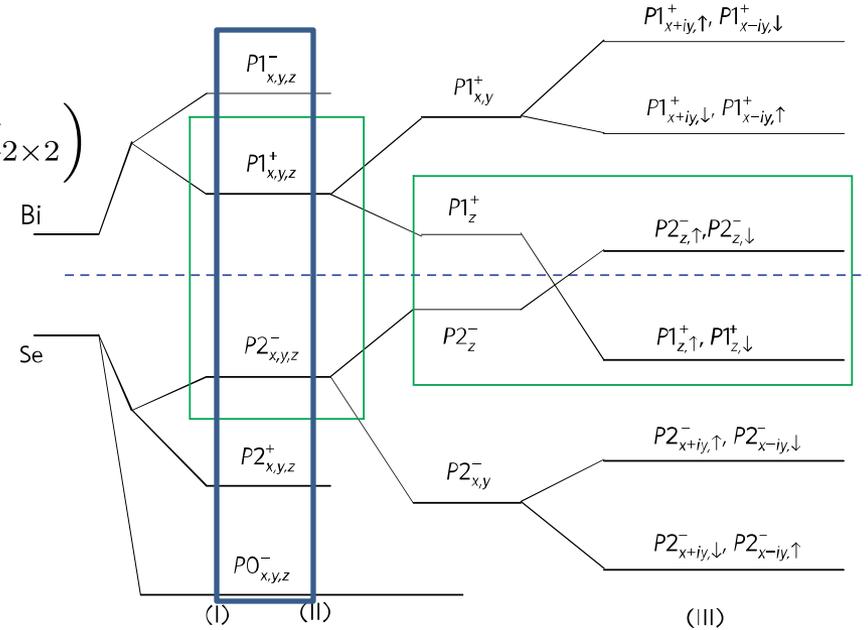
- The model Hamiltonian in the above basis can be written as

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

Parameters determined by comparison to *ab initio* calculations

$$k_{\pm} = k_x \pm ik_y, \quad \epsilon_0(\mathbf{k}) = C + D_1 k_z^2 + D_2 k_{\perp}^2, \quad \mathcal{M}(\mathbf{k}) = M - B_1 k_z^2 - B_2 k_{\perp}^2$$

- Hamiltonian is like a 3D anisotropic Dirac model but with \mathbf{k} -dependent mass
- Extra cubic terms \rightarrow reduce rotational symmetry about z -axis from $SO(2)$ to C_3



II. Three-Dimensional Topological Insulators

B. Surface states with a single Dirac cone

- Similar to the HgTe case split the Hamiltonian into portions with and without k_z since we break translational symmetry along the z -axis

$$\tilde{H}_0 = \tilde{\epsilon}(k_z) + \begin{pmatrix} \tilde{M}(k_z) & A_1 k_z & 0 & 0 \\ A_1 k_z & -\tilde{M}(k_z) & 0 & 0 \\ 0 & 0 & \tilde{M}(k_z) & -A_1 k_z \\ 0 & 0 & -A_1 k_z & -\tilde{M}(k_z) \end{pmatrix}, \quad \begin{aligned} \tilde{\epsilon}(k_z) &= C + D_1 k_z^2 \\ \tilde{M}(k_z) &= M - B_1 k_z^2 \end{aligned}$$

$$\tilde{H}_1 = D_2 k_\perp^2 + \begin{pmatrix} -B_2 k_\perp^2 & 0 & 0 & A_2 k_- \\ 0 & B_2 k_\perp^2 & A_2 k_- & 0 \\ 0 & A_2 k_+ & -B_2 k_\perp^2 & 0 \\ A_2 k_+ & 0 & 0 & B_2 k_\perp^2 \end{pmatrix},$$

- The form of the first Hamiltonian is similar to the one in QSHE
- Surface state at $k_x = k_y = 0$ is determined by the same equation as the QSHE
- Surface state exists for $M/B_1 > 0$. In the examples below $B_1 B_2 > 0$, $A_1 A_2 > 0$
- **Note:** surface **helicity** is determined by sign of A_1/B_1 ; here spins have more than 2 polarization states

Once again projection of bulk Hamiltonian on to surface states we get

$$H_{\text{surf}}(k_x, k_y) = C + A_2 (\sigma^x k_y - \sigma^y k_x)$$

- For $A_2 = 4.1$ eV, $v_F = A_2/\hbar = 6.2 \times 10^5$ m/s vs. ab initio result of $v_F = 5 \times 10^5$ m/s

II. Three-Dimensional Topological Insulators

C. Crossover from three dimensions to two dimensions

- The models describing 2D and 3D topological insulators are quite similar
- But is a thin 3D film a trivial or nontrivial insulator?
- Consider a 3D TI with finite thickness d in the z -direction

• For $k_x = k_y = 0$ we have

$$\tilde{H}_0 = \tilde{\epsilon}(k_z) + \begin{pmatrix} \tilde{M}(k_z) & A_1 k_z & 0 & 0 \\ A_1 k_z & -\tilde{M}(k_z) & 0 & 0 \\ 0 & 0 & \tilde{M}(k_z) & -A_1 k_z \\ 0 & 0 & -A_1 k_z & -\tilde{M}(k_z) \end{pmatrix},$$

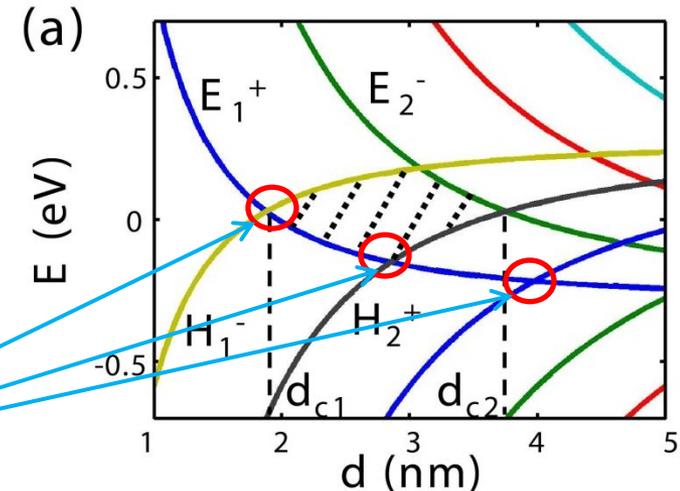
- For $A_1 = 0$ the Hamiltonian is diagonal and we can compute the eigenstates as

$$|E_n\rangle = \sqrt{\frac{2}{d}} \sin\left(\frac{n\pi z}{d} + \frac{n\pi}{2}\right) |P1_z^+, \uparrow (\downarrow)\rangle \quad |H_n\rangle = \sqrt{\frac{2}{d}} \sin\left(\frac{n\pi z}{d} + \frac{n\pi}{2}\right) |P2_z^-, \uparrow (\downarrow)\rangle$$

$$E_e(n) = C + M + (D_1 - B_1) \left(\frac{n\pi}{d}\right)^2 \quad E_h(n) = C - M + (D_1 + B_1) \left(\frac{n\pi}{d}\right)^2$$

- For $M < 0$ and a small enough d the subbands are *normally ordered*
- As d increases there must be an electron-hole subband crossing at some $d = d_c$
- For $A_1 = 0$ the subband energies as a function of distance look similar to the HgTe QW

Note: multiple crossings



II. Three-Dimensional Topological Insulators

C. Crossover from three dimensions to two dimensions

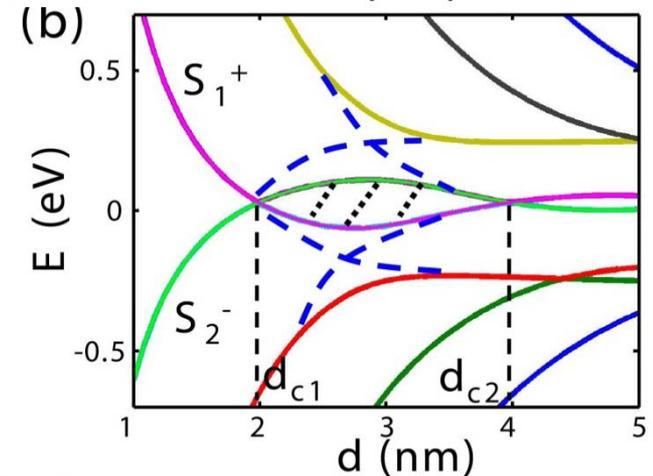
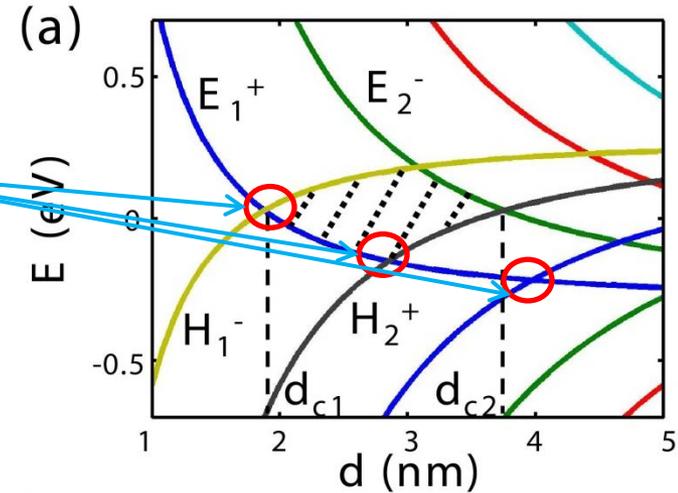
- For $k_x = k_y = 0$ we have
$$\tilde{H}_0 = \tilde{\epsilon}(k_z) + \begin{pmatrix} \tilde{M}(k_z) & A_1 k_z & 0 & 0 \\ A_1 k_z & -\tilde{M}(k_z) & 0 & 0 \\ 0 & 0 & \tilde{M}(k_z) & -A_1 k_z \\ 0 & 0 & -A_1 k_z & -\tilde{M}(k_z) \end{pmatrix},$$

- For $A_1 = 0$ the subband energies as a function of distance look similar to the HgTe QW

Note: multiple crossings

- For $A_1 \neq 0$ the subbands on the right (for $A_1 = 0$) hybridize
- Hybridization gives special states $|S_1^+\rangle$, which is superposition of $|E_{2n-1}\rangle$ and $|H_{2n}\rangle$ (for $n = 1, 2, \dots$), and $|S_2^-\rangle$ (superposition of $|H_{2n-1}\rangle$ and $|E_{2n}\rangle$)
- Crossing is permitted only with the *next closest* subband and they intersect multiple times
- Thin film oscillates between trivial and nontrivial with transition points given by ($A_1 \rightarrow 0$)

$$d_{cn} = n\pi \sqrt{\frac{B_1}{|M|}}$$

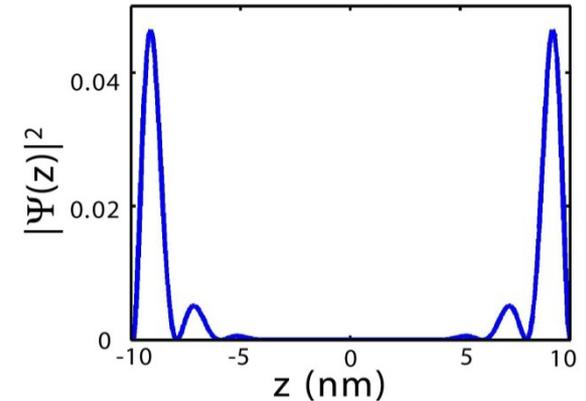
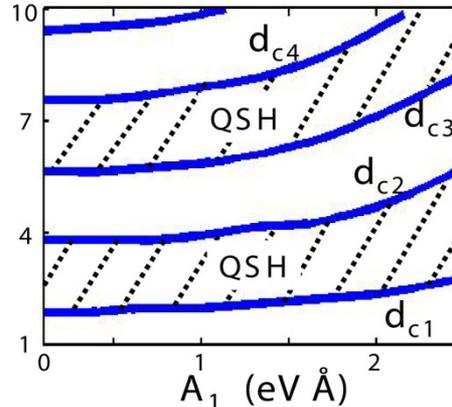
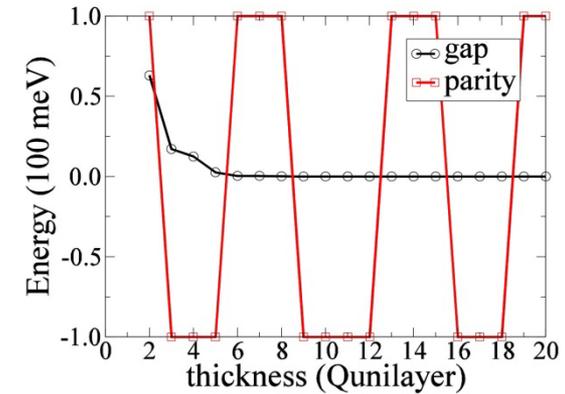
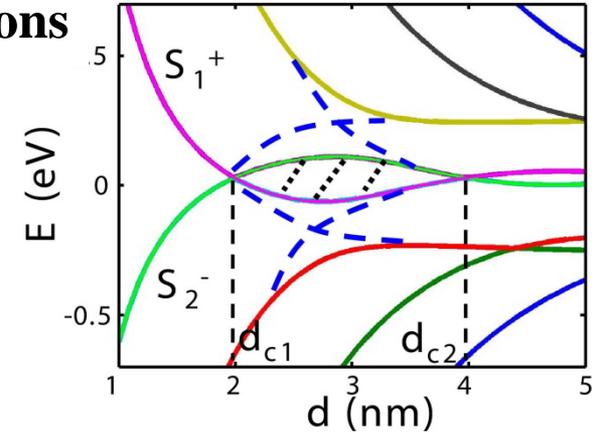


II. Three-Dimensional Topological Insulators

C. Crossover from three dimensions to two dimensions

- For $k_x = k_y = 0$

$$\tilde{H}_0 = \tilde{\epsilon}(k_z) + \begin{pmatrix} \tilde{M}(k_z) & A_1 k_z & 0 & 0 \\ A_1 k_z & -\tilde{M}(k_z) & 0 & 0 \\ 0 & 0 & \tilde{M}(k_z) & -A_1 k_z \\ 0 & 0 & -A_1 k_z & -\tilde{M}(k_z) \end{pmatrix},$$
- Hybridization gives special states $|S_1^+\rangle$, which is superposition of $|E_{2n-1}\rangle$ and $|H_{2n}\rangle$ (for $n = 1, 2, \dots$), and $|S_2^-\rangle$ (superposition of $|H_{2n-1}\rangle$ and $|E_{2n}\rangle$)
- Multiple crossings give relative parity oscillations with thickness
- $|S_1^+\rangle$ and $|S_2^-\rangle$ are localized at the opposite surfaces of the 3D TI slab; oscillations in wave function also go as $\sim \pi(B_1/|M|)^{1/2}$
- Dependence of critical thickness on A_1 is shown in the figure to the right
- As $d \rightarrow \infty$, $|S_1^+\rangle$ and $|S_2^-\rangle$ decouple and become surface state of the 3D TI



II. Three-Dimensional Topological Insulators

C. Crossover from three dimensions to two dimensions

- Relation between electron and hole subbands in the $d \rightarrow \infty$ limit suggests another way to describe 3D to 2D crossover
- The surface is described by

$$H_{\text{surf}}(k_x, k_y) = A_2 \begin{pmatrix} 0 & ik_- & 0 & 0 \\ -ik_+ & 0 & 0 & 0 \\ 0 & 0 & 0 & -ik_- \\ 0 & 0 & ik_+ & 0 \end{pmatrix}$$

- The upper and lower block diagonal elements correspond to the two surfaces
- For slabs of finite thickness a coupling term $M_{2\text{D}}(\mathbf{k})$ can be added

$$H_{\text{surf}}(k_x, k_y) = A_2 \begin{pmatrix} 0 & ik_- & M_{2\text{D}} & 0 \\ -ik_+ & 0 & 0 & M_{2\text{D}} \\ M_{2\text{D}} & 0 & 0 & -ik_- \\ 0 & M_{2\text{D}} & ik_+ & 0 \end{pmatrix}$$

- Changes in sign of $M_{2\text{D}}$ tell if phase is trivial or not. $M_{2\text{D}}$ oscillates with d since the surface wave functions oscillate
- In other words, both top-down and bottom-up approaches agree
- In real materials, like Bi_2Se_3 we can expect the nontrivial phase to first occur at a thickness of ~ 3 nm or three quintuple layers

II. Three-Dimensional Topological Insulators

D. Electromagnetic properties

1. Half quantum Hall effect on the surface

- The only momentum independent term one can add is $H_1 = \sum_a m_a \sigma^a$
- The perturbed Hamiltonian has the spectrum

$$E_{\mathbf{k}} = \pm \sqrt{(A_2 k_y + m_x)^2 + (A_2 k_x - m_y)^2 + m_z^2}$$

- Only parameter m_z can open a gap and destabilize the surface states
- The term $m_z \sigma^z$ breaks TRS; but (say) with 2 identical Dirac cones, with imaginary coupling, we have gapped system with TRS

$$H'_{\text{surf}} = \begin{pmatrix} A_2 (\sigma^x k_y - \sigma^y k_x) & -im\sigma^z \\ im\sigma^z & A_2 (\sigma^x k_y - \sigma^y k_x) \end{pmatrix}$$

- But with term $m_z \sigma^z$ the surface will be

$$H_{\text{surf}}(\mathbf{k}) = A_2 \sigma^x k_y - A_2 \sigma^y k_x + m_z \sigma^z$$

- With the generic two-band model we consider the winding of: $\mathbf{d}(\mathbf{k}) = \begin{pmatrix} A_2 k_y \\ -A_2 k_x \\ m_z \end{pmatrix}$
- A “meron” configuration $\mathbf{d}(\mathbf{k})$ covers half the unit sphere
- With winding number $\pm 1/2$ we have Hall conductance (valid for $m_z \rightarrow 0$)

$$\sigma_H = \frac{m_z}{|m_z|} \frac{e^2}{2h}$$

- Parity anomaly in high energy physics
- Above analysis only applies in continuum, i.e. $|m_z|/A_2 \ll 2\pi/a$
- Unlike QAHE, where $M \rightarrow 0$, Hall conductance = 0 or 1 instead of $\pm 1/2$

II. Three-Dimensional Topological Insulators

D. Electromagnetic properties

1. Half quantum Hall effect on the surface

- Deviations from the Dirac effective model at large momenta \rightarrow corrections to the Hall conductance

$$\Delta\sigma_H = \sigma_H(m_z \rightarrow 0^+) - \sigma_H(m_z \rightarrow 0^-) = \frac{m_z}{|m_z|} \frac{e^2}{h}$$

is independent of large momentum contributions

- The effect of the mass term $m_z\sigma^z$ on the large-momentum sector of the theory is negligible for $m_z \rightarrow 0$
- Contributions to σ_H from large momenta \rightarrow continuous functions of m_z ; therefore $\Delta\sigma_H$ should not be affected
- TR transforms the system with mass m_z to that with mass $-m_z$
$$\sigma_H(m_z \rightarrow 0^+) = -\sigma_H(m_z \rightarrow 0^-)$$
- **Note:** unlike QAHE upper and lower 2×2 blocks are **not** TR conjugate
- Disorder: Nomura, Koshino, and Ryu showed that the surface state is metallic even for an arbitrary impurity strength
- TR breaking disorder \rightarrow unitary class
- For infinitesimal TR breaking $\sigma_{xx} = 0$ and $\sigma_{xy} = \pm e^2/2h$
- Exchange interaction with impurity given by $H_{\text{int}} = \sum_i J_i \mathbf{S}_i \cdot \psi^\dagger \boldsymbol{\sigma} \psi(\mathbf{R}_i)$

II. Three-Dimensional Topological Insulators

D. Electromagnetic properties

1. Half quantum Hall effect on the surface

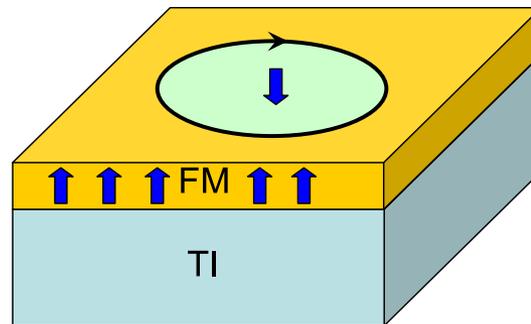
- In a usual Fermi liquid, if the surface state has a finite k_F , an RKKY interaction between the impurity spins is introduced
- The sign of RKKY oscillates with wave length $\propto 1/2k_F$
- For $k_F \rightarrow 0$ the sign of the RKKY interaction does not oscillate but is uniform
- The resulting uniform spin-spin interaction (ferromagnetic) is determined by the coupling to the surface electrons
- A uniform spin polarization can maximize the gap opened on the surface \rightarrow energetically favorable
- Therefore, the system can order ferromagnetically when the chemical potential is near the Dirac point
- This mechanism provides a way to generate a surface TR symmetry breaking field by
 - Coating the surface with magnetic impurities
 - Tuning the chemical potential near the Dirac point

II. Three-Dimensional Topological Insulators

D. Electromagnetic properties

2. Topological magnetoelectric effect

- Unlike QHE in the pure 2D system surface quantum Hall cannot be measured using DC transport for the reasons:
 - Surface of a 3D TI is a closed manifold (i.e. no edges)
 - If TRS is broken only on a partial patch of the surface chiral states on the domain wall give $\sigma_H = e^2/h$ and not $e^2/2h$
- The TRS broken patch (right) is like the boundary between n and $n+1$ level QHE

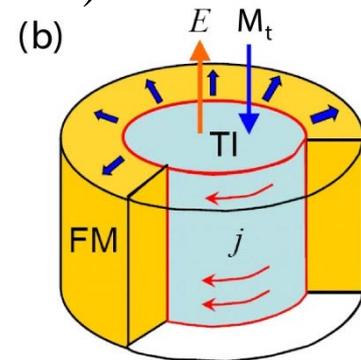


- A new probe is needed \rightarrow Topological Magnetoelectric Effect (TME)

$$\mathbf{j} = \frac{m}{|m|} \frac{e^2}{2h} \hat{\mathbf{n}} \times \mathbf{E} \quad \mathbf{M}_t = -\frac{m}{|m|} \frac{e^2}{2hc} \mathbf{E}$$

- The complete EM response of the system is described by the modified constituent equations ($P_3 = \pm 1/2$)

$$\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M} + 2P_3\alpha\mathbf{E} \quad \mathbf{D} = \mathbf{E} + 4\pi\mathbf{P} - 2P_3\alpha\mathbf{B}$$



II. Three-Dimensional Topological Insulators

D. Electromagnetic properties

3. Image magnetic monopole effect

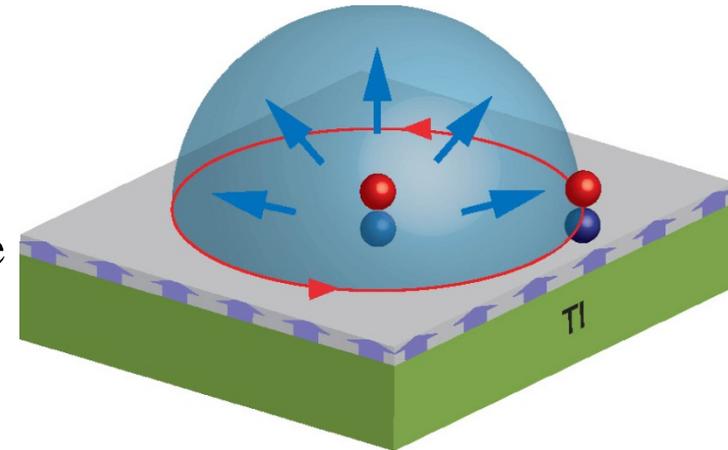
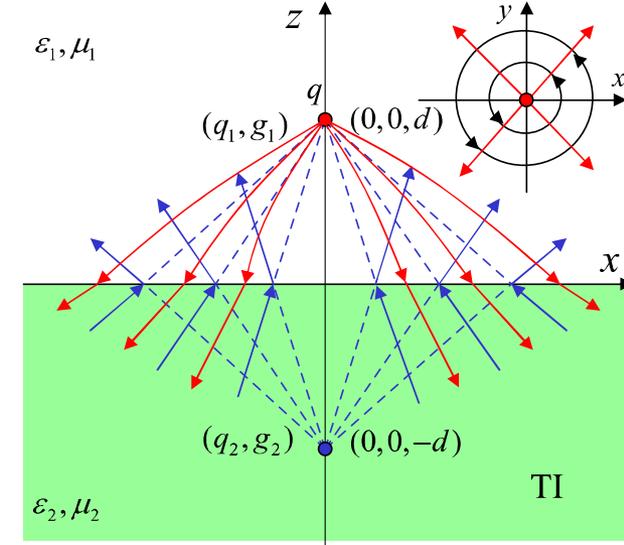
- Direct consequences of the TME effect is the image magnetic monopole effect

$$q_1 = q_2 = \frac{1}{\epsilon_1} \frac{(\epsilon_1 - \epsilon_2)(1/\mu_1 + 1/\mu_2) - 4\alpha^2 P_3^2}{(\epsilon_1 + \epsilon_2)(1/\mu_1 + 1/\mu_2) + 4\alpha^2 P_3^2} q$$

$$g_1 = -g_2 = -\frac{4\alpha P_3}{(\epsilon_1 + \epsilon_2)(1/\mu_1 + 1/\mu_2) + 4\alpha^2 P_3^2} q$$

- Interesting phenomena appear when we consider the dynamics of the external charge
- For 2DEG at a distance d above the surface of the 3D TI and if the motion of the 2DEG electrons is slow enough compared to \hbar/m the image monopoles will follow the electrons adiabatically
- The electron forms an electron-monopole composite, i.e. a “dyon”
- When 2 electrons wind around each other, each electron perceives the magnetic flux of the image monopole attached to the other electron

$$\theta = \frac{g_1 q}{2\hbar c} = \frac{2\alpha^2 P_3}{(\epsilon_1 + \epsilon_2)(1/\mu_1 + 1/\mu_2) + 4\alpha^2 P_3^2} q$$



II. Three-Dimensional Topological Insulators

D. Electromagnetic properties

4. Topological Kerr and Faraday rotation

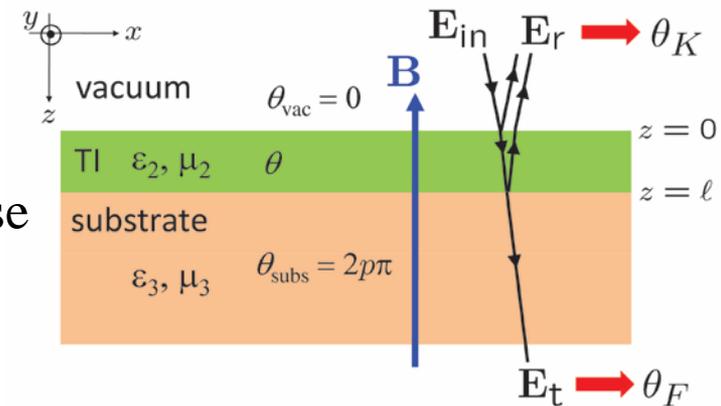
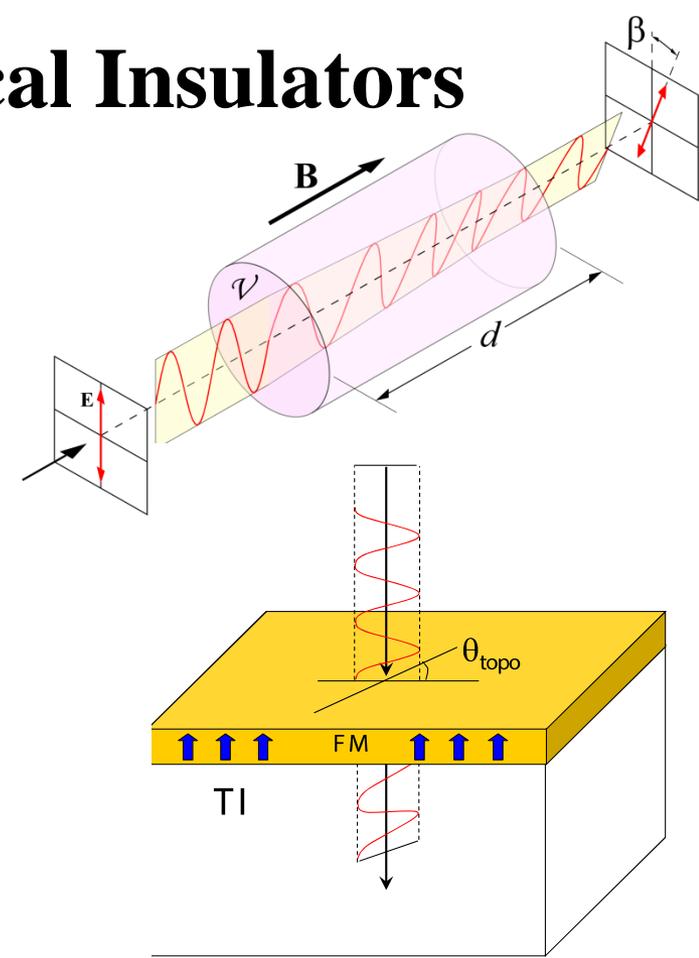
- Another TME effect is through the transmission and reflection of polarized light
- Standard Faraday effect requires an external \mathbf{B} field
- For TME we Faraday rotation occurs due to unusual boundary conditions at the interface of the TI and ferromagnetic insulator (FMI)
- The rotation angles for the Kerr and Faraday effect are

$$\tan(\theta_K) = \frac{4\alpha P_3 \sqrt{\epsilon_1/\mu_1}}{\epsilon_2/\mu_2 - \epsilon_1/\mu_1 + 4\alpha^2 P_3^2},$$

$$\tan(\theta_F) = \frac{2\alpha P_3}{\sqrt{\epsilon_1/\mu_1} + \sqrt{\epsilon_2/\mu_2}}$$

- Problems:
 - dependence on material parameters
 - Detection obscured by standard EM response
- New scheme: combine Faraday and Kerr

$$\frac{\cot(\theta_F) + \cot(\theta_K)}{1 + \cot^2(\theta_F)} = 2\alpha P_3$$



II. Three-Dimensional Topological Insulators

D. Electromagnetic properties

5. Related Effects

- The magnetic monopole carries a charge, i.e. monopole with unit flux carries $e/2$ charge
$$q = e \frac{\theta}{2\pi} \frac{g}{\phi_0}$$
- There is a charge pumping effect when monopole motion \rightarrow couples to electric charge
- When electron-electron interaction is considered interesting new effects can occur
- We can get a so-called axion from fluctuations of P_3 due coupling between spin-waves and the electromagnetic field
- Polariton can be formed by the hybridization of the spin-wave and photon
- The polariton gap is controlled by the magnetic field, which may realize a tunable optical modulator
- Inter-surface exciton condensate can be formed
- Charge current on the surface can flip the magnetic moment of the magnetic layer
- In other words, charge density is coupled to magnetic textures such as domain walls and vortices
- Potential applications in spintronics

II. Three-Dimensional Topological Insulators

E. Experimental results

1. Material growth

- Cava group (Princeton): Bulk materials were first grown for experiments on topological insulators ($\text{Bi}_{1-x}\text{Sb}_x$, Bi_2Se_3 , Bi_2Te_3 , and Sb_2Te_3)
- Fisher group (Stanford): Bi_2Te_3
- Cui group (Stanford): Bi_2Se_3 nanoribbons
- Xue group (Tsinghua): MBE grown thin films of Bi_2Se_3 , Bi_2Te_3
- Due to layered structure thin films can also be obtained by exfoliation from bulk samples
- Stoichiometric compounds relatively easy to grow
- Due to intrinsic doping from vacancy and anti-site defects Bi_2Se_3 , Bi_2Te_3 , are n -type and Sb_2Te_3 are p -type in the bulk
- Controlled doping of Bi_2Se_3 with Sb and Ca and Bi_2Te_3 with Sn gives control over the chemical potential
- Cu doping causes Bi_2Se_3 to become superconducting (nontrivial?)
- Fe and Mn dopants may yield ferromagnetism

II. Three-Dimensional Topological Insulators

E. Experimental results

2. ARPES

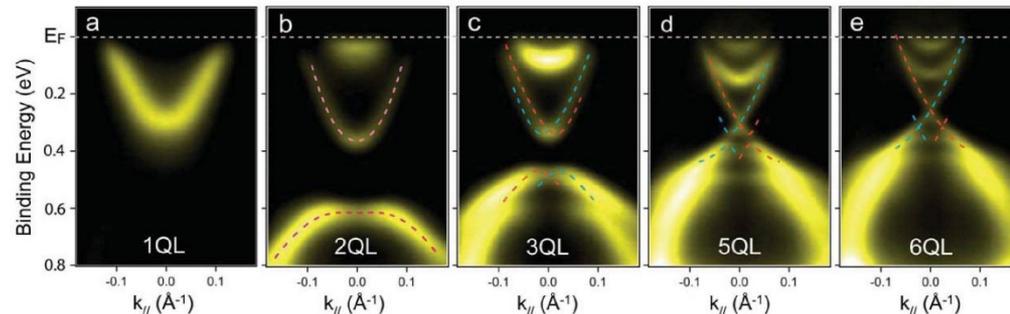
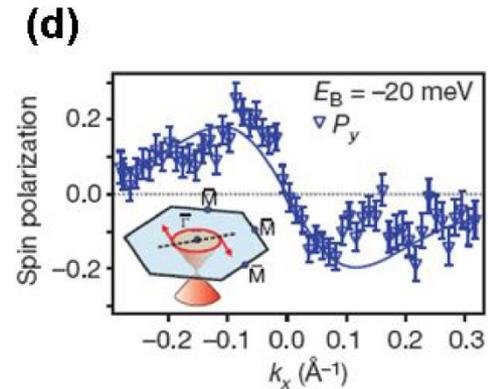
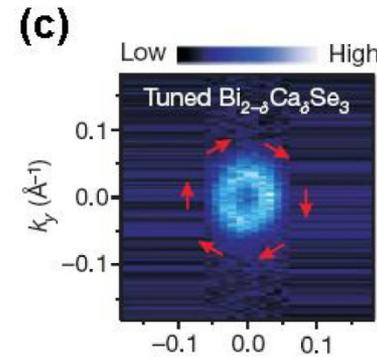
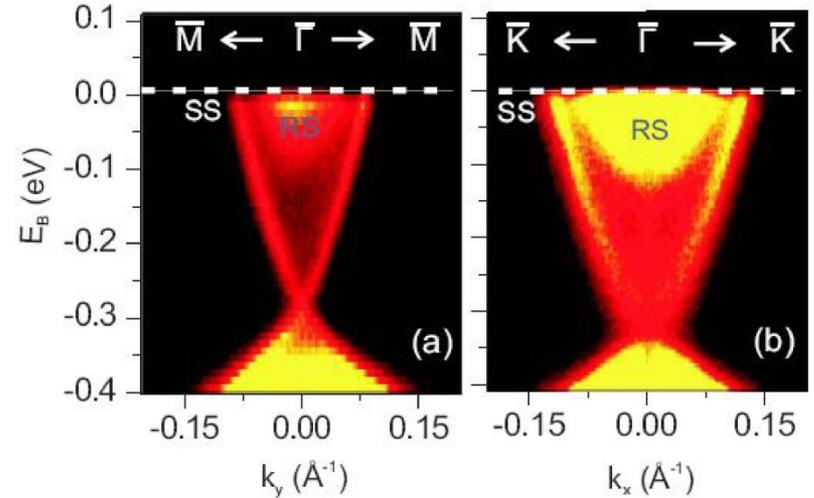
- Unlike $\text{Bi}_{1-x}\text{Sb}_x$ second generation TIs have only one Dirac cone
- Spin-resolved ARPES can show spin polarization of surface states
- However, “hexagonal warping” effects appear in the data away from the Dirac point

$$H(\mathbf{k}) = E_0(\mathbf{k}) + v_{\mathbf{k}}(k_x\sigma^y - k_y\sigma^x) + \frac{\lambda}{2}(k_+^3 + k_-^3)\sigma^z$$

$$v_{\mathbf{k}} = v(1 + \alpha\mathbf{k}^2)$$

$$E_0(\mathbf{k}) = \mathbf{k}^2/(2m^*)$$

- ARPES spectra are shown for several thicknesses of a Bi_2Se_3 thin film, which show the evolution of the surface states.

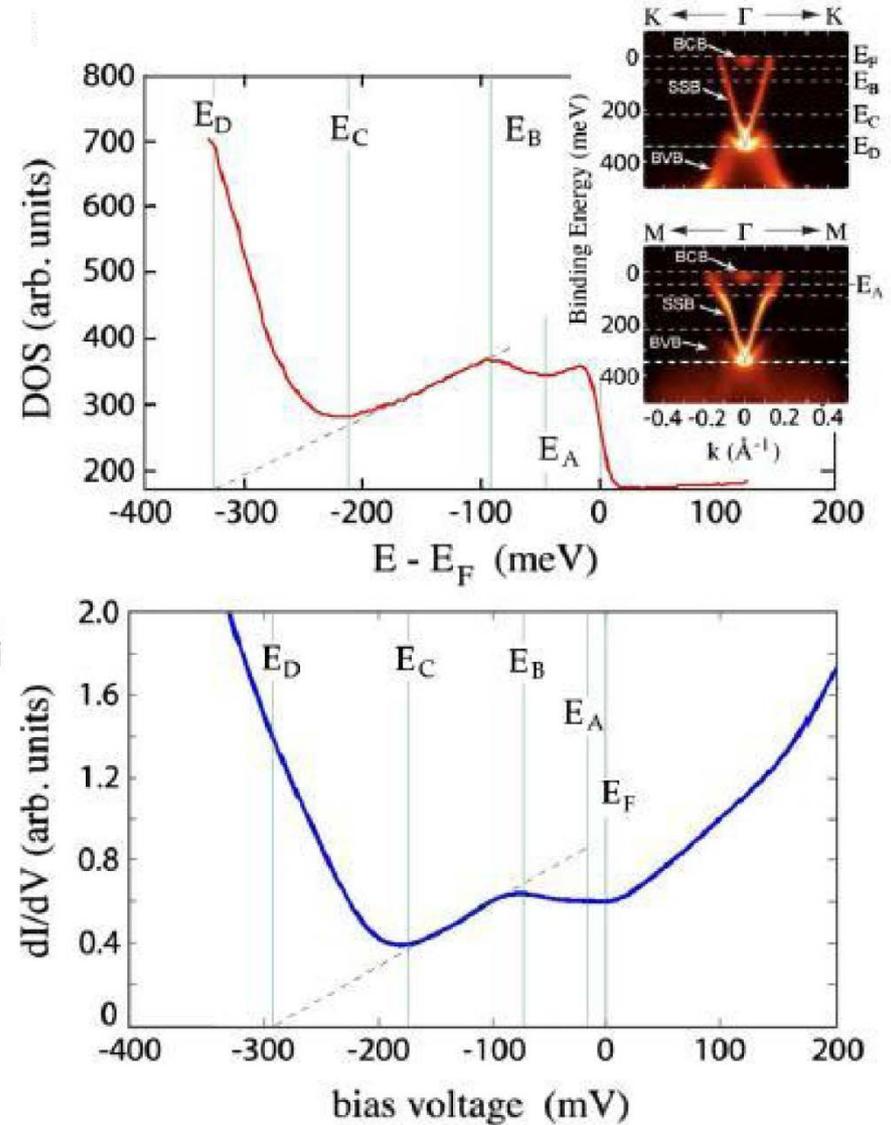
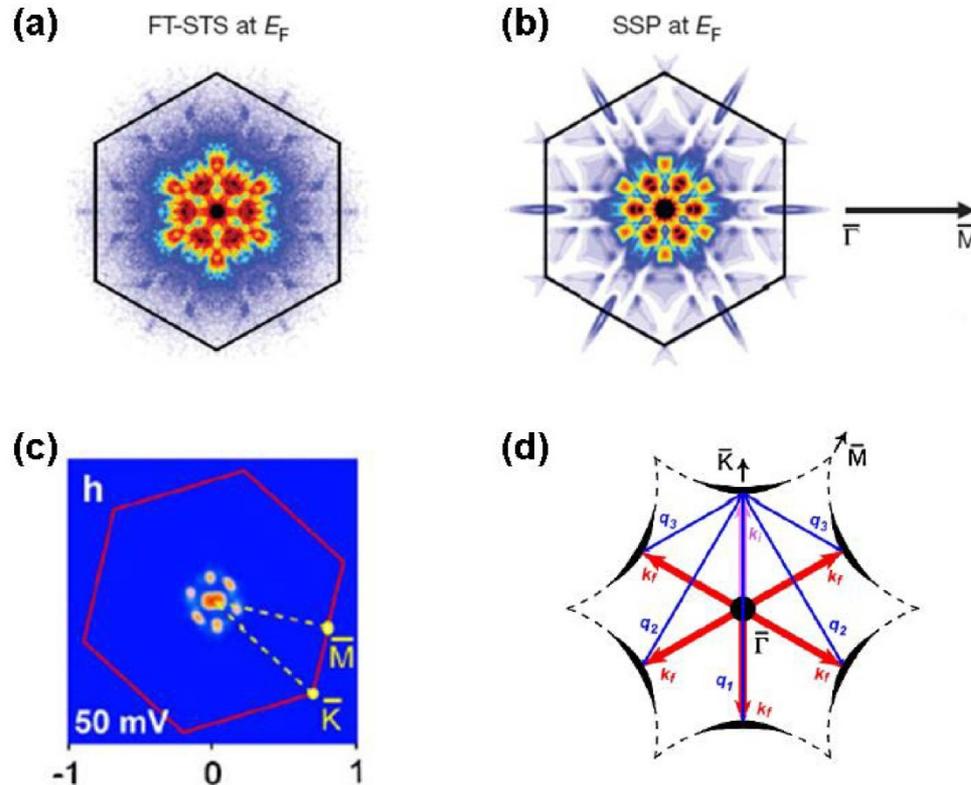


II. Three-Dimensional Topological Insulators

E. Experimental results

3. STM

- Good agreement is found between the integrated density of states from ARPES and STM
- STM also shows protection against backscattering

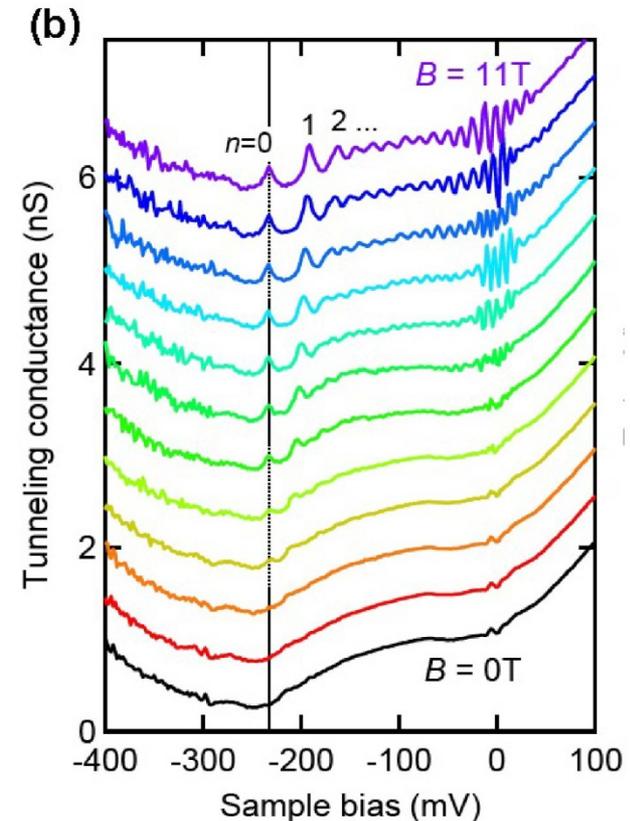
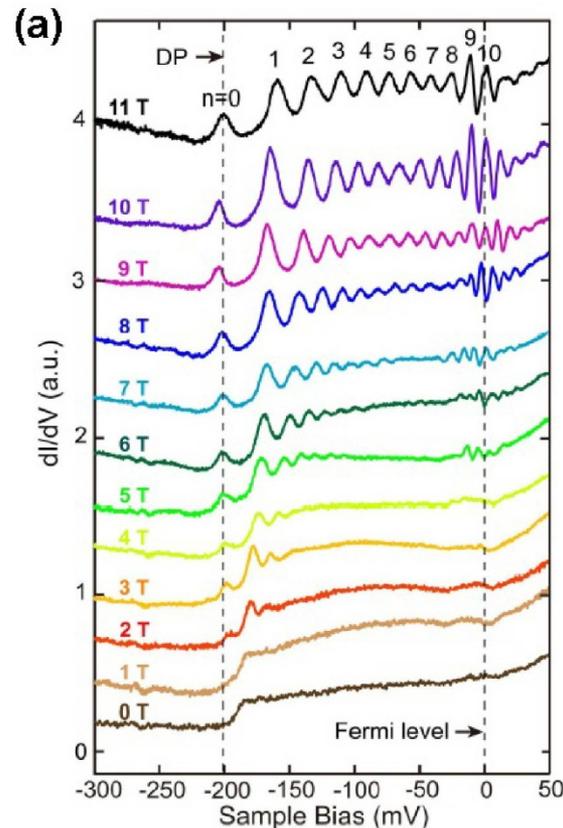


II. Three-Dimensional Topological Insulators

E. Experimental results

3. STM

- Good agreement is found between the integrated density of states from ARPES and STM
- STM also shows protection against backscattering
- Like graphene surface states would have a relativistic (Dirac-like) Landau level spectrum
- We can also observe Landau levels in a magnetic field

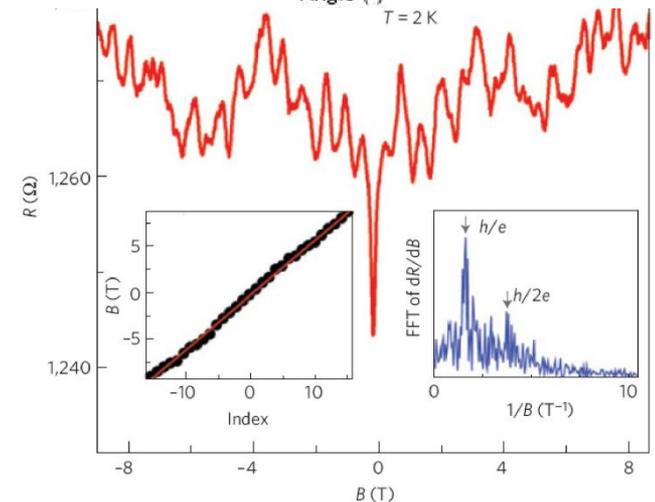
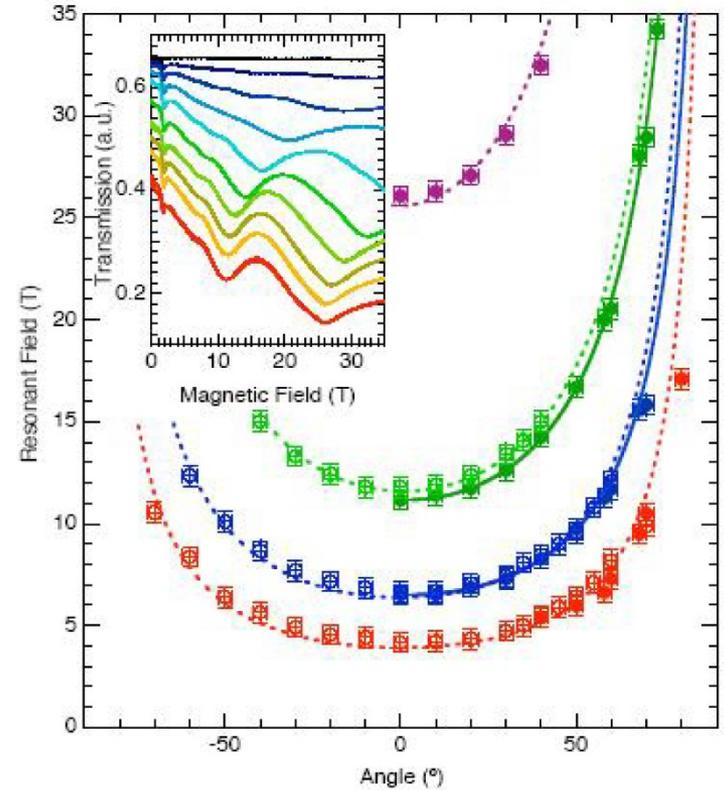


II. Three-Dimensional Topological Insulators

E. Experimental results

2. Transport

- The fact that cyclotron resonance frequency only scales with perpendicular magnetic field shows 2D nature of surface states
- One way to reduce bulk doping is using thin films obtained by mechanically exfoliation or epitaxial growth
- An important advantage of a sample of mesoscopic size is the possibility of tuning the carrier density by an external gate voltage
- Magnetoresistance of a nanoribbon exhibits a primary hc/e oscillation, which corresponds to Aharonov-Bohm oscillations of the surface state around the surface of the nanoribbon

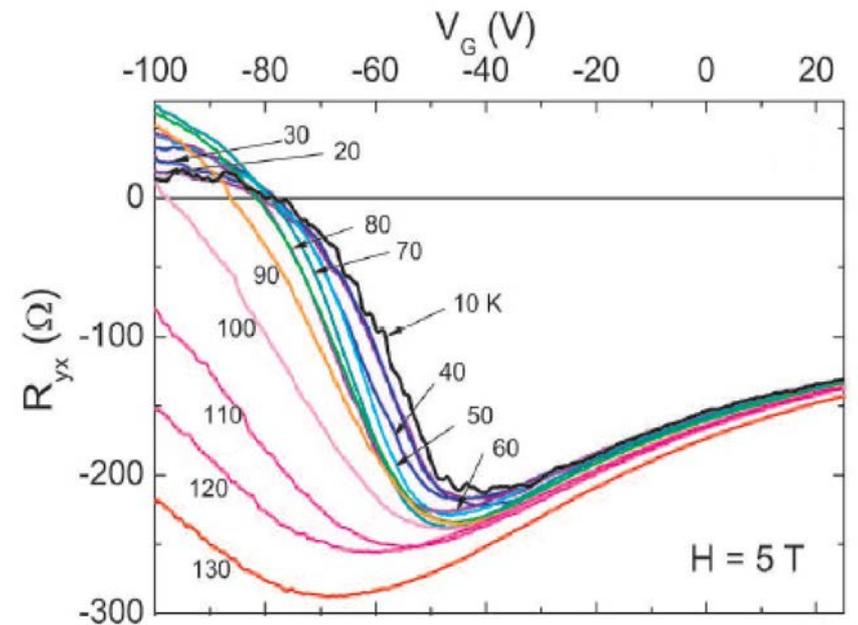
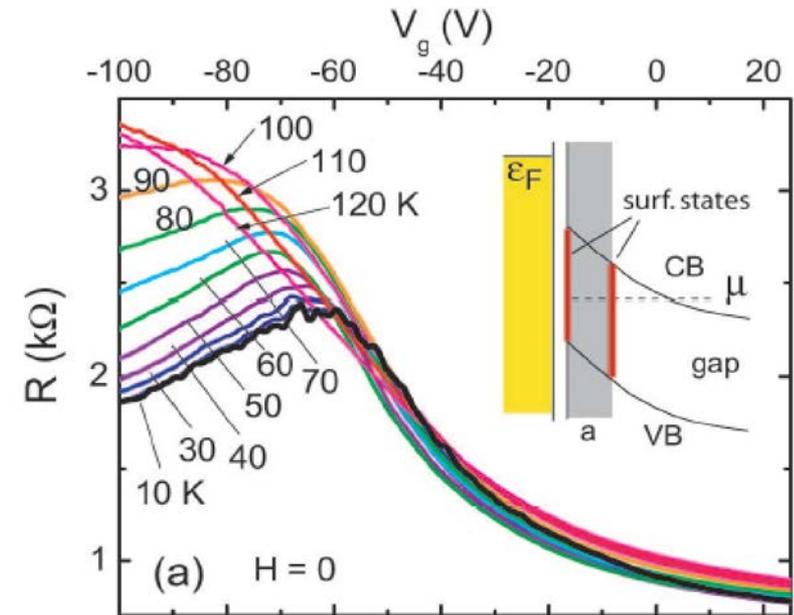


II. Three-Dimensional Topological Insulators

E. Experimental results

2. Transport

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II. Three-Dimensional Topological Insulators

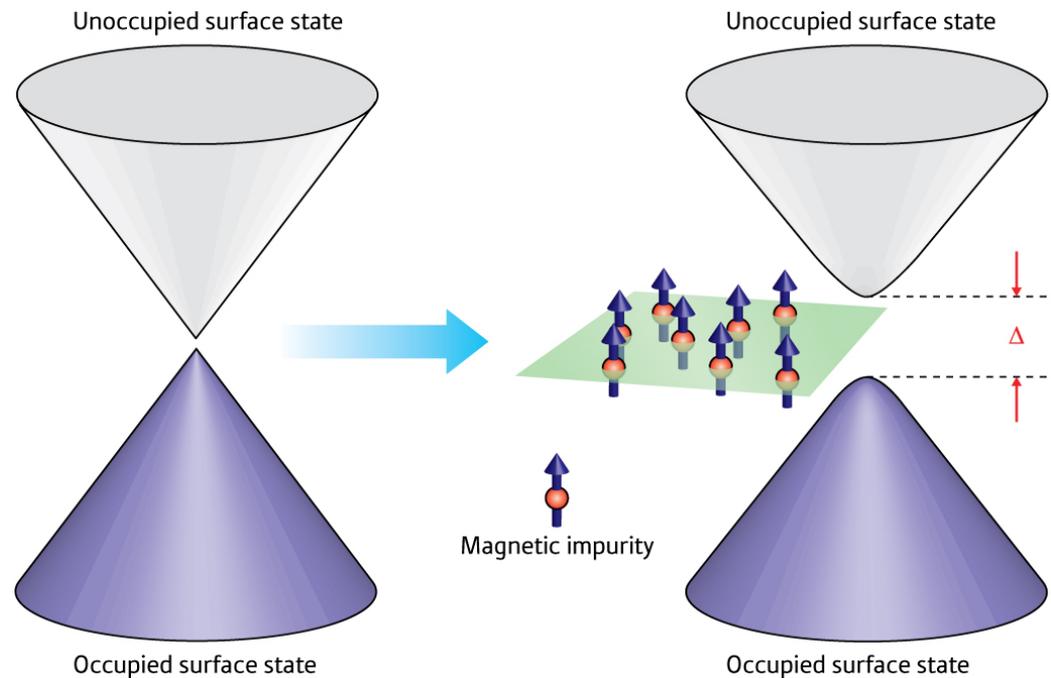
F. Other topological insulator materials

- Topological materials HgTe, Bi₂Se₃, Bi₂Te₃, and Sb₂Te₃ provided us with a prototype material for 2D and 3D TIs
- Other 3D TIs: tetradymite semiconductors like Thallium-based III-V-VI₂ ternary chalcogenides
- Strained bulk HgTe is a topological insulator; distortion along [111] opens a gap between LH and HH bands
- A similar band structure also exists in ternary Heusler compounds; fifty of them are found to exhibit band inversion; other interesting properties
 - Superconductivity
 - Magnetism
 - Heavy-fermion behavior
- QSHE has been proposed in Na₂IrO₃
- Topological Mott insulator phases have been proposed in Ir-based pyrochlore oxides Ln₂Ir₂O₇ with Ln = Nd, Pr
- SmB₆ was recently verified as a Kondo topological insulator

IV. General Theory of Topological Insulators

A. Topological field theory

- Interested in long-wavelength and low-energy properties of a condensed matter system
- In this limit details of the microscopic Hamiltonian are **not** important
- Broken symmetry states \rightarrow order parameter, symmetry and dimensionality
- SPT states \rightarrow coefficient of the topological term identified as the topological order parameter
- Topological Field Theory (TFT) can be developed for topological insulators
- Unlike Topological Band Theory (TBT), TFT can accommodate interactions and disorder
- In the limit of no interactions and disorder TFT reduces to TBT



IV. General Theory of Topological Insulators

A. Topological field theory

1. Chern-Simons insulator in 2+1 dimensions

- TFT for the QH system in 2+1 D

$$S_{\text{eff}} = \frac{C_1}{4\pi} \int d^2x \int dt \epsilon^{\mu\nu\tau} A_\mu \partial_\nu A_\tau$$

- TFT for the QH system in 2+1 D

$$C_1 = \frac{\pi}{3} \int \frac{d^3k}{(2\pi)^3} \text{Tr} [\epsilon^{\mu\nu\rho} G \partial_\mu G^{-1} G \partial_\nu G^{-1} G \partial_\rho G^{-1}],$$

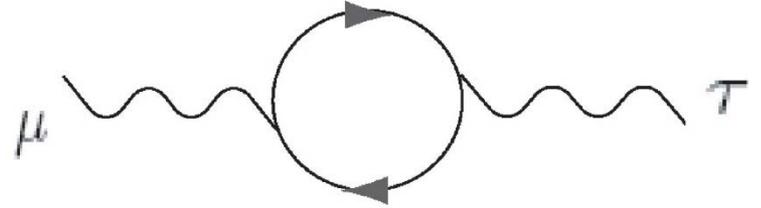
where $G(\mathbf{k}, \omega)$ is imaginary-time single-particle Green's function $\mu, \nu, \rho = 0, 1, 2 \equiv t, x, y$

- For an interacting system we can have a map from k-space to space of nonsingular Green functions in the group $GL(n, \mathbb{C})$; 3rd homotopy group labeled by an integer $\pi_3(GL(n, \mathbb{C})) \cong \mathbb{Z}$
- The winding number for this homotopy class is exactly measured by C_1 , where $n \geq 3$ is the number of bands

- For $G \rightarrow G_0$, integral over ω gives $C_1 = \frac{1}{2\pi} \int dk_x \int dk_y f_{xy}(\mathbf{k}) \in \mathbb{Z}$

$$f_{xy}(\mathbf{k}) = \frac{\partial a_y(\mathbf{k})}{\partial k_x} - \frac{\partial a_x(\mathbf{k})}{\partial k_y}$$

$$a_i(\mathbf{k}) = -i \sum_{\alpha \in \text{occ}} \langle \alpha \mathbf{k} | \frac{\partial}{\partial k_i} | \alpha \mathbf{k} \rangle, \quad i = x, y.$$



IV. General Theory of Topological Insulators

A. Topological field theory

1. Chern-Simons insulator in 2+1 dimensions

- Under TR, since $A_0 \rightarrow A_0$ and $\mathbf{A} \rightarrow -\mathbf{A}$, Chern-Simons theory breaks TRS in 2+1 D
- Taking a functional derivative with respect to A_μ we get:

$$j_\mu = \frac{C_1}{2\pi} \epsilon^{\mu\nu\tau} \partial_\nu A_\tau$$

- Splitting into temporal component we get charge accumulated:

$$j_0 = \frac{C_1}{2\pi} \epsilon^{ij} \partial_i A_j = \frac{C_1}{2\pi} B$$

- Charge accumulated due to magnetic field; i.e. magnetic flux pumps charge
- The spatial component of the space-time current gives

$$j_i = \frac{C_1}{2\pi} \epsilon^{ij} E_j$$

- Electric field gives transverse current with $\sigma_{xy} = (C_1/2\pi) e^2/h$
- At least in the non-interacting case it's easy to see that $C_1 = 2\pi n$ since the Berry phase is quantized
- This is the usual quantum Hall response, i.e. $\sigma_{xy} = ne^2/h$ (with $n \in \mathbb{Z}$)

$$S_{\text{eff}} = \frac{C_1}{4\pi} \int d^2x \int dt \epsilon^{\mu\nu\tau} A_\mu \partial_\nu A_\tau$$

IV. General Theory of Topological Insulators

A. Topological field theory

2. Chern-Simons insulator in 4+1 dimensions

- Advantage of TFT of QHE → Generalization to all odd space-time dimensions

$$S_{\text{eff}} = \frac{C_2}{24\pi^2} \int d^4x dt \epsilon^{\mu\nu\rho\sigma\tau} A_\mu \partial_\nu A_\rho \partial_\sigma A_\tau$$

- The action is explicitly invariant under TR
- C_2 is written in terms of *full* Green's functions

$$C_2 \equiv \frac{\pi^2}{15} \int \frac{d^5k}{(2\pi)^5} \text{Tr} [\epsilon^{\mu\nu\rho\sigma\tau} (G\partial_\mu G^{-1}) (G\partial_\nu G^{-1}) (G\partial_\rho G^{-1}) (G\partial_\sigma G^{-1}) (G\partial_\tau G^{-1})]$$

- This labels the homotopy group $\pi_5(\text{GL}(n, \mathbb{C})) \cong \mathbb{Z}$
- For a non-interacting system, C_2 can be obtained by explicit integration over ω to give a Berry-like integration in \mathbf{k} -space for $i, j, k, \ell = 1, 2, 3, 4$

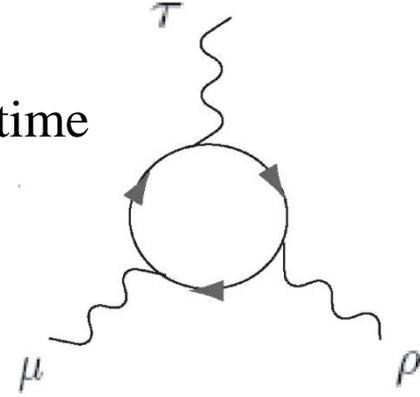
$$C_2 = \frac{1}{32\pi^2} \int d^4k \epsilon^{ijkl} \text{tr}[f_{ij} f_{kl}] \quad f_{ij}^{\alpha\beta} = \partial_i a_j^{\alpha\beta} - \partial_j a_i^{\alpha\beta} + i [a_i, a_j]^{\alpha\beta}$$

$$a_i^{\alpha\beta}(\mathbf{k}) = -i \langle \alpha, \mathbf{k} | \frac{\partial}{\partial k_i} | \beta, \mathbf{k} \rangle$$

- The physical response of 4+1 D Chern-Simons insulators is given by

$$j^\mu = \frac{C_2}{2\pi^2} \epsilon^{\mu\nu\rho\sigma\tau} \partial_\nu A_\rho \partial_\sigma A_\tau$$

which is the nonlinear response to the external field A_μ



IV. General Theory of Topological Insulators

A. Topological field theory

2. Chern-Simons insulator in 4+1 dimensions

- Advantage of TFT of QHE \rightarrow Generalization to all odd space-time dimensions

$$S_{\text{eff}} = \frac{C_2}{24\pi^2} \int d^4x dt \epsilon^{\mu\nu\rho\sigma\tau} A_\mu \partial_\nu A_\rho \partial_\sigma A_\tau$$

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$$j^\mu = \frac{C_2}{2\pi^2} \epsilon^{\mu\nu\rho\sigma\tau} \partial_\nu A_\rho \partial_\sigma A_\tau$$

which is the nonlinear response to the external field A_μ

- To understand this response better, consider a special field configuration

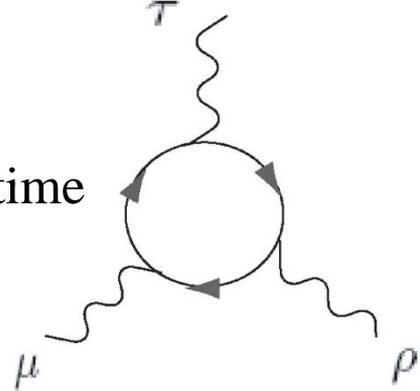
$$A_x = 0, A_y = B_z x, A_z = -E_z t, A_w = A_t = 0$$

- Non-zero components $\rightarrow F_{xy} = B_z$ and $F_{zt} = -E_z$

$$j_w = \frac{C_2}{4\pi^2} B_z E_z$$

- Integrating in the x, y dimensions we get

$$\int dx dy j_w = \frac{C_2}{4\pi^2} \left(\int dx dy B_z \right) E_z \equiv \frac{C_2 N_{xy}}{2\pi} E_z$$

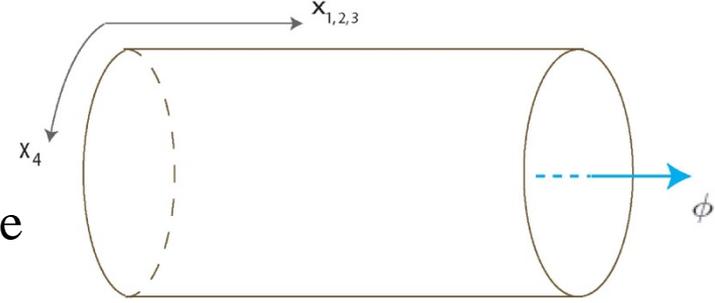


IV. General Theory of Topological Insulators

A. Topological field theory

3. Dimensional reduction to the three-dimensional \mathbb{Z}_2 topological insulator

- 3D and 2D TIs can be obtained by dimensional reduction on the 4D QHE
- Only consider $A_\mu \equiv A(x_0, x_1, x_2, x_3)$
- Consider a geometry where x_4 forms a small circle
- For fixed k_4 we obtain an effective TFT in 3+1 D



$$S_\theta = \frac{\alpha}{32\pi^2} \int d^3x dt \theta(x, t) \epsilon^{\mu\nu\rho\tau} F_{\mu\nu} F_{\rho\tau}(x, t)$$

- The flux due to $A_4(x, t, x_4)$ through the compact extra dimension is

$$\theta(x, t) \equiv C_2 \phi(x, t) = C_2 \oint dx_4 A_4(x, t, x_4)$$

- TRS constrains the value of the flux to two values: 0 and π (for $C_2 = 1$)
- Using a model 3D Hamiltonian (general interacting) is more practical; need to define an order parameter

$$P_3 \equiv \frac{\theta}{2\pi} = \frac{\pi}{6} \int_0^1 du \int \frac{d^4\mathbf{k}}{(2\pi)^4} \text{Tr} \left\{ \epsilon^{\mu\nu\rho\sigma} \left[(G\partial_\mu G^{-1}) (G\partial_\nu G^{-1}) (G\partial_\rho G^{-1}) (G\partial_\sigma G^{-1}) (G\partial_u G^{-1}) \right] \right\}$$

where $G(\mathbf{k}, u = 0) \equiv G(k_0, \mathbf{k}, u = 0) \equiv G(k_0, \mathbf{k})$ is the imaginary-time single-particle Green's function of the fully interacting many-body system; $u = 1$ is topologically trivial

IV. General Theory of Topological Insulators

A. Topological field theory

3. Dimensional reduction to the three-dimensional \mathbb{Z}_2 topological insulator

- Topological order parameter

$$P_3 \equiv \frac{\theta}{2\pi} = \frac{\pi}{6} \int_0^1 du \int \frac{d^4\mathbf{k}}{(2\pi)^4} \text{Tr} \left\{ \epsilon^{\mu\nu\rho\sigma} \left[(G\partial_\mu G^{-1}) (G\partial_\nu G^{-1}) (G\partial_\rho G^{-1}) (G\partial_\sigma G^{-1}) (G\partial_u G^{-1}) \right] \right\}$$

- The following identity is essential for the definition of P_3

$$G(k_0, -\mathbf{k}) = TG(k_0, \mathbf{k})^T T^{-1}$$

- Unlike the Chern-Simons insulator P_3 is not strictly quantized; it can vary continuously between 1/2 and 0 when TRS is broken
- For a non-interacting system, integrating out ω , we get the elegant formula

$$P_3 = \frac{1}{16\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left\{ \left[f_{ij}(\mathbf{k}) - \frac{2}{3} i a_i(\mathbf{k}) a_j(\mathbf{k}) \right] a_k(\mathbf{k}) \right\}$$

- For the model of 2nd generation 3D TIs the above formula can be evaluated explicitly as $P_3 = \theta/2\pi = 1/2$

- The θ -term for 3D TI vs. 2+1 D QH

- θ -term dominates Maxwell term at low energies in 2+1 D by dimensional analysis
- In 3D TI θ - and Maxwell terms have same scaling dimension

- The full set of modified Maxwell's equations + θ -term:

$$\frac{1}{4\pi} \partial_\nu F^{\mu\nu} + \partial_\nu \mathcal{P}^{\mu\nu} + \frac{\alpha}{4\pi} \epsilon^{\mu\nu\sigma\tau} \partial_\nu (P_3 F_{\sigma\tau}) = \frac{1}{c} j^\mu$$

IV. General Theory of Topological Insulators

A. Topological field theory

3. Dimensional reduction to the three-dimensional \mathbb{Z}_2 topological insulator

- The full set of modified Maxwell's equations + θ -term:

$$\frac{1}{4\pi} \partial_\nu F^{\mu\nu} + \partial_\nu \mathcal{P}^{\mu\nu} + \frac{\alpha}{4\pi} \epsilon^{\mu\nu\sigma\tau} \partial_\nu (P_3 F_{\sigma\tau}) = \frac{1}{c} j^\mu$$

- In component form

$$\nabla \cdot \mathbf{D} = 4\pi\rho + 2\alpha(\nabla P_3 \cdot \mathbf{B})$$

$$\nabla \times \mathbf{H} - \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} = \frac{4\pi}{c} \mathbf{j} - 2\alpha \left((\nabla P_3 \times \mathbf{E}) + \frac{1}{c} (\partial_t P_3) \mathbf{B} \right)$$

$$\nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

where $\mathbf{D} = \mathbf{E} + 4\pi\mathbf{P}$ and $\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M}$

- Alternatively one could absorb the topological terms while defining \mathbf{D} and \mathbf{H} (previous section)

$$\mathbf{H} = \mathbf{B} - 4\pi\mathbf{M} + 2P_3\alpha\mathbf{E} \quad \mathbf{D} = \mathbf{E} + 4\pi\mathbf{P} - 2P_3\alpha\mathbf{B}$$

- The topological response can be determined by taking a functional derivative of the topological action with respect to A_μ

$$j^\mu = \frac{1}{2\pi} \epsilon^{\mu\nu\sigma\tau} \partial_\nu P_3 \partial_\sigma A_\tau$$

IV. General Theory of Topological Insulators

A. Topological field theory

3. Dimensional reduction to the three-dimensional \mathbb{Z}_2 topological insulator

1. Half-QH effect on the surface of a 3D topological insulator

- When $P_3 = P_3(z)$ the topological response equation becomes

$$j^\mu = \frac{\partial_z P_3}{2\pi} \epsilon^{\mu\nu\rho} \partial_\nu A_\rho, \quad \mu, \nu, \rho = t, x, y$$

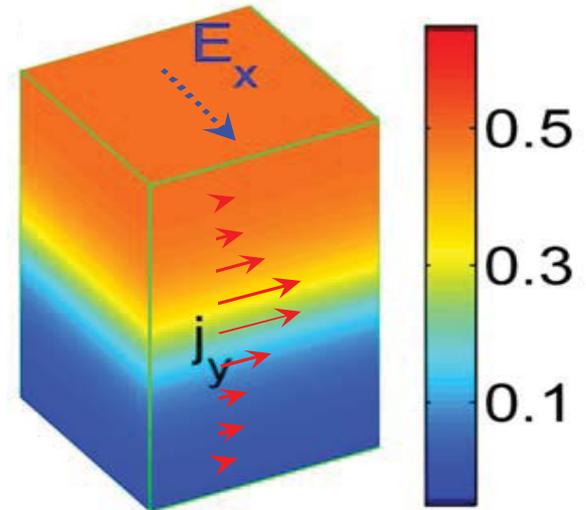
- Integration along the z -direction gives the total Hall current

$$J_y^{2D} = \int_{z_1}^{z_2} dz j_y = \frac{1}{2\pi} \left(\int_{z_1}^{z_2} dP_3 \right) E_x$$

with total 2D Hall conductance

$$\sigma_{xy}^{2D} = \int_{z_1}^{z_2} dP_3 / 2\pi$$

- For a interface between a topologically nontrivial insulator with $P_3=1/2$ and a topologically trivial insulator with $P_3=0$ (say vacuum) the Hall conductance is $\sigma = \Delta P_3 = \pm 1/2$
- Aside from an integer ambiguity, the QH conductance is *exactly* quantized, independent of the details of the interface



IV. General Theory of Topological Insulators

A. Topological field theory

3. Dimensional reduction to the three-dimensional \mathbb{Z}_2 topological insulator

2. Topological magnetoelectric effect induced by a temporal gradient of P_3

- When $P_3 = P_3(t)$ the topological response equation:

$$j^i = -\frac{\partial_t P_3}{2\pi} \epsilon^{ijk} \partial_j A_k, \quad i, j, k = x, y, z$$

which can be compactly written as

$$\mathbf{j} = -\frac{\partial_t P_3}{2\pi} \mathbf{B}$$

- Since $\mathbf{j} = \partial_t \mathbf{P}$, for a constant static magnetic field, we can write $\partial_t \mathbf{P} = -\partial_t (P_3 \mathbf{B} / 2\pi)$

$$\mathbf{P} = -\frac{\mathbf{B}}{2\pi} (P_3 + \text{const.})$$

- This can also be viewed as the higher dimensional charge pumping
- Witten Effect:** assume we have magnetic charge distribution, i.e. $\nabla \cdot \mathbf{B} \neq 0$

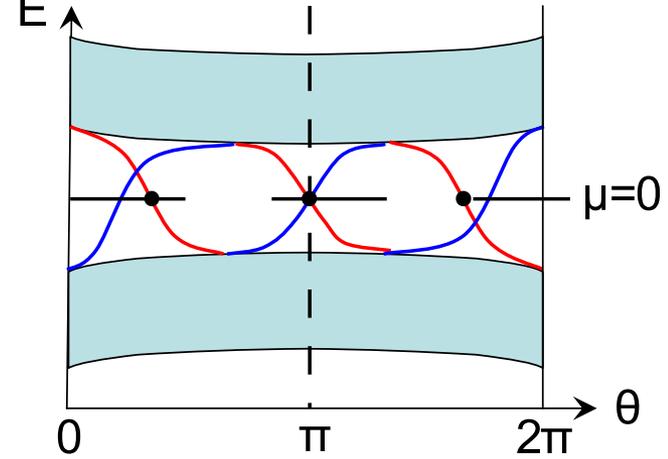
$$\nabla \cdot \mathbf{j} = -\frac{\partial_t P_3}{2\pi} \nabla \cdot \mathbf{B}.$$

- The monopole density is given by $\rho_m = \nabla \cdot \mathbf{B} / 2\pi$

$$\partial_t \rho_e = (\partial_t P_3) \rho_m$$

- When P_3 is changed adiabatically from 0 to $\Theta/2\pi$ the monopole acquires an electric charge

$$Q_e = \frac{\Theta}{2\pi} Q_m$$



IV. General Theory of Topological Insulators

A. Topological field theory

4. Further dimensional reduction to the two-dimensional \mathbb{Z}_2 topological insulator

- Similar to 3D TIs, topological order parameter can be defined for 2D TIs
- We need two Wess-Zumino-Witten extension parameters (u, v) since dimensional reduction needs to be performed twice on the 4D QH state
- For a general interacting insulator, the 2+1 D topological order parameter is expressed as

$$P_2 = \frac{1}{120} \epsilon^{\mu\nu\rho\sigma\tau} \int_{-1}^1 du \int_{-1}^1 dv \int \frac{d^3\mathbf{k}}{(2\pi)^3} \text{Tr} [(G\partial_\mu G^{-1}) (G\partial_\nu G^{-1}) (G\partial_\rho G^{-1}) (G\partial_\sigma G^{-1}) (G\partial_\tau G^{-1})]$$
$$= 0 \text{ or } 1/2 \pmod{\mathbb{Z}}$$

where $\epsilon^{\mu\nu\rho\sigma\tau}$ is the totally antisymmetric tensor in five dimensions, taking value 1 when the variables are an even permutation of (k_0, k_1, k_2, u, v)

- This topological order parameter is valid for interacting QSH systems in 2+1 D, including states in the Mott regime
- **Note:** This is not true for *all* Mott insulators; P_3 might not be a good topological order parameter for some 3D Mott insulators

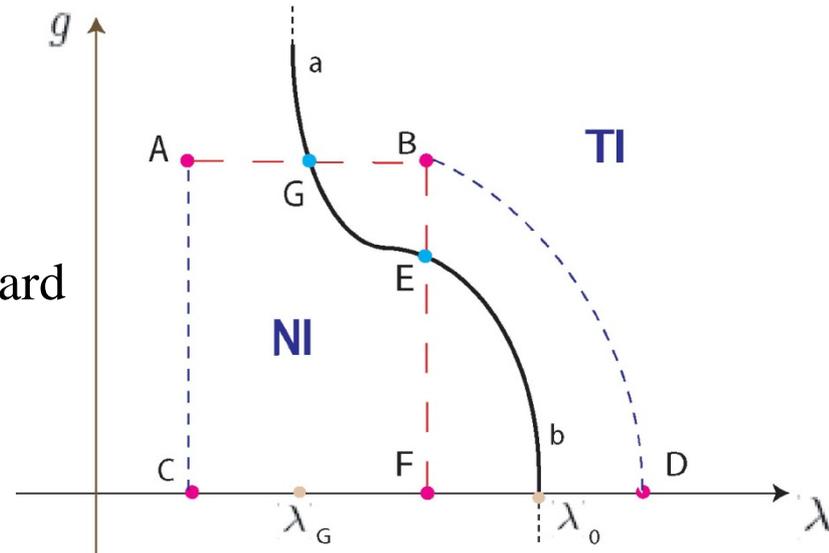
IV. General Theory of Topological Insulators

A. Topological field theory

5. General phase diagram of topological Mott insulator and topological Anderson insulator

- Topological order parameter defined earlier **not** applicable to *all* interacting systems
- For example, Topological order parameter difficult to compute when we have ground state degeneracy or *intrinsic* topological order; TFT is still possible
- In 3D, Fractional TIs (FTIs) have $P_3 =$ rational multiple of $1/2$
- Breaking TRS on the surface of FTI \rightarrow half of Fractional QHE (FQHE)
- In general, consider $H = H_0(\lambda_1, \lambda_2, \dots) + H_1(g_1, g_2, \dots)$
- For $F \rightarrow B$ we have *dynamically generated SOC*
- Several proposals
 - Topological Mott insulators (TMI)
 - Topological Kondo insulators (TKI)
 - ...
- For example, consider the Kane-Mele-Hubbard model

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + i\lambda \sum_{\langle\langle i,j \rangle\rangle} c_i^\dagger \nu_{ij} \sigma_z c_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



IV. General Theory of Topological Insulators

A. Topological field theory

5. General phase diagram of topological Mott insulator and topological Anderson insulator

- For example, consider the Kane-Mele-Hubbard model

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- Interactions can be dealt with TFT by solving for full Green's function
- **Useful simplification:** when there is an adiabatic connection to non-interacting system we can define a “topological Hamiltonian”

$$\tilde{h}(\mathbf{k}) = -G^{-1}(0, \mathbf{k}) = h_0(\mathbf{k}) + \Sigma(0, \mathbf{k})$$

- Remarkably, the topological Hamiltonian captures the topological invariant of the full interacting problem
- **Other simplifications:** Self-energy is *local* like in Dynamical Mean Field Theory (DMFT), i.e. $\Sigma(\omega, \mathbf{k}) \approx \Sigma(\omega)$

$$H_{\mathbf{k}} = \sum_{a=1}^5 h_{\mathbf{k}}^a \Gamma^a \quad G^{-1} = i\omega - h_{\mathbf{k}}^a \Gamma^a - \Sigma(\omega) \equiv G_{\text{atom}}^{-1} - h_{\mathbf{k}}^a \Gamma^a$$

- Expression for topological order parameter

$$n = \frac{2}{\pi^2} \int_{\text{BZ}} d^4k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{\partial_\omega G_{\text{atom}}^{-1}}{(G_{\text{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3} \varepsilon_{abcde} h_{\mathbf{k}}^a \partial_{k_x} h_{\mathbf{k}}^b \partial_{k_y} h_{\mathbf{k}}^c \partial_{k_z} h_{\mathbf{k}}^d \partial_{k_\lambda} h_{\mathbf{k}}^e$$

IV. General Theory of Topological Insulators

A. Topological field theory

5. General phase diagram of topological Mott insulator and topological Anderson insulator

- **Other simplifications:** Self-energy is *local* like in Dynamical Mean Field Theory (DMFT), i.e. $\Sigma(\omega, \mathbf{k}) \approx \Sigma(\omega)$

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- Expression for topological order parameter

$$n = \frac{2}{\pi^2} \int_{\text{BZ}} d^4k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{\partial_{\omega} G_{\text{atom}}^{-1}}{(G_{\text{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3} \varepsilon_{abcde} h_{\mathbf{k}}^a \partial_{k_x} h_{\mathbf{k}}^b \partial_{k_y} h_{\mathbf{k}}^c \partial_{k_z} h_{\mathbf{k}}^d \partial_{k_{\lambda}} h_{\mathbf{k}}^e$$

- Integrate out frequency part

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{\partial_{\omega} G_{\text{atom}}^{-1}}{(G_{\text{atom}}^{-2} - |h_{\mathbf{k}}|^2)^3} = \frac{3}{16|h_{\mathbf{k}}|^5} \gamma$$

- Winding number becomes

$$n = \gamma \times \frac{3}{8\pi^2} \int_{\text{BZ}} d^4k \varepsilon_{abcde} \hat{h}_{\mathbf{k}}^a \partial_{k_x} \hat{h}_{\mathbf{k}}^b \partial_{k_y} \hat{h}_{\mathbf{k}}^c \partial_{k_z} \hat{h}_{\mathbf{k}}^d \partial_{k_{\lambda}} \hat{h}_{\mathbf{k}}^e$$

- When $\Sigma(\omega)$ is diagonal in orbital space:

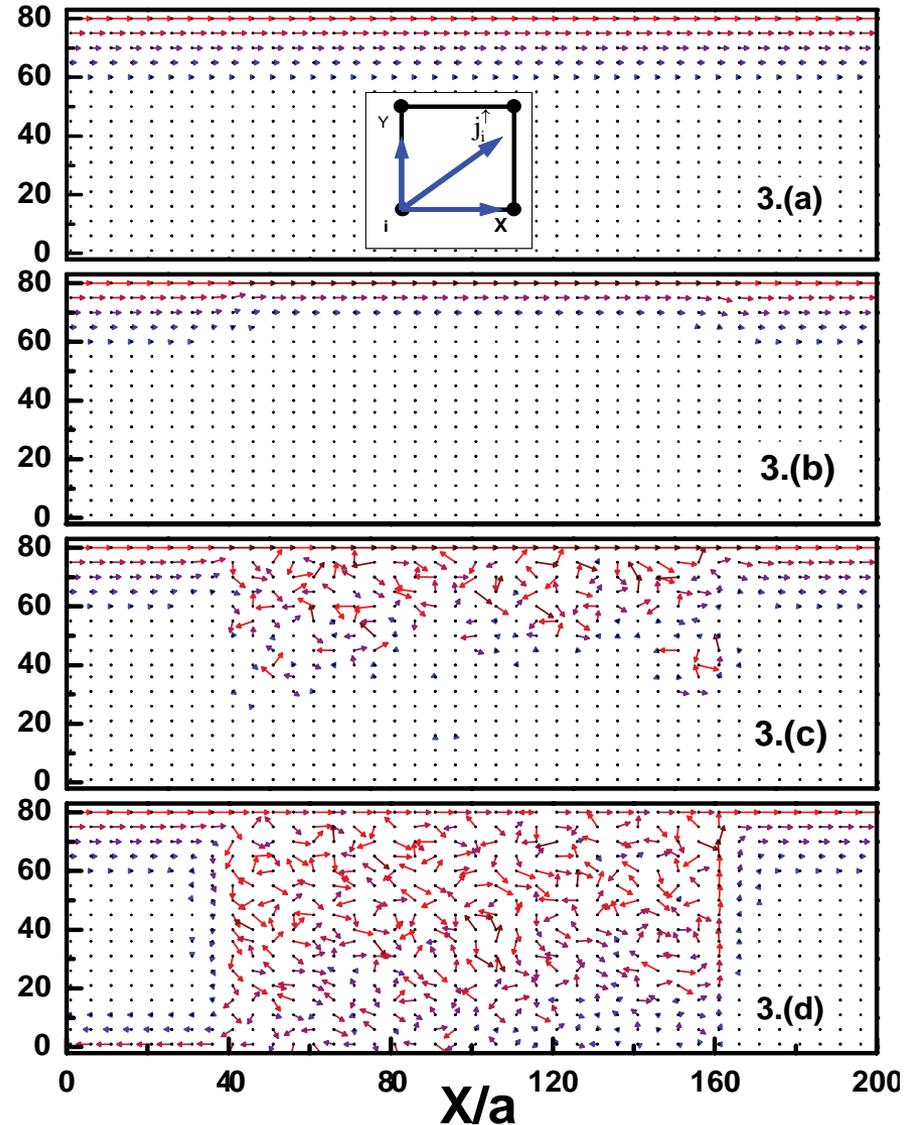
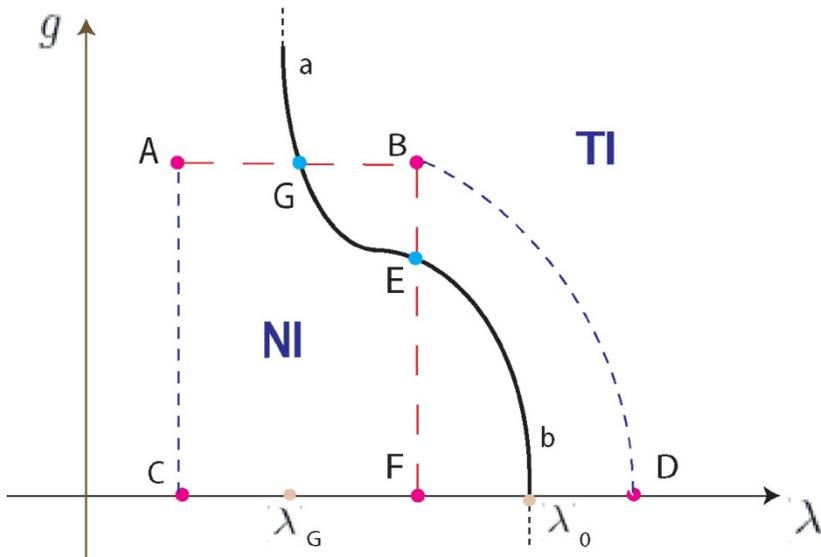
Chern number = Frequency-Domain Winding Number \times Chern number of a mean-field Hamiltonian

IV. General Theory of Topological Insulators

A. Topological field theory

5. General phase diagram of topological Mott insulator and topological Anderson insulator

- For disordered systems, we can use TFT by replacing Green's functions by the disorder-averaged Green's functions
- Interpret g as the disorder strength in the phase diagram
- Effect of disorder on QSHE



IV. General Theory of Topological Insulators

B. Topological band theory

- Only works for non-interacting system
- Important tool in the discovery of new topological materials
- Difficult to evaluate \mathbb{Z}_2 invariants for a generic band structure
- Three approaches
 - Spin Chern numbers
 - Topological invariants constructed from Bloch wave functions
 - Discrete indices calculated from single-particle states at Time-Reversal

Invariant Momentum (TRIM) in the Brillouin zone

- Consider the matrix $B_{\alpha\beta}(\mathbf{k}) = \langle -\mathbf{k}, \alpha | T | \mathbf{k}, \beta \rangle$
- At the TRIM $B(\Gamma_i)$ is antisymmetric; we can define

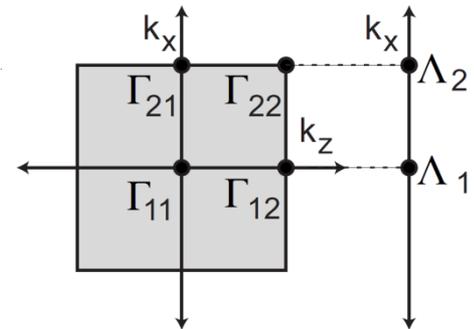
$$\delta_i = \frac{\sqrt{\det[B(\Gamma_i)]}}{\text{Pf}[B(\Gamma_i)]}$$

- In 1D, there are only two TRIM, and a “TR polarization” can be defined as the product of δ_i : $\pi \equiv (-1)^{P_\theta} = \delta_1 \delta_2$

- Similarly for 2D we can define $(-1)^{\nu_{2D}} = (-1)^{P_\theta(k_2=0) - P_\theta(k_2=\pi)}$

$$(-1)^{\nu_{2D}} = \prod_{i=1}^4 \delta_i$$

- Trivial: $(-1)^{\nu_{2D}} = +1$ and Non-trivial: $(-1)^{\nu_{2D}} = -1$



IV. General Theory of Topological Insulators

B. Topological band theory

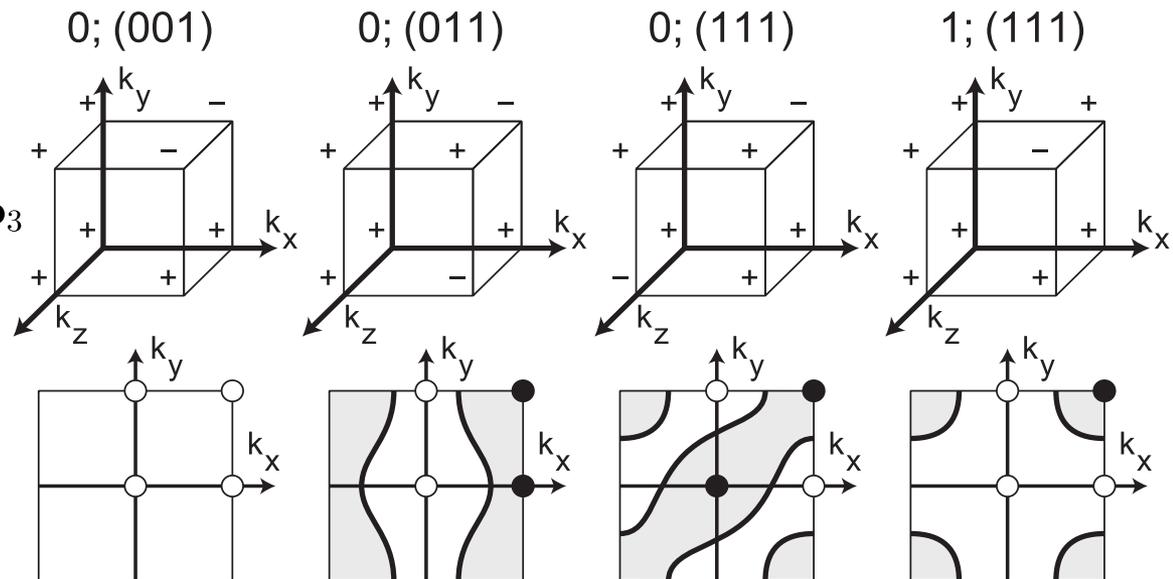
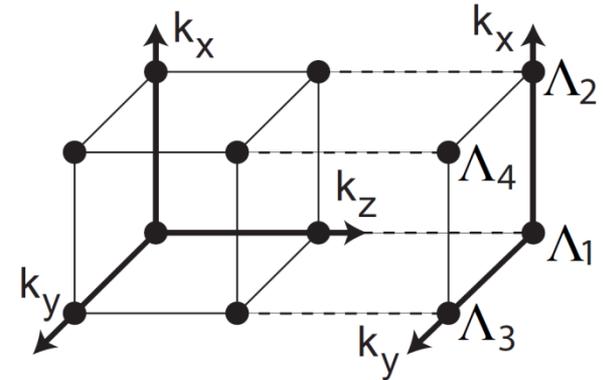
- “Dimensional increase” to 3D

$$(-1)^{\nu_{3D}} = \prod_{i=1}^8 \delta_i$$

- Weak TI: $(-1)^{\nu_{3D}} = +1$ and Strong TI: $(-1)^{\nu_{3D}} = -1$
- Product of any four δ_i for which Γ_i lie in the same plane are gauge invariant
- Therefore we get 3 more invariants defined by

$$(-1)^{\nu_k} = \prod_{n_k=1; n_{j \neq k}=0,1} \delta_{i=(n_1 n_2 n_3)}$$

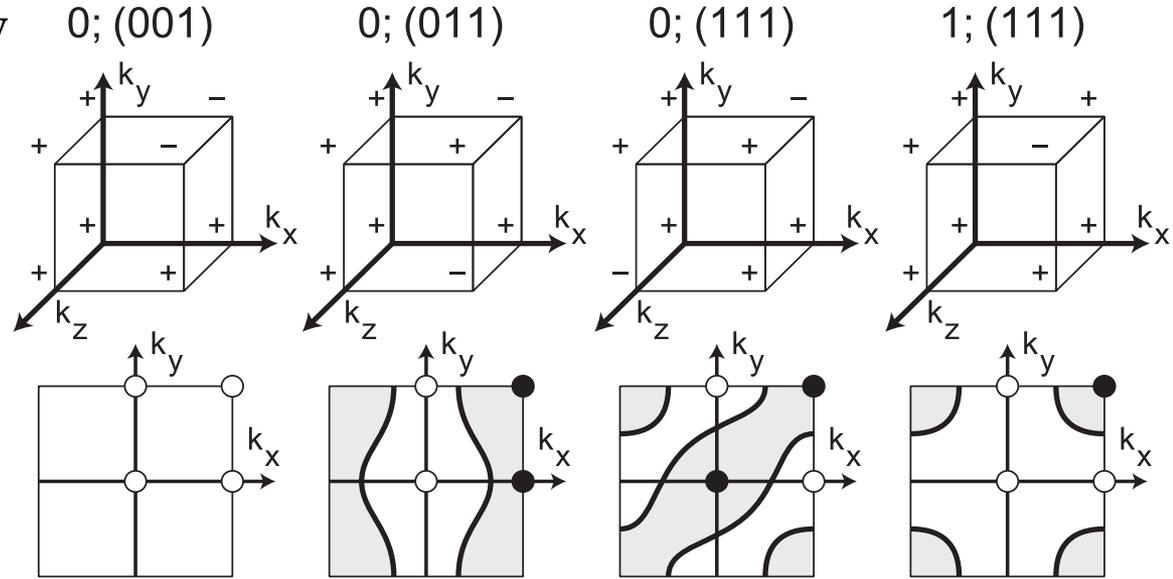
- It is useful to view these invariants as components of a mod 2 reciprocal lattice vector $\mathbf{G}_\nu = \nu_1 \mathbf{b}_1 + \nu_2 \mathbf{b}_2 + \nu_3 \mathbf{b}_3$
- For a dislocation with Burgers vector \mathbf{b} it was shown that there will be gapless modes on the dislocation if $\mathbf{G}_\nu \cdot \mathbf{b} = (2n+1)\pi$ for integer n



IV. General Theory of Topological Insulators

B. Topological band theory

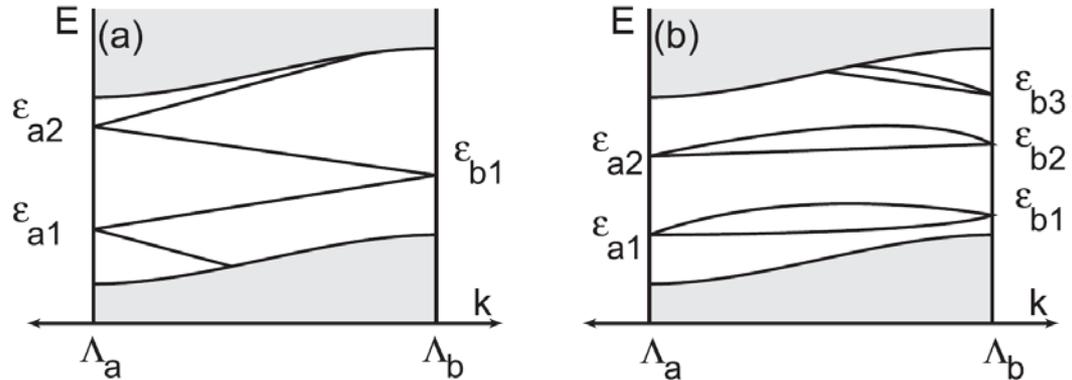
- The surface band structure (bottom figures) will resemble
 - (a): paths connecting a filled circle to an empty circle
 - (b): paths connecting two filled circles or two empty circles



- With inversion symmetry rewrite δ_i as

$$\delta_i = \prod_{m=1}^N \xi_{2m}(\Gamma_i)$$

where $\xi_{2m}(\Gamma_i) = \pm 1$ is the parity eigenvalue of the $2m^{\text{th}}$ band at Γ_i and $\xi_{2m} = \xi_{2m-1}$ are Kramers pairs



- This algorithm also applies to non-inversion symmetric materials which can adiabatically deformed into inversion symmetric ones without closing the energy gap

IV. General Theory of Topological Insulators

C. Reduction from topological field theory to topological band theory

- It's intuitive that there's a connection between TBT and TFT in the non-interacting limit
- TFT requires knowledge of the band structure over the **entire** Brillouin zone
- Recall the matrix

$$B_{\alpha\beta}(\mathbf{k}) = \langle -\mathbf{k}, \alpha | T | \mathbf{k}, \beta \rangle$$

- The TFT formula for P_3 then reduces to

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

- The TFT formula for P_3 gives $\text{deg}(f)$, where $f: T^3 \rightarrow SU(2)$
- Due to TR symmetry, if we choose the image point as one of the two antisymmetric matrices in $SU(2)$ (e.g. $i\sigma_y$) we have an interesting “pair annihilation” of those points other than the eight TRIM
- In other words, Brillouin zone has redundancy in the non-interacting limit
- The explicit relation between TFT and TBT is

$$(-1)^{2P_3} = (-1)^{\nu_{3D}}$$

V. Topological Superconductors and Superfluids

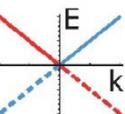
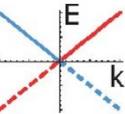
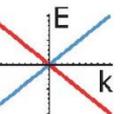
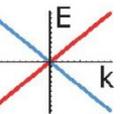
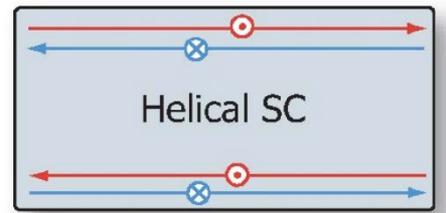
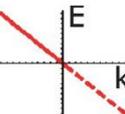
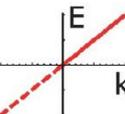
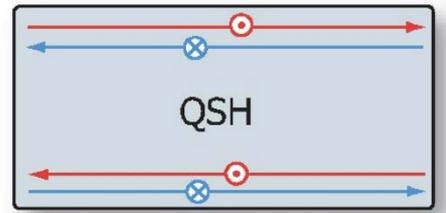
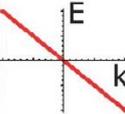
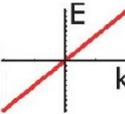
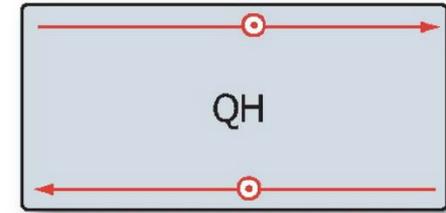
- Superconducting gap, in Bogoliubov-de Gennes (BdG) Hamiltonian, is analogous to *band* gap of insulators
- $^3\text{He-B}$ is a topological superfluid state; BdG Hamiltonian identical to 3D TI
- Classification similar for Topological Superconductors (TSCs) and TIs in 2D
- TRS breaking **2D TSCs** are classified by \mathbb{Z} like **IQHE**
- TRS preserving **2D TSCs** and **2D TIs** are both \mathbb{Z}_2
- TSCs in 1D are always \mathbb{Z}_2 with or without TRS
- Subtlety: **3D TSC** is \mathbb{Z} while **3D TI** is \mathbb{Z}_2
- Aside from striking similarities between time-reversal symmetric TSCs and TIs, TRS breaking TSCs are interesting due to non-Abelian statistics and their potential application to Topological Quantum Computation (TQC)
- p_x+ip_y TSC with \mathcal{N} vortices has that many Majorana Zero Modes (MZMs)
- Braiding vortices gives non-Abelian statistics
- Simplest $\mathcal{N} = 1$ spinless chiral TSC first proposed by Read and Green in 2000
- Spinful version predicted in Sr_2RuO_4 ; very little experimental progress
- New proposals based on *conventional* superconductors proposed by including elements with high Spin-Orbit Coupling (SOC)

AZ\ d	0	1	2	3
A	\mathbb{Z}	0	\mathbb{Z}	0
AIII	0	\mathbb{Z}	0	\mathbb{Z}
AI	\mathbb{Z}	0	0	0
BDI	\mathbb{Z}_2	\mathbb{Z}	0	0
D	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}	0
DIII	0	\mathbb{Z}_2	\mathbb{Z}_2	\mathbb{Z}
AII	\mathbb{Z}	0	\mathbb{Z}_2	\mathbb{Z}_2
CII	0	\mathbb{Z}	0	\mathbb{Z}_2
C	0	0	\mathbb{Z}	0
CI	0	0	0	\mathbb{Z}

V. Topological Superconductors and Superfluids

A. Effective models of time-reversal invariant superconductors

- The simplest way to understand TRI TSCs is through their analogy with TIs
- Similar to TRS breaking example: just as a QH state with Chern number N has N chiral edge states, a chiral TSC with topological invariant \mathcal{N} has \mathcal{N} chiral Majorana edge states
- However, unlike IQHE, chiral Majoranas have half the Degrees of Freedom (DOF) as chiral *electron* edge states
- Therefore, the chiral superconductor is the “minimal” topological state in 2D
- Superconducting analogue of QSH state: a “helical” superconductor
- Spin up: $p_x + ip_y$; spin down: $p_x - ip_y$
- Counter-propagating Majorana Kramer’s pairs
- These “Majorana *modes*,” and **not** “Majorana fermions,” superficially have the same Dirac-like dispersion as Majorana fermions in high energy



V. Topological Superconductors and Superfluids

A. Effective models of time-reversal invariant superconductors

- Hamiltonian of the simplest nontrivial TRS breaking superconductor, the $p+ip$ superconductor for spinless fermions

$$H = \frac{1}{2} \sum_p \begin{pmatrix} c_{\mathbf{p}}^\dagger & c_{-\mathbf{p}} \end{pmatrix} \begin{pmatrix} \epsilon_{\mathbf{p}} & \Delta p_+ \\ \Delta^* p_- & -\epsilon_{\mathbf{p}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{p}} \\ c_{-\mathbf{p}}^\dagger \end{pmatrix}$$

where $\epsilon_{\mathbf{p}} = \mathbf{p}^2/2m - \mu$ and $p_{\pm} = p_x \pm ip_y$

- In the weak pairing phase with $\mu > 0$ the $p_x + ip_y$ chiral superconductor is known to have chiral Majorana edge states propagating on each boundary, described by the Hamiltonian $H_{\text{edge}} = \sum_{k_y \geq 0} v_F k_y \psi_{-k_y} \psi_{k_y}$ where $\psi_{-k_y} = \psi_{k_y}^\dagger$
- Simplest model for the topologically nontrivial TRI superconductor in 2D:

$$H = \frac{1}{2} \sum_p \tilde{\Psi}^\dagger \begin{pmatrix} \epsilon_{\mathbf{p}} & \Delta p_+ & 0 & 0 \\ \Delta^* p_- & -\epsilon_{\mathbf{p}} & 0 & 0 \\ 0 & 0 & \epsilon_{\mathbf{p}} & -\Delta^* p_- \\ 0 & 0 & -\Delta p_+ & -\epsilon_{\mathbf{p}} \end{pmatrix} \tilde{\Psi} \quad \text{with } \tilde{\Psi}(\mathbf{p}) \equiv \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\uparrow}^\dagger \\ c_{\mathbf{p}\downarrow} \\ c_{-\mathbf{p}\downarrow}^\dagger \end{pmatrix}$$

- Note that upper (lower) block, with $p_x + ip_y$ ($p_x - ip_y$) pairing, is analogous to spin up (down) Kramer partner
- Hamiltonian has same form as BHZ model with PHS and \mathbf{k} -dependent mass term $M(\mathbf{k}) = M - 2B(2 - \cos(k_x) - \cos(k_y))$ replaced by $\epsilon_{\mathbf{p}} = \mathbf{p}^2/2m - \mu$

V. Topological Superconductors and Superfluids

A. Effective models of time-reversal invariant superconductors

- Simplest model for the topologically nontrivial TRI superconductor in 2D:

$$H = \frac{1}{2} \sum_{\mathbf{p}} \tilde{\Psi}^\dagger \begin{pmatrix} \epsilon_{\mathbf{p}} & \Delta p_+ & 0 & 0 \\ \Delta^* p_- & -\epsilon_{\mathbf{p}} & 0 & 0 \\ 0 & 0 & \epsilon_{\mathbf{p}} & -\Delta^* p_- \\ 0 & 0 & -\Delta p_+ & -\epsilon_{\mathbf{p}} \end{pmatrix} \tilde{\Psi} \quad \text{with } \tilde{\Psi}(\mathbf{p}) \equiv \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{-\mathbf{p}\uparrow}^\dagger \\ c_{\mathbf{p}\downarrow} \\ c_{-\mathbf{p}\downarrow}^\dagger \end{pmatrix}$$

- The *form* of this model is similar to 2D TIs; i.e. Bogoliubov quasiparticles behave like electrons in a TI
- Although *free electron* edge states protected by TRS in TIs, is it also true for Bogoliubov quasiparticles?
- Consider the edge state Hamiltonian

$$H_{\text{edge}} = \sum_{k_y \geq 0} v_F k_y (\psi_{-k_y\uparrow} \psi_{k_y\uparrow} - \psi_{-k_y\downarrow} \psi_{k_y\downarrow})$$

- The Bogoliubov quasiparticles $\psi_{k_y\uparrow}$, $\psi_{k_y\downarrow}$ in terms of electron operators

$$\begin{aligned} \psi_{k_y\uparrow} &= \int d^2x \left(u_{k_y}(x) c_\uparrow(x) + v_{k_y}(x) c_\uparrow^\dagger(x) \right) \\ \psi_{k_y\downarrow} &= \int d^2x \left(u_{-k_y}^*(x) c_\downarrow(x) + v_{-k_y}^*(x) c_\downarrow^\dagger(x) \right) \end{aligned}$$

Eigenstates of BdG Hamiltonian

- Time-reversal transformation of electron states implies $T\psi_{k_y\uparrow}T^{-1} = \psi_{-k_y\downarrow}$ and $T\psi_{k_y\downarrow}T^{-1} = -\psi_{-k_y\uparrow}$

V. Topological Superconductors and Superfluids

A. Effective models of time-reversal invariant superconductors

- Similar to 2D, the 3D TSC Hamiltonian can be written as

$$H = \frac{1}{2} \sum_p \Psi^\dagger \begin{pmatrix} \epsilon_p \mathbb{I}_{2 \times 2} & i\sigma^2 \sigma^\alpha (\Delta^{\alpha j} p_j) \\ \text{h.c.} & -\epsilon_p \mathbb{I}_{2 \times 2} \end{pmatrix} \Psi \quad \text{with } \Psi(\mathbf{p}) \equiv \begin{pmatrix} c_{\mathbf{p}\uparrow} \\ c_{\mathbf{p}\downarrow} \\ c_{-\mathbf{p}\uparrow}^\dagger \\ c_{-\mathbf{p}\downarrow}^\dagger \end{pmatrix}$$

where $\Delta^{\alpha j} = \Delta u^{\alpha j}$ is a 3×3 matrix with $u \in SO(3)$

- Ignoring dipole-dipole interaction term, and performing a spin rotation, $\Delta^{\alpha j}$ can be diagonalized to $\Delta^{\alpha j} = \Delta \delta^{\alpha j}$

$$H = \frac{1}{2} \int d^2\mathbf{x} \Psi^\dagger \begin{pmatrix} \epsilon_p & 0 & \Delta p_+ & -\Delta p_z \\ 0 & \epsilon_p & -\Delta p_z & -\Delta p_- \\ \Delta^* p_- & -\Delta^* p_z & -\epsilon_p & 0 \\ -\Delta^* p_z & -\Delta^* p_+ & 0 & -\epsilon_p \end{pmatrix} \Psi$$

where $\epsilon_p = \mathbf{p}^2/2m - \mu$ and $p_\pm = p_x \pm ip_y$

- For $\mu > 0$ the surface states are Majorana *mode* described by

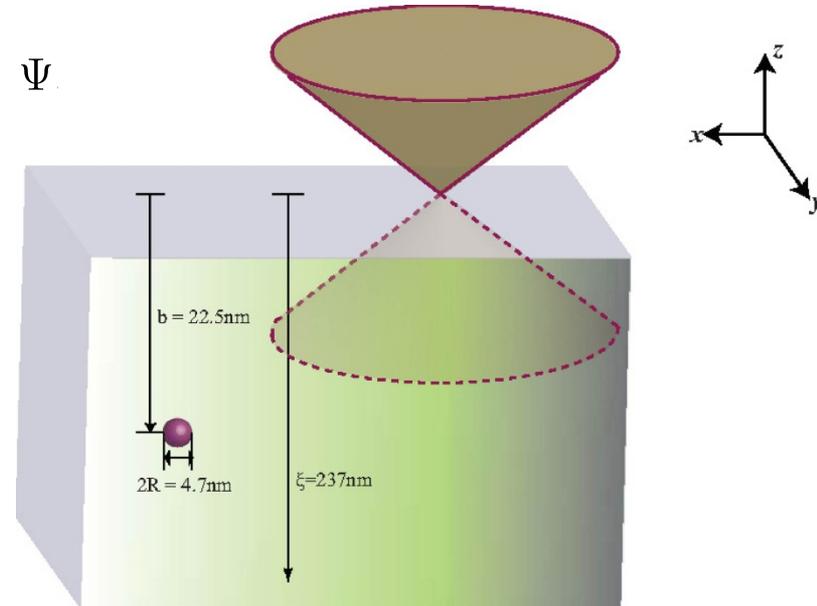
$$H_{\text{surf}} = \frac{1}{2} \sum_{\mathbf{k}} v_F \psi_{-\mathbf{k}}^T (k_x \sigma_y - k_y \sigma_x) \psi_{\mathbf{k}}$$

with the Majorana condition $\psi_{-\mathbf{k}} = \sigma_x \psi_{\mathbf{k}}^{\dagger T}$

- Particle-hole symmetry enforces

- Chemical potential at the Dirac point ($\mu = 0$)
- Spin lies in the surface plane

- Spin winding around the momentum is well-defined and gives invariant \mathbb{Z}



V. Topological Superconductors and Superfluids

B. Topological invariants

- TSCs with and without TRS in 1, 2, or 3 dimensions is either \mathbb{Z}_2 or \mathbb{Z}
- Generic mean-field BdG Hamiltonian for a 3D TR invariant superconductor

$$H = \sum_{\mathbf{k}} \left[\psi_{\mathbf{k}}^\dagger h_{\mathbf{k}} \psi_{\mathbf{k}} + \frac{1}{2} \left(\psi_{\mathbf{k}}^\dagger \Delta_{\mathbf{k}} \psi_{-\mathbf{k}}^{\dagger T} + \text{h.c.} \right) \right]$$

- In a different basis we have $H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger H_{\mathbf{k}} \Psi_{\mathbf{k}}$

$$H_{\mathbf{k}} = \frac{1}{2} \begin{pmatrix} 0 & h_{\mathbf{k}} + i\mathcal{T} \Delta_{\mathbf{k}}^\dagger \\ h_{\mathbf{k}} - i\mathcal{T} \Delta_{\mathbf{k}}^\dagger & 0 \end{pmatrix} \quad \Psi_{\mathbf{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi_{\mathbf{k}} - i\mathcal{T} \psi_{-\mathbf{k}}^\dagger \\ \psi_{\mathbf{k}} + i\mathcal{T} \psi_{-\mathbf{k}}^\dagger \end{pmatrix}$$

where $\psi_{\mathbf{k}}$ is an N -component vector and $h_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ are $N \times N$ matrices

- The time-reversal matrix satisfies: $\mathcal{T}^\dagger h_{\mathbf{k}} \mathcal{T} = h_{-\mathbf{k}}^T$, $\mathcal{T}^2 = -\mathbb{I}$, and $\mathcal{T}^\dagger \mathcal{T} = \mathbb{I}$
- The above *off-diagonal* form is only possible with TRS + PHS
- These two conditions also require hermiticity of $\mathcal{T} \Delta_{\mathbf{k}}^\dagger$; this means generic non-hermiticity of $h_{\mathbf{k}} + i\mathcal{T} \Delta_{\mathbf{k}}^\dagger$
- Using singular value decomposition we can write $h_{\mathbf{k}} + i\mathcal{T} \Delta_{\mathbf{k}}^\dagger = U_{\mathbf{k}}^\dagger D_{\mathbf{k}} V_{\mathbf{k}}$; we can deform (diagonal) matrix $D_{\mathbf{k}}$ into the identity without closing the bulk gap
- Then defining $Q_{\mathbf{k}} = U_{\mathbf{k}}^\dagger V_{\mathbf{k}} \in U(N)$ integer-valued topological invariant can be defined as

$$N_W = \frac{1}{24\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left[Q_{\mathbf{k}}^\dagger \partial_i Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_j Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_k Q_{\mathbf{k}} \right]$$

- 1D and 2D invariants can be obtained by dimensional reduction

V. Topological Superconductors and Superfluids

B. Topological invariants

$$N_W = \frac{1}{24\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left[Q_{\mathbf{k}}^\dagger \partial_i Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_j Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_k Q_{\mathbf{k}} \right]$$

- Consider $Q_{\mathbf{k}}$ in the weak pairing limit
- When the Fermi Surfaces (FSs) are non-degenerate, and $\Delta_{\mathbf{k}}$ is only turned on around the FSs, the matrix elements of $\mathcal{T} \Delta_{\mathbf{k}}^\dagger$ between different bands are negligible; to leading order we have

$$h_{\mathbf{k}} + i\mathcal{T} \Delta_{\mathbf{k}}^\dagger \simeq \sum_n (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) |n, \mathbf{k}\rangle \langle n, \mathbf{k}|$$

$$\delta_{n\mathbf{k}} \equiv \langle n, \mathbf{k}| \mathcal{T} \Delta_{\mathbf{k}}^\dagger |n, \mathbf{k}\rangle \in \mathbb{R}$$

$\delta_{n\mathbf{k}}$ are simply matrix elements of $\Delta_{\mathbf{k}}^\dagger$ between $|n, \mathbf{k}\rangle$ and its Kramers partner

where $|n, \mathbf{k}\rangle$ are eigenvectors of $h_{\mathbf{k}}$

- In this approximation $Q_{\mathbf{k}}$ are given by

$$Q_{\mathbf{k}} = \sum_n e^{i\theta_{n\mathbf{k}}} |n, \mathbf{k}\rangle \langle n, \mathbf{k}| \quad e^{i\theta_{n\mathbf{k}}} = (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) / |\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}|$$

- Plugging the above expression for $Q_{\mathbf{k}}$ into the general formula for N_W we get

$$N_W = \frac{1}{24\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left[\left(\sum_{n_1} e^{-i\theta_{n_1\mathbf{k}}} |n_1, \mathbf{k}\rangle \langle n_1, \mathbf{k}| \right) \partial_i \left(\sum_{n_2} e^{i\theta_{n_2\mathbf{k}}} |n_2, \mathbf{k}\rangle \langle n_2, \mathbf{k}| \right) \left(\sum_{n_3} e^{-i\theta_{n_3\mathbf{k}}} |n_3, \mathbf{k}\rangle \langle n_3, \mathbf{k}| \right) \right. \\ \left. \times \partial_j \left(\sum_{n_4} e^{i\theta_{n_4\mathbf{k}}} |n_4, \mathbf{k}\rangle \langle n_4, \mathbf{k}| \right) \left(\sum_{n_5} e^{-i\theta_{n_5\mathbf{k}}} |n_5, \mathbf{k}\rangle \langle n_5, \mathbf{k}| \right) \partial_k \left(\sum_{n_6} e^{i\theta_{n_6\mathbf{k}}} |n_6, \mathbf{k}\rangle \langle n_6, \mathbf{k}| \right) \right]$$

$$N_W = \frac{i}{2\pi^2} \int d^3\mathbf{k} \sum_{n,s} \epsilon^{ijk} \left[\partial_i \theta_n \left(a_j^{ns} \sin \left(\frac{\theta_{ns}}{2} \right) \right) \left(a_k^{sn} \sin \left(\frac{\theta_{sn}}{2} \right) \right) \right. \\ \left. - \frac{2i}{3} \sum_p \left(a_i^{pn} \sin \left(\frac{\theta_{pn}}{2} \right) \right) \left(a_j^{ns} \sin \left(\frac{\theta_{ns}}{2} \right) \right) \left(a_k^{sp} \sin \left(\frac{\theta_{sp}}{2} \right) \right) \right]$$

V. Topological Superconductors and Superfluids

B. Topological invariants

$$N_W = \frac{1}{24\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left[Q_{\mathbf{k}}^\dagger \partial_i Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_j Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_k Q_{\mathbf{k}} \right]$$

- Formulas from the last slide

$$h_{\mathbf{k}} + iT\Delta_{\mathbf{k}}^\dagger \simeq \sum_n (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) |n, \mathbf{k}\rangle \langle n, \mathbf{k}|$$

$$Q_{\mathbf{k}} = \sum_n e^{i\theta_{n\mathbf{k}}} |n, \mathbf{k}\rangle \langle n, \mathbf{k}|$$

$$\delta_{n\mathbf{k}} \equiv \langle n, \mathbf{k} | T \Delta_{\mathbf{k}}^\dagger | n, \mathbf{k} \rangle \in \mathbb{R}$$

$$e^{i\theta_{n\mathbf{k}}} = (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) / |\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}|$$

$$N_W = \frac{i}{2\pi^2} \int d^3\mathbf{k} \sum_{n,s} \epsilon^{ijk} \left[\partial_i \theta_n \left(a_j^{ns} \sin \left(\frac{\theta_{ns}}{2} \right) \right) \left(a_k^{sn} \sin \left(\frac{\theta_{sn}}{2} \right) \right) \right. \\ \left. - \frac{2i}{3} \sum_p \left(a_i^{pn} \sin \left(\frac{\theta_{pn}}{2} \right) \right) \left(a_j^{ns} \sin \left(\frac{\theta_{ns}}{2} \right) \right) \left(a_k^{sp} \sin \left(\frac{\theta_{sp}}{2} \right) \right) \right]$$

$\theta_{ns} = \theta_n - \theta_s$

$a_j^{ns} = -i \langle n, \mathbf{k} | \partial_j | s, \mathbf{k} \rangle$

- Restrict the pairing to an energy shell $-\epsilon < \epsilon_{n\mathbf{k}} < \epsilon$; means only $\delta_{n\mathbf{k}}$ is non-zero
- This means $\theta_{m\mathbf{k}}$ outside this energy range is an integer multiple of π
- Standard (but not simple!) trigonometry gives

$$\sin \left(\frac{\theta_{pn}}{2} \right) \sin \left(\frac{\theta_{ns}}{2} \right) \sin \left(\frac{\theta_{sp}}{2} \right) = -\frac{1}{4} [\cancel{\sin(\theta_{sp})} + \cancel{\sin(\theta_{ns})} + \cancel{\sin(\theta_{pn})}]$$

in the limit $\epsilon \rightarrow 0$ we have $\theta_n \rightarrow 0$ the remaining two terms vanish

- Therefore, the entire 2nd term of N_W vanishes

- First term? $\propto -\partial_i \theta_n \sin^2 \left(\frac{\theta_{ns}}{2} \right)$
 $\rightarrow \infty?$

V. Topological Superconductors and Superfluids

B. Topological invariants

$$N_W = \frac{1}{24\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left[Q_{\mathbf{k}}^\dagger \partial_i Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_j Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_k Q_{\mathbf{k}} \right]$$

- Main formulas

$$h_{\mathbf{k}} + iT \Delta_{\mathbf{k}}^\dagger \simeq \sum_n (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) |n, \mathbf{k}\rangle \langle n, \mathbf{k}|$$

$$Q_{\mathbf{k}} = \sum_n e^{i\theta_{n\mathbf{k}}} |n, \mathbf{k}\rangle \langle n, \mathbf{k}|$$

$$\delta_{n\mathbf{k}} \equiv \langle n, \mathbf{k} | T \Delta_{\mathbf{k}}^\dagger |n, \mathbf{k}\rangle \in \mathbb{R}$$

$$e^{i\theta_{n\mathbf{k}}} = (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) / |\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}|$$

$$N_W = -\frac{i}{2\pi^2} \int d^3\mathbf{k} \sum_{n,s} \epsilon^{ijk} \underbrace{\partial_i \theta_n}_{\rightarrow \infty?} \left[a_j^{ns} a_k^{sn} \sin^2 \left(\frac{\theta_{ns}}{2} \right) \right]$$

$$a_j^{ns} = -i \langle n, \mathbf{k} | \partial_j |s, \mathbf{k}\rangle$$

$$\theta_{ns} = \theta_n - \theta_s$$

- To the leading order, near the Fermi surface we have

$$e^{i\theta_{n\mathbf{k}}} \simeq \frac{v_F (k_\perp - k_F) + i\delta_{nk_F}}{\sqrt{v_F^2 (k - k_F)^2 + \delta_{nk_F}^2}}$$

- In the limit $\delta_{nk_F} \rightarrow 0$ we have $e^{i\theta_{n\mathbf{k}}} \simeq -1 \pm i0$; more precisely we have

$$\lim_{\delta_{nk_F} \rightarrow 0} \theta_{n\mathbf{k}} = \pi \text{sgn}(\delta_{nk_F}) \eta(k_F - k_\perp)$$

- On differentiating we get

$$\partial_{k_\perp} \theta_{n\mathbf{k}} = -\pi \text{sgn}(\delta_{n\mathbf{k}}) \delta(k_\perp - k_F)$$

which, in the vector form, looks like

$$\nabla \theta_{n\mathbf{k}} = -\pi \mathbf{v}_{n\mathbf{k}} \text{sgn}(\delta_{n\mathbf{k}}) \delta(\epsilon_{n\mathbf{k}})$$

- The $\partial_i \theta_n$ term does indeed blow up at the Fermi surface

V. Topological Superconductors and Superfluids

B. Topological invariants

$$N_W = \frac{1}{24\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left[Q_{\mathbf{k}}^\dagger \partial_i Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_j Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_k Q_{\mathbf{k}} \right]$$

- Main formulas

$$\begin{aligned}
 h_{\mathbf{k}} + iT\Delta_{\mathbf{k}}^\dagger &\simeq \sum_n (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) |n, \mathbf{k}\rangle \langle n, \mathbf{k}| & Q_{\mathbf{k}} &= \sum_n e^{i\theta_{n\mathbf{k}}} |n, \mathbf{k}\rangle \langle n, \mathbf{k}| \\
 \delta_{n\mathbf{k}} &\equiv \langle n, \mathbf{k} | T\Delta_{\mathbf{k}}^\dagger |n, \mathbf{k}\rangle \in \mathbb{R} & e^{i\theta_{n\mathbf{k}}} &= (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) / |\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}| \\
 N_W &= -\frac{i}{2\pi^2} \int d^3\mathbf{k} \sum_{n,s} \epsilon^{ijk} \partial_i \theta_n \left[a_j^{ns} a_k^{sn} \sin^2 \left(\frac{\theta_{ns}}{2} \right) \right] & a_j^{ns} &= -i \langle n, \mathbf{k} | \partial_j |s, \mathbf{k}\rangle \\
 \partial_{k_\perp} \theta_{n\mathbf{k}} &= -\pi \text{sgn}(\delta_{n\mathbf{k}}) \delta(k_\perp - k_F) & \theta_{ns} &= \theta_n - \theta_s
 \end{aligned}$$

- Plugging in all the formulas

$$\begin{aligned}
 N_W &= -\frac{i}{2\pi^2} \int_{FS} d^2\mathbf{k}_\parallel \int_{k_F - \epsilon/v_F}^{k_F + \epsilon/v_F} dk_\perp \sum_{n,s} \partial_\perp \theta_n \sin^2 \left(\frac{\theta_{ns}}{2} \right) (a_1^{ns} a_2^{sn} - a_2^{ns} a_1^{sn}) \\
 &= -\frac{i}{2\pi^2} \int_{FS} d^2\mathbf{k}_\parallel \sum_{n,s} \left[\int d\theta_\beta \sin^2 \left(\frac{\theta_n - \theta_s}{2} \right) \right] (a_1^{ns} a_2^{sn} - a_2^{ns} a_1^{sn}) \\
 &= -\frac{i}{2\pi^2} \int_{FS} d^2\mathbf{k}_\parallel \sum_{n,s} \frac{\theta_n - \sin(\theta_n - \theta_s)}{2} \Big|_{\theta_n^-}^{\theta_n^+} (a_1^{ns} a_2^{sn} - a_2^{ns} a_1^{sn})
 \end{aligned}$$

- Labeling the single band crossing the Fermi surface with $n = 0$

$$N_W = -\frac{i}{2\pi^2} \int_{FS} d^2\mathbf{k}_\parallel \sum_{s \neq 0} \frac{\theta_0 - \sin(\theta_0 - \theta_s)}{2} \Big|_{\theta_0^-}^{\theta_0^+} (a_1^{0s} a_2^{s0} - a_2^{0s} a_1^{s0})$$

V. Topological Superconductors and Superfluids

B. Topological invariants

$$N_W = \frac{1}{24\pi^2} \int d^3\mathbf{k} \epsilon^{ijk} \text{Tr} \left[Q_{\mathbf{k}}^\dagger \partial_i Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_j Q_{\mathbf{k}} Q_{\mathbf{k}}^\dagger \partial_k Q_{\mathbf{k}} \right]$$

- Main formulas

$$\begin{aligned}
 h_{\mathbf{k}} + iT\Delta_{\mathbf{k}}^\dagger &\simeq \sum_n (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) |n, \mathbf{k}\rangle \langle n, \mathbf{k}| & Q_{\mathbf{k}} &= \sum_n e^{i\theta_{n\mathbf{k}}} |n, \mathbf{k}\rangle \langle n, \mathbf{k}| \\
 \delta_{n\mathbf{k}} &\equiv \langle n, \mathbf{k} | T\Delta_{\mathbf{k}}^\dagger |n, \mathbf{k}\rangle \in \mathbb{R} & e^{i\theta_{n\mathbf{k}}} &= (\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}) / |\epsilon_{n\mathbf{k}} + i\delta_{n\mathbf{k}}| \\
 N_W &= -\frac{i}{2\pi^2} \int d^3\mathbf{k} \sum_{n,s} \epsilon^{ijk} \partial_i \theta_n \left[a_j^{ns} a_k^{sn} \sin^2 \left(\frac{\theta_{ns}}{2} \right) \right] & a_j^{ns} &= -i \langle n, \mathbf{k} | \partial_j |s, \mathbf{k}\rangle \\
 \partial_{k_\perp} \theta_{n\mathbf{k}} &= -\pi \text{sgn}(\delta_{n\mathbf{k}}) \delta(k_\perp - k_F) & \theta_{ns} &= \theta_n - \theta_s
 \end{aligned}$$

- Labeling the single band crossing the Fermi surface with $n = 0$

$$\begin{aligned}
 N_W &= -\frac{i}{2\pi^2} \int_{FS} d^2\mathbf{k}_\parallel \sum_{s \neq 0} \frac{\theta_0 - \cancel{\sin(\theta_0 - \theta_s)}}{2} \Big|_{\theta_0^-}^{\theta_0^+} (a_1^{0s} a_2^{s0} - a_2^{0s} a_1^{s0}) \\
 &= -\frac{i}{4\pi^2} \int_{FS} d^2\mathbf{k}_\parallel \sum_{s \neq 0} \Delta\theta_0 (a_1^{0s} a_2^{s0} - a_2^{0s} a_1^{s0}) \\
 &= \frac{1}{4\pi} \sum_{FS} \text{sgn}(\delta_{s\mathbf{k}}) \int_{FS} d^2\mathbf{k}_\parallel (\partial_1 a_2^{00} - \partial_2 a_1^{00}) \\
 &= \frac{1}{2} \sum_s \text{sgn}(\delta_s) C_{1s}
 \end{aligned}$$

- Formal expression for the Chern number: $C_{1s} = \frac{1}{2\pi} \int_{\text{FS}_s} d\Omega^{ij} (\partial_i a_{sj}(\mathbf{k}) - \partial_j a_{si}(\mathbf{k}))$

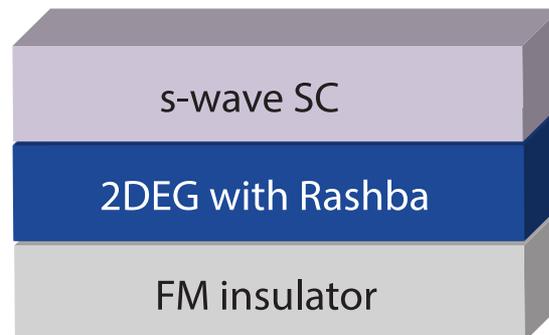
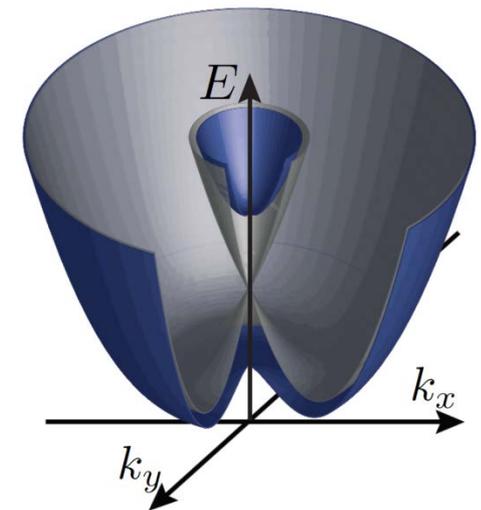
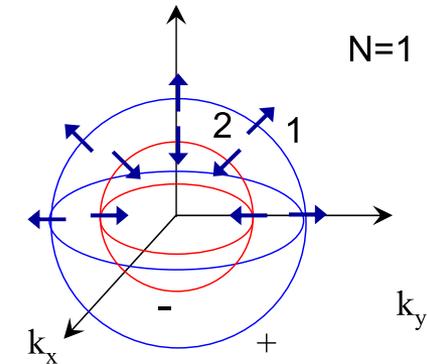
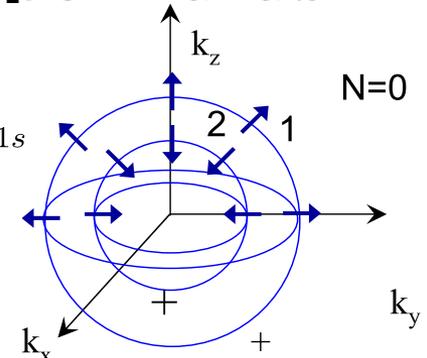
V. Topological Superconductors and Superfluids

B. Topological invariants

- Topological invariant or winding number: $N_W = \frac{1}{2} \sum_s \text{sgn}(\delta_s) C_{1s}$
- Chern number:

$$C_{1s} = \frac{1}{2\pi} \int_{\text{FS}_s} d\Omega^{ij} (\partial_i a_{sj}(\mathbf{k}) - \partial_j a_{si}(\mathbf{k})) \quad a_{si} = -i \langle s\mathbf{k} | \frac{\partial}{\partial k_i} | s\mathbf{k} \rangle$$

- Consider an example: $h_{\mathbf{k}} = \mathbf{k}^2/2m - \mu + \alpha \mathbf{k} \cdot \boldsymbol{\sigma}$
- Rashba spin-orbit coupling gives two spin-polarized Fermi surfaces with *opposite* Chern numbers of ± 1
- Consider a pairing function $\Delta_{\mathbf{k}} = i\Delta_0 \sigma^y$
- The pairing function *cannot* be constant; it must change sign between different Fermi surfaces
- Now, consider *unconventional*, i.e. momentum dependent pairing $\Delta_{\mathbf{k}} = i\Delta_0 \sigma^y \boldsymbol{\sigma} \cdot \mathbf{k}$
- Consider analogy to TRS breaking counterpart



V. Topological Superconductors and Superfluids

B. Topological invariants

- Topological invariant of 2D and 1D TSCs obtained by dimensional reduction

- Consider 3D Hamiltonian with k_z replaced by θ

- Topological invariant in 2D:

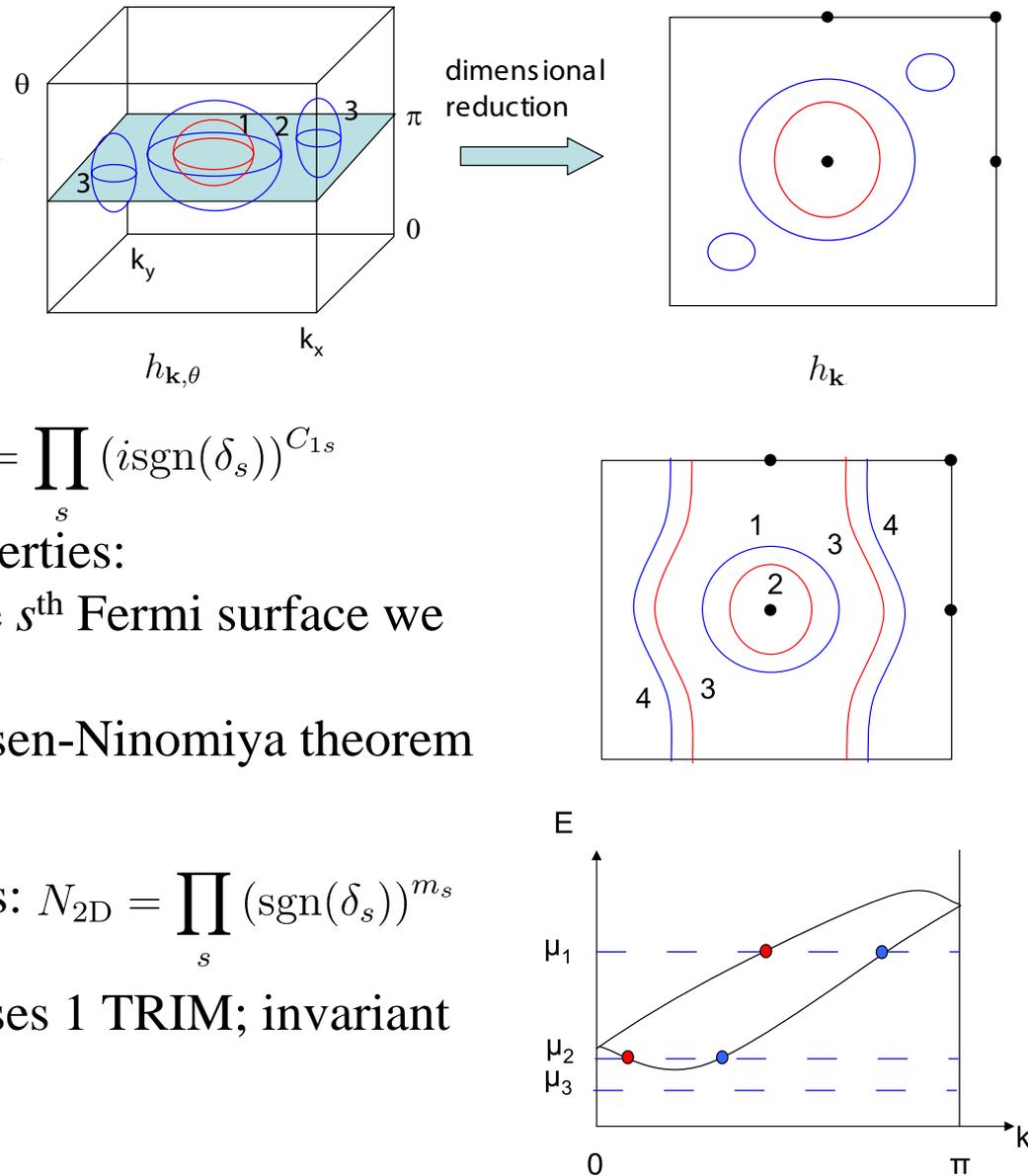
$$N_{2D} = (-1)^{N_W} = (-1)^{\frac{1}{2} \sum_s \text{sgn}(\delta_s) C_{1s}} = \prod_s (i \text{sgn}(\delta_s))^{C_{1s}}$$

- The Chern number obeys the properties:

- For m_s TRIMs enclosed in the s^{th} Fermi surface we have $(-1)^{C_{1s}} = (-1)^{m_s}$
- As a consequence of the Nielsen-Ninomiya theorem we have $\sum_s C_{1s} = 0$

- Topological invariant for 2D TSCs: $N_{2D} = \prod_s (\text{sgn}(\delta_s))^{m_s}$

- In 1D each Fermi “surface” encloses 1 TRIM; invariant for 1D TSCs is $N_{1D} = \prod_s (\text{sgn}(\delta_s))$

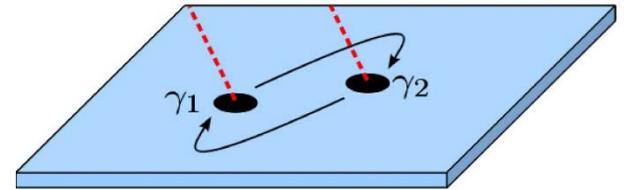


V. Topological Superconductors and Superfluids

C. Majorana zero modes in topological superconductors

1. Majorana zero modes in $p+ip$ superconductors

- The core of a $p+ip$ superconducting vortex contains a localized quasiparticle with exactly zero energy: the Majorana Zero Mode (MZM)
- The quasiparticle operator γ is the Majorana *mode* obeying $[\gamma, H] = 0$ and $\gamma^\dagger = \gamma$
- When two vortices are exchanged, since the phase of charge- $2e$ order parameter winds by 2π , electron picks up a phase π
- Since Majoranas are superposition of electron creation and annihilation operators, we get $\gamma_1 \rightarrow -\gamma_2$ and $\gamma_2 \rightarrow \gamma_1$
- Two vortices actually share two internal states labeled by $i\gamma_1\gamma_2 = \pm 1$
- With $2N$ vortices the core states span a 2^N -dimensional Hilbert space
- The braiding of vortices leads to non-Abelian unitary transformations in this Hilbert space
- Non-locality of the internal states of vortices ensures their coupling to the environment to be exponentially small \Rightarrow fault-tolerant quantum computation at the *hardware* level
- Natural $p+ip \rightarrow \text{Sr}_2\text{RuO}_4$; many properties of this system remain unclear
- Artificial $p+ip$: proximity effect on (i) surface of 3D TI (ii) TRS breaking 2D TI (iii) semiconductors with strong Rashba SOC



V. Topological Superconductors and Superfluids

C. Majorana zero modes in topological superconductors

2. Majorana fermions in surface states of the topological insulator

- Fu and Kane proposed MZM in superconducting vortex using surface states of a 3D topological insulator
- Consider (say) the surface of Bi_2Se_3

$$H = \sum_{\mathbf{p}} \psi^\dagger [v(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{\mathbf{z}} - \mu] \psi \quad \text{with } \psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$$

- Considering proximity to an s -wave superconductor we add $H_\Delta = \Delta \psi_\uparrow^\dagger \psi_\downarrow^\dagger + \text{h.c.}$
- The BdG Hamiltonian is given by $H_{\text{BdG}} = \frac{1}{2} \sum_{\mathbf{p}} \Psi^\dagger H_{\mathbf{p}} \Psi$ where $\Psi^\dagger \equiv (\psi^\dagger \quad \psi)$

$$H_{\mathbf{p}} \equiv \begin{pmatrix} v(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{\mathbf{z}} - \mu & i\sigma^y \Delta \\ -i\sigma^y \Delta^* & -v(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{\mathbf{z}} + \mu \end{pmatrix}$$

- With a finite μ and a TRS breaking mass term $m\sigma^z$ we can write

$$H = \sum_{\mathbf{p}} \psi^\dagger [v(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{\mathbf{z}} + m\sigma^z - \mu] \psi \quad \text{with } \mu > m > 0, \mu - m \ll m$$

$$\simeq \int d^2x \psi_+^\dagger \left(\frac{\mathbf{p}^2}{2m} + m - \mu \right) \psi_+ \quad \leftarrow \text{“nonrelativistic approximation” to the massive Dirac Hamiltonian}$$

where ψ_+ is the positive energy branch of the surface states; in momentum space

$$\psi_{+\mathbf{p}} = u_{\mathbf{p}} \psi_\uparrow + v_{\mathbf{p}} \psi_\downarrow \quad \text{with } u_{\mathbf{p}} = \sqrt{\frac{1}{2} + \frac{m}{2\sqrt{\mathbf{p}^2 + m^2}}} \quad \text{and } v_{\mathbf{p}} = \frac{p_+}{|\mathbf{p}|} \sqrt{\frac{1}{2} - \frac{m}{2\sqrt{\mathbf{p}^2 + m^2}}}$$

V. Topological Superconductors and Superfluids

C. Majorana zero modes in topological superconductors

2. Majorana fermions in surface states of the topological insulator

- Nonrelativistic approximation

$$H \simeq \int d^2x \psi_+^\dagger \left(\frac{\mathbf{p}^2}{2m} + m - \mu \right) \psi_+ \quad \text{with } \mu > m > 0, \mu - m \ll m$$

where ψ_+ is the positive energy branch of the surface states; in momentum space

$$\psi_{+\mathbf{p}} = u_{\mathbf{p}}\psi_\uparrow + v_{\mathbf{p}}\psi_\downarrow \quad \text{with} \quad u_{\mathbf{p}} = \sqrt{\frac{1}{2} + \frac{m}{2\sqrt{\mathbf{p}^2 + m^2}}} \quad \text{and} \quad v_{\mathbf{p}} = \frac{p_+}{|\mathbf{p}|} \sqrt{\frac{1}{2} - \frac{m}{2\sqrt{\mathbf{p}^2 + m^2}}}$$

- The projection of the pairing term H_Δ onto the ψ_+ band we get

$$\begin{aligned} H_\Delta &\simeq \sum_{\mathbf{p}} \psi_{+,\mathbf{p}}^\dagger \psi_{+,-\mathbf{p}}^\dagger \Delta u_{\mathbf{p}} v_{\mathbf{p}} + \text{h.c.} && \text{Precisely the} \\ &\simeq \sum_{\mathbf{p}} \frac{\Delta p_+}{2m} \psi_{+,\mathbf{p}}^\dagger \psi_{+,-\mathbf{p}}^\dagger + \text{h.c.} && \text{Hamiltonian for a} \\ &&& \text{\(\mathit{p}+i\mathit{p}\) superconductor} \end{aligned}$$

- As we tune $m \rightarrow 0$, we can still tune $\mu \rightarrow 0$ while satisfying $\mu > m > 0$, $\mu - m \ll m$ and keeping superconducting gap finite; i.e. MZM still exists with TRS and $\mu = 0$
- Lower dimensional analogue of this system \rightarrow pairing on the edges of QSHE
- MZM appears on the domain wall between s -wave superconductor and ferromagnetic insulator on the QSHE edge

V. Topological Superconductors and Superfluids

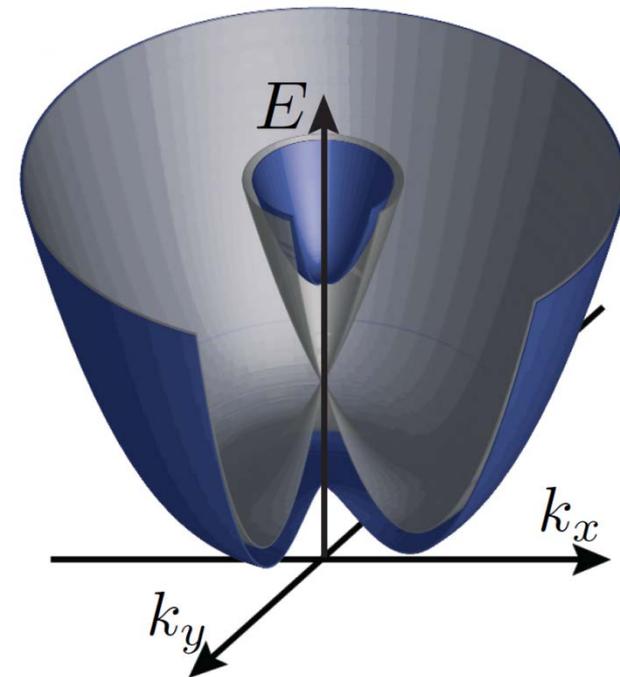
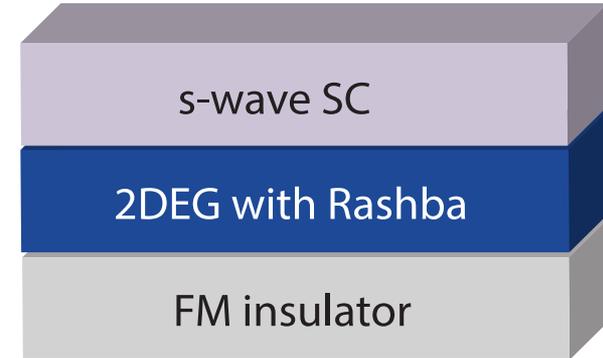
C. Majorana zero modes in topological superconductors

3. Majorana fermions in semiconductors with Rashba spin-orbit coupling

- 2D electron gas with Rashba SOC: system which is described by a Hamiltonian very similar to the surface of a 3D TI

$$H = \int d^2\mathbf{x} \psi^\dagger \left(\frac{\mathbf{p}^2}{2m} + \alpha(\boldsymbol{\sigma} \times \mathbf{p}) \cdot \hat{\mathbf{z}} - \mu \right) \psi$$

- When s -wave pairing is introduced, each of the two spin-split Fermi surfaces forms a nontrivial superconductor
- The Majoranas from these two Fermi surfaces annihilate each other so that the s -wave superconductor in the Rashba system is trivial
- Breaking TRS opens a gap at $\mathbf{k} = 0$; if chemical potential lies in the gap *only one* Fermi surface exists
- Alternative to Ferromagnetic (FM) insulator: in-plane magnetic field + Dresselhaus SOC
- Similar scheme possible in 1D: semiconductor nanowires with Rashba SOC
- Non-Abelian statistics still possible in 1D nanowire “T junctions”



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4. Majorana fermions in quantum Hall and quantum anomalous Hall insulators

- A proposal based on proximity effect to a 2D QH or QAH insulator
- Consider a QH insulator with Hall conductance Ne^2/h in close proximity to a superconductor
- For infinitesimally small pairing we get chiral TSC with invariant $\mathcal{N} = 2N$
- The edge state Hamiltonian, in terms of creation/annihilation operators for a complex spinless fermion, of a QH state with Chern number $N = 1$ is described by $H_{\text{edge}} = \sum_{p_y} v p_y \eta_{p_y}^\dagger \eta_{p_y}$ where $\{\gamma_{-p_y a}, \gamma_{p'_y b}\} = \delta_{ab} \delta_{p_y p'_y}$ and $\gamma_{p_y a}^\dagger = \gamma_{-p_y a}$
- Split into Majorana operators $\eta_{p_y} = \frac{1}{\sqrt{2}}(\gamma_{p_y 1} + i\gamma_{p_y 2})$ and $\eta_{p_y} = \frac{1}{\sqrt{2}}(\gamma_{-p_y 1} - i\gamma_{-p_y 2})$

$$H_{\text{edge}} = \sum_{p_y \geq 0} p_y (\gamma_{-p_y 1} \gamma_{p_y 1} + \gamma_{-p_y 2} \gamma_{p_y 2})$$

- QH plateau transition from $N = 1$ to $N = 0$ will generically split into two transitions when superconducting pairing is introduced
- However, **large** external magnetic field suppresses superconductivity
- Can induce superconductivity in QAHE in Mn-doped HgTe QWs, and Cr- or Fe-doped Bi_2Se_3 thin films

V. Topological Superconductors and Superfluids

C. Majorana zero modes in topological superconductors

5. Detection of Majorana fermions

- Consider the geometry shown in the figure to the right
- An incident electron, with $E = 0$, splits into two chiral Majoranas at point “a,” with each Majorana following a path “b” and “c,” and recombining at point “d”
- Say the ring encloses a flux $\Phi = nhc/2e$
- For odd (even) n we get a (an) hole (electron) at point “d”
- Other proposals
 - Charging energy effects in mesoscopic superconductors
 - Doubled period of the Josephson tunneling current as a function of flux (i.e. Fraunhofer pattern) in 1D and 2D junctions

