Periodic table for topological insulators and superconductors

Main themes:

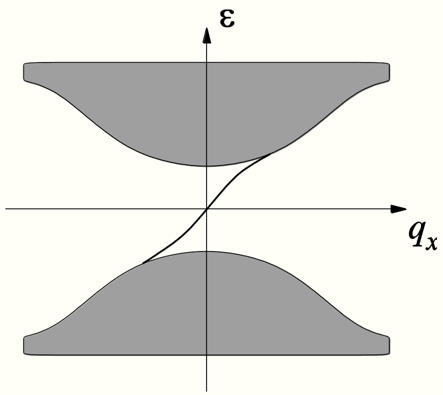
Periodic table:

ОПЫТЪ СИСТЕМЫ ЭЛЕМЕНТОВЪ,

ОСНОВАННОЙ НА ИХЪ АТОМНОМЪ ВѢСѢ И ХИМИЧЕСКОМЪ СХОДСТВѢ.

			Ti=50	Zr=90	?=180.
			V=51	Nb=94	Ta=182.
			Cr=52	Mo=96	W=186.
			Mn=55	Rh=104,4	Pt=197,
			Fe=56	Ru=104,4	Ir=198.
			Ni=Co=59	Pl=106,6	Os=199.
H=1			Cu=63,4	Ag=108	Hg=200.
	Be=9,4	Mg=24	Zn=65,2	Cd=112	
	B=11	Al=27,4	?=68	Ur=116	Au=197?
	C=12	Si=28	?=70	Sn=118	
	N=14	P=31	As=75	Sb=122	Bi=210?
	O=16	S=32	Se=79,4	Te=128?	
	F=19	Cl=35,5	Br=80	I=127	
Li=7	Na=23	K=39	Rb=85,4	Cs=133	Tl=204.
		Ca=40	Sr=87,6	Ba=137	Pb=207.
		?=45	Ce=92		
		?Er=56	La=94		
		?Yt=60	Di=95		
		?In=75,6	Th=118?		

Topological features of electron spectrum



Bott periodicity:

$$\tilde{K}^{n+2}_{\mathbb{C}}(X) \cong \tilde{K}^{n}_{\mathbb{C}}(X)$$

$$\tilde{K}^{n+8}_{\mathbb{R}}(X) \cong \tilde{K}^{n}_{\mathbb{R}}(X)$$

Topological phases

Examples:

- Free fermions: IQHE, $p_x + ip_y$ superconductors, etc.
- ~~Strongly correlated: FQHE, $\mathbb{Z}_2$ gauge (e.g., gapped RVB)~~

(We are only classifying phases of weakly interacting fermions. . .)

Properties:

- Energy gap in the bulk
- Gapless edge modes (IQHE, FQHE)
- ~~Anyons (exist in strongly correlated phases: FQHE, $\mathbb{Z}_2$)~~
- Topological (e.g., Chern-Simons) action

Free electron Hamiltonians

- Using creation and annihilation operators:
  - $\widehat{H} = \sum_{j,k} B_{j,k} a_j^\dagger a_k$ (suitable when charge is conserved).
  - The ground state is characterized by a k-dimensional subspace $\mathcal{L} \subseteq \mathbb{C}^{m+k}$;
  - parametrized by $U(k+m)/(U(k) \times U(m))$.

Majorana operators:

$$c_{2l-1} = a_l + a_l^\dagger, \quad c_{2l} = \tfrac{1}{i}(a_l - a_l^\dagger)$$

$$c_j c_k + c_k c_j = 2\delta_{jk}$$

- Using Majorana operators:
  - $\widehat{H} = \frac{i}{4} \sum_{j,k} A_{jk} c_j c_k$.
  - The ground state is parametrized by $O(2n)/U(n)$.

The elements (topological phases to classify)

- IQHE systems (GaAs-AlGaAs heterostructures, graphene)
- 2D spin-Hall insulators (HgTe)
- 3D topological insulators (BiSb)
- 1D triplet superconductors ($(\mathrm{TMTSF})_2\mathrm{X}$)
- $p_x + ip_y$ superconductors (SrRu)
- Superfluid ^{3}He-B

Yet undiscovered:

- $(p_x + ip_y) \times (p_x - ip_y)$ superconductors
- Majorana chains

The table(s)

First table: complex K-theory

Stable equivalence classes of complex vector bundles on a topological space X are given by homotopy classes of maps $X \to C_0$.

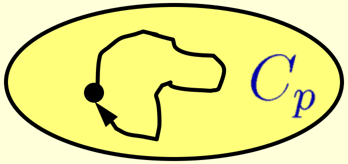
p	Classifying space C_p	$\pi_0(C_p)$	invariant
0	$\bigoplus_k \lim_{n\to\infty} U(k+2n)/(U(k+n)\times U(n))$	$\mathbb{Z}$	$k \in \mathbb{Z}$
1	$\lim_{n\to\infty} U(n)$	0	

C_0 parametrizes $k+n$-dimensional linear subspaces in $\mathbb{C}^{k+2n}$

C_1 parametrizes unitary matrices

Bott periodicity: $C_1 \sim \Omega(C_0), \quad C_0 \sim \Omega(C_1).$

loop spaces



Second table: real K-theory

p	Classifying space R_p	$\pi_0(R_p)$	invariant
0	$O(k+2n)/(O(k+n)\times O(n))$	$\mathbb{Z}$	$k\in\mathbb{Z}$
1	$O(n)$	$\mathbb{Z}_2$	$\det S=\pm 1$
2	$O(2n)/U(n)$	$\mathbb{Z}_2$	$\mathrm{Pf}\,A=\pm 1$
3	$U(2n)/Sp(n)$	0	
4	$Sp(k+2n)/(Sp(k+n)\times Sp(n))$	$\mathbb{Z}$	$k\in\mathbb{Z}$
5	$Sp(n)$	0	
6	$Sp(n)/U(n)$	0	
7	$U(n)/O(n)$	0	

The real Grassmanian R_0 classifies real vector bundles.

$R_p\sim\Omega^p(R_0)$; Bott periodicity: $R_{p+8}\sim R_p$.

The space R_p classifies *Clifford extensions* $\mathrm{Ciff}^{p,0}\setminus\mathrm{Ciff}^{p+1,0}$, which are closely related to free fermionic Hamiltonians with symmetries.

The classification

p	$\pi_0(C_p)$	$d=1$	$d=2$	$d=3$
0	$\mathbb{Z}$		IQHE	
1	0			

$U(1)$ symmetry, or conserved charge (Q); no time-reveral symmetry (T).

p	$\pi_0(R_p)$	$d=1$	$d=2$	$d=3$
0	$\mathbb{Z}$	$* * *$	$p_x + ip_y$ (SrRu)	T (^{3}He-B)
1	$\mathbb{Z}_2$	Majorana chain	T-invariant triplet superconductors $((p_x+ip_y)\times(p_x-ip_y))$	T, Q insulators (BiSb)
2	$\mathbb{Z}_2$	T-inv. triplet superconductors ($(\mathrm{TMTSF})_2\mathrm{X}$)	T, Q insulators (spin-Hall in HgTe)	
3	0			
4	$\mathbb{Z}$			

Summary of the classification

- All the phases (except $***$) belong to 4 symmetry classes:
  - Q (Hall insulators) — (mod 2) table

$$\left.\begin{array}{ll} -\ \text{no symmetry} & \text{(superconductors)} \\ -\ T & \text{(TRI superconductors)} \\ -\ T, Q & \text{(TRI insulators)} \end{array}\right\} \text{(mod 8) table}$$

- Symmetries are described by Clifford algebras
- Topological methods:
  - Vector bundles on the momentum space (works for translationally invariant systems)
  - Dirac operators (on spin manifolds)
  - K-homology (disordered system on any reasonable space, not necessarily a manifold)

Previous classification schemes

- Random matrix ensembles: the same 10 classes, but no dimension shift or periodicity.

- Recent results:

  Qi, Hughes, Zhang (2008) – Z_2 insulators

  Qi, Hughes, Raghu, Zhang (2008) – Z_2 superconductors:

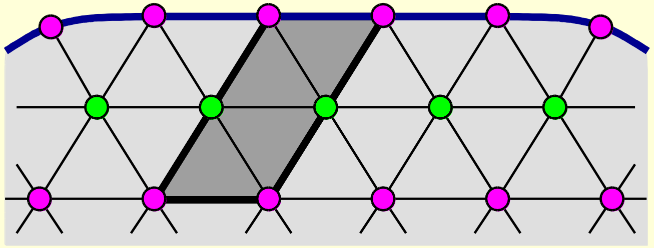
explicit dimension shift but no “grand unification”

Integer quantum Hall effect

Electromagnetic response: $j_\alpha = \sigma_{\alpha\beta} E_\beta, \quad \sigma_{xy} = \frac{e^2}{2\pi\hbar}\nu, \quad \sigma_{xx} = 0.$

$$S = \frac{\nu}{4\pi} \int \epsilon^{\mu\nu\lambda} A_\mu \, \partial_\nu A_\lambda \, d^3x$$

Tight-binding model:



$\pi/2$ flux per triangle

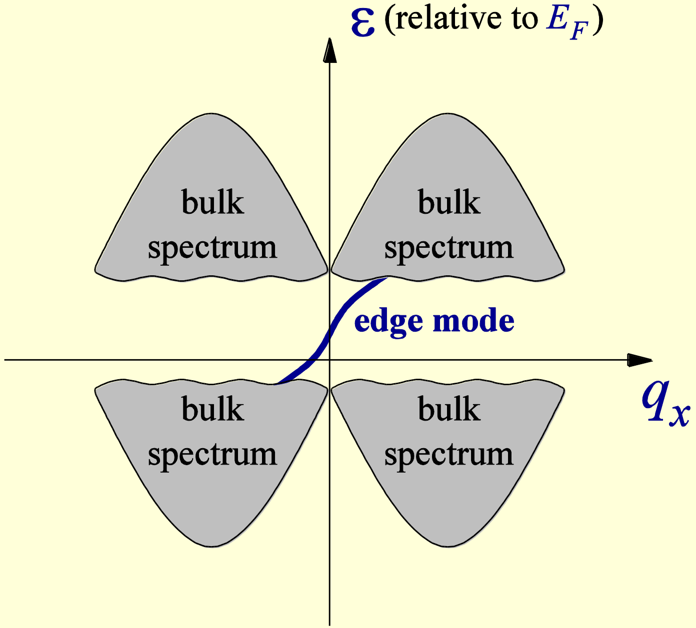
unit cell $= 4$ triangles

$$\widehat{H} = \sum_{j,k} B_{j,k} \, a_j^\dagger a_k$$

$$= \sum_{j,\alpha;k,\beta} B_{j,\alpha;k,\beta} \, a_{j,\alpha}^\dagger a_{k,\beta}$$

$$= \sum_{q;\alpha,\beta} B_{\alpha,\beta}(q) \, a_{q,\alpha}^\dagger a_{q,\beta}$$

Spectrum: $\varepsilon(q) = \text{eigenvalue}\Big(\underbrace{B(q)}_{2\times 2 \text{ matrix}} \Big)$



Topological invariant: Chern number

- Abstract notion:

Occupied states: $\mathcal{L}(q) \subseteq \mathbb{C}^2$ (eigenvectors corresponding to negative eigenvalues of $\widetilde{B}(q)$)

$$q \mapsto \mathcal{L}(q)$$

momentum space $\rightarrow$ complex Grassmanian C_0

- Calculation using spectrum flattening:

$$\widetilde{B}(q) = \operatorname{sgn}(B(q))$$ (same eigenvectors; eigenvalues $= \pm 1$)

Note that $\widetilde{B}(q) = 1 - 2P(q)$, where $P(q)$ is the projector onto the occupied electron states.

$$\nu = \frac{i}{16\pi} \int \mathrm{Tr}\left(\widetilde{B} \left(\frac{\partial \widetilde{B}}{\partial q_x} \frac{\partial \widetilde{B}}{\partial q_y} - \frac{\partial \widetilde{B}}{\partial q_y} \frac{\partial \widetilde{B}}{\partial q_x} \right) \right) dq_x\, dq_y.$$

(Thouless, Komoto, Nightingale, den Nijs, 1982)

Dealing with disorder: Real-space expression for the Chern number

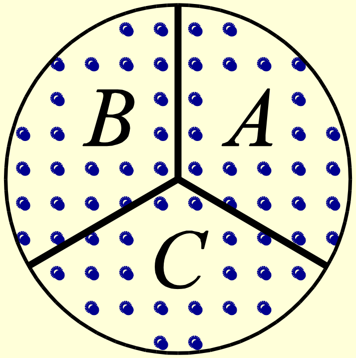
- If electrons are localized, the Hall conductivity is quantized (rigorous proof by Bellissard at al (1994))

- Let $\widehat{H} = \sum_{j,k} B_{jk} a_j^\dagger a_k$. A sufficient localization condition is this:

spatial dimension

$$\widetilde{B}_{jk} \le c\left|\vec{r}_j - \vec{r}_k\right|^{-(2+\varepsilon)}, \quad \text{where } \widetilde{B} = \operatorname{sgn} B. \qquad (\widetilde{B}^2 = 1,\ \widetilde{B}^\dagger = \widetilde{B})$$

- A quantized quantity (related to the Hall conductivity in the adiabatic approximation) may be defined as follows:

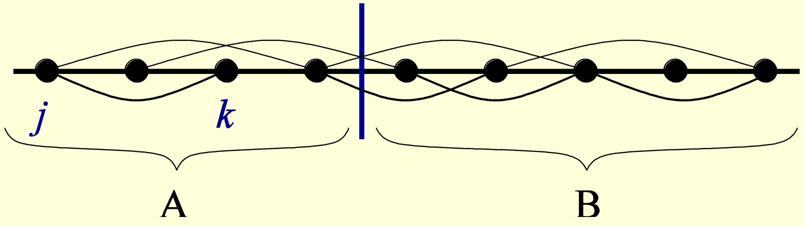


$$\nu = \sum_{j\in A} \sum_{k\in B} \sum_{l\in C} h_{jkl}, \qquad \text{where}$$

$$h_{jkl} = \frac{3\pi i}{4}\left(\widetilde{B}_{jk}\widetilde{B}_{kl}\widetilde{B}_{lj} - \widetilde{B}_{jl}\widetilde{B}_{lk}\widetilde{B}_{kj}\right).$$

One-dimensional analogue:

Matrix U on an infinite chain:



- U is unitary;
- U is quasidiagonal: $|U_{jk}| \leq c|j-k|^{-(1+\varepsilon)}$.

Definition: $f_{jk} = |U_{jk}|^2 - |U_{kj}|^2$ — "current" from j to k.

Theorem: The current is conserved: $\sum_k f_{jk} = 0$.

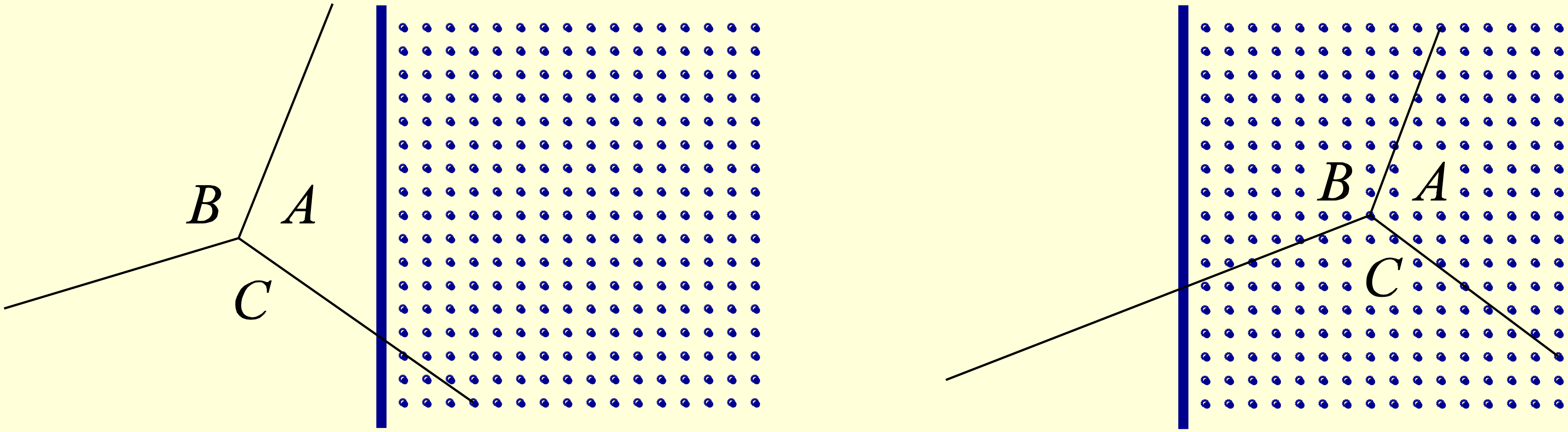
The total flow, $\mathcal{F} = \sum_{j \in A} \sum_{k \in B} f_{jk}$ is *constant* along the chain and has *integer* value.

Corollary: It is impossible to define a unitary quasidiagonal matrix on a *half-infitite* chain.

(The faliure of unitarity at the end of the chain is described by the difference of two projectors.)

Application to IQHE

- Similarly, the real-space Chern number is constant if the electrons are localized everywhere. Thus they must be **delocalized** at the edge.



$\nu = 0$

$\nu \neq 0$

- This is an abstract proof: It does not really tell what happens at the edge.

Generalization (leading to K-homology)

- Integer topological invariants can be defined for quasidiagonal matrices of two kinds:
  - *Unitary matrices* have a nontrivial topological invariant in *odd* dimensions.
  - *Hermitian matrices* $\widetilde{B}$ *such that* $\widetilde{B}^2 = 1$ have a nontrivial invariant in *even* dimensions. Such matrices describe **insulators without** T **symmetry**.

- That is a manifestation of the $(\mathrm{mod}\ 2)$ Bott periodicity.

- The faluire of the specified matrix properties at the boundary is characterized by an *even or odd Fredholm module.*

- Quasidiagonal matrices on a compact manifold or cell complex X may be classified by K-homology groups $K_1(X)$ or $K_0(X)$ (though less rigorously).

Summary of the classification

(where we are now)

- Symmetries are described by Clifford algebras
- Topological methods:
  - ✓ Vector bundles on the momentum space (works for translationally invariant systems)
  - – **Dirac operators**
  - ✓ K-homology (disordered system on any reasonable space, not necessarily a manifold)

Majorana chain

(No symmetry at all: spin-polarized superconductor)

$$\widehat{H} = \frac{i}{4}\sum_{j,k} A_{jk} c_j c_k$$

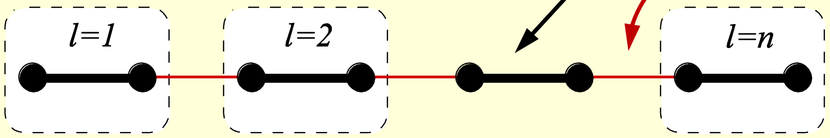
real skew-symmetric matrix

Majorana operators:

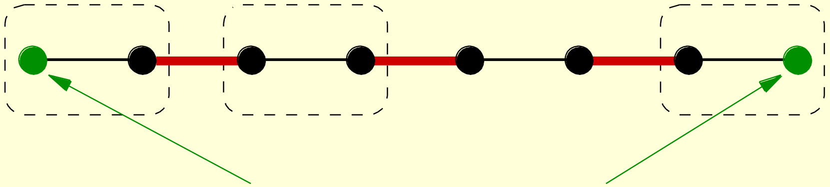
$$c_{2l-1} = a_l + a_l^\dagger, \quad c_{2l} = \frac{1}{i}(a_l - a_l^\dagger)$$

$$c_j c_k + c_k c_j = 2\delta_{jk}$$

For example, $H = \frac{i}{2}\left(u \sum_{l=1}^{n} c_{2l-1} c_{2l} + v \sum_{l=1}^{n-1} c_{2l} c_{2l+1} \right)$



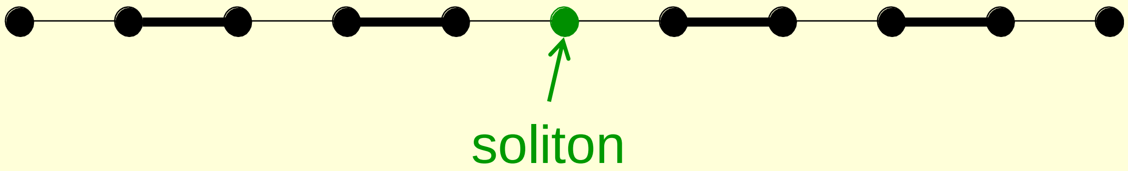
$u > v$



$u < v$: The ground state is 2-fold degenerate: $\Delta E \sim e^{-n/\xi}$.

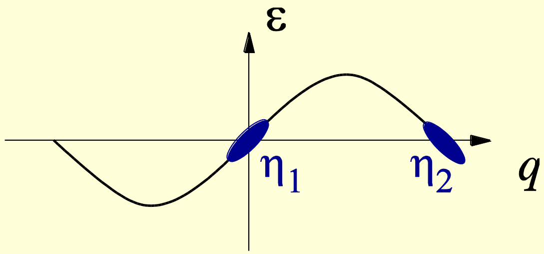
upaired Majorana modes

Soliton and a Dirac operator

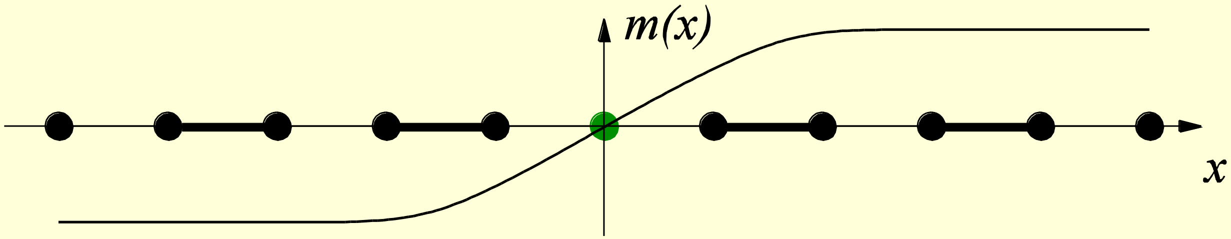


- Consider the case $u = v$ (gapless system)

- Take the continuum limit (fields η_1, η_2)



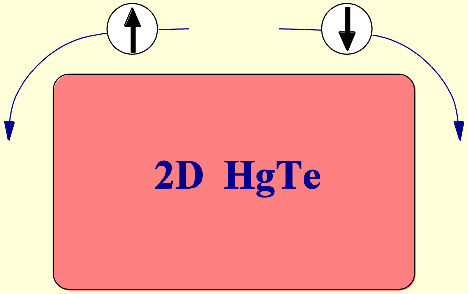
- Introduce a mass term, $m(x) \sim u - v$



$$\widehat{H} = \frac{i}{2} \int \eta^T \begin{pmatrix} \partial & m \\ -m & -\partial \end{pmatrix} \eta \, dx, \qquad \eta = \begin{pmatrix} \eta_1(x) \\ \eta_2(x) \end{pmatrix}$$

$m(x)$ changes sign ⇒ **zero mode** (by the index theorem)

A more realistic example



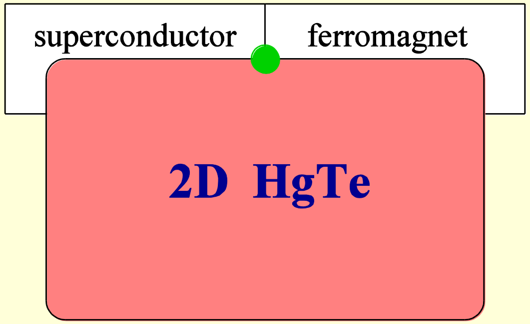
$$\widehat{H} = \int \Big(i(\psi_\uparrow^\dagger \partial \psi_\uparrow - \psi_\downarrow^\dagger \partial \psi_\downarrow) + h_x(\psi_\uparrow^\dagger \psi_\downarrow + \psi_\downarrow^\dagger \psi_\uparrow) + \Delta(\psi_\uparrow^\dagger \psi_\downarrow^\dagger + \psi_\downarrow \psi_\uparrow) \Big)\, dx$$

$$= \frac{i}{2} \int \eta^T \left(\Gamma \partial + M(x)\right) \eta \, dx, \qquad \text{where} \quad \eta = \begin{pmatrix} \psi_\uparrow + \psi_\uparrow^\dagger \\ -i(\psi_\uparrow - \psi_\uparrow^\dagger) \\ \psi_\downarrow + \psi_\downarrow^\dagger \\ -i(\psi_\downarrow - \psi_\downarrow^\dagger) \end{pmatrix}.$$

$$\Gamma = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \qquad M = \begin{pmatrix} 0 & 0 & 0 & h_x - \Delta \\ 0 & 0 & -h_x - \Delta & \\ 0 & h_x + \Delta & 0 & 0 \\ -h_x + \Delta & 0 & 0 & 0 \end{pmatrix}$$

$\mathrm{Pf}(M(x)) = \Delta^2 - h_x^2$ changes sign

$\Rightarrow$ **zero mode**



Symmetries

Charge operator: $\widehat{Q} = \sum_l (a_l^\dagger a_l - \frac{1}{2}) = \frac{i}{2} \sum_l c_l' c_l'' = \frac{i}{4} \sum_{j,k} Q_{jk} c_j c_k$

$$\boxed{\begin{aligned} c_l' &= a_l + a_l^\dagger \\ c_l'' &= \tfrac{1}{i}(a_l - a_l^\dagger) \end{aligned}}$$

$$Q = \begin{pmatrix} 0 & 1 & & & \\ -1 & 0 & & & \\ & & 0 & 1 & \\ & & -1 & 0 & \\ & & & & \ddots \end{pmatrix}$$

Time-reversal operator (defined implicitly: $T(x) = \widehat{T} X \widehat{T}^{-1}$)

$$\begin{aligned} T(i) &= -i \\ T(a_\uparrow) &= a_\downarrow \\ T(a_\downarrow) &= -a_\uparrow \\ T(a_\uparrow^\dagger) &= a_\downarrow^\dagger \\ T(a_\downarrow^\dagger) &= -a_\uparrow^\dagger \end{aligned}$$

$$T(c_k) = \sum_j T_{jk} c_j$$

real skew-symmetric matrix

Properties of the matrices Q and T

- Q, T are real skew-symmetric matrices
- $Q^2 = T^2 = -1, \quad QT = -TQ$
- Let $\widehat{H} = \frac{i}{4}\sum_{j.k} A_{jk} c_j c_k$.
  - If $\widehat{H}$ is Q-invariant, then $QA = AQ$;
  - If $\widehat{H}$ is T-invariant, then $TA = -AT$.

Q and T generate a *Clifford algebra*

- Let $e_1 = T, \quad e_2 = QT$, and let $\widetilde{A} = -i\,\mathrm{sgn}(iA)$.

No symmetry:	$\widetilde{A}^2 = -1$
T only:	$e_1^2 = \widetilde{A}^2 = -1, \quad e_1\widetilde{A} = -\widetilde{A}e_1$
T and Q:	$e_1^2 = e_2^2 = \widetilde{A}^2 = -1,$ $e_1e_2 = -e_2e_1,$ $e_j\widetilde{A} = -\widetilde{A}e_j \ \ (j = 1, 2)$

e_1, e_2 generate a Clifford algebra, and $\widetilde{A}$ *extends* it.

Extension type $\mathrm{Cliff}^{0,q} \setminus \mathrm{Cliff}^{0,q+1}$ $(q = 0, 1, 2)$

Clifford algebras (with real coefficients)

$\mathrm{Ciff}^{p,q}$: Generators: $e_1, \ldots, e_{p+q}$

$$e_1^2 = \cdots = e_p^2 = 1, \quad e_{p+1}^2 = \cdots = e_{p+q}^2 = -1,$$
$$e_j e_k = -e_k e_j \quad (\text{for } j \neq k)$$

Examples:

- $\mathrm{Ciff}^{1,0} \cong \mathbb{R} \oplus \mathbb{R} \quad = \left\{ x\frac{1+e_1}{2} + y\frac{1-e_2}{2} \;:\; x, y \in \mathbb{R} \right\}$
- $\mathrm{Ciff}^{1,0} \cong \mathbb{C} \quad (e_1^2 = -1 \;;\; e_1$ is like $i)$
- $\mathrm{Ciff}^{2,0} \cong \mathbb{R}(2) \quad$ (the algebra of 2×2 real matrices, $e_1 = \sigma^z,\; e_2 = \sigma^x$)
- $\mathrm{Ciff}^{1,1} \cong \mathbb{R}(2) \quad (e_1 = \sigma^z,\; e_2 = i\sigma^y)$
- $\mathrm{Ciff}^{0,2} \cong \mathbb{H} \quad$ (the algebra of quaternions)

Periodicity:

- $\mathrm{Ciff}^{p+1,q+1} \cong \mathrm{Ciff}^{p,q} \otimes \mathbb{R}(2) \sim \mathrm{Ciff}^{p,q}$

Morita equivalence

- $\mathrm{Ciff}^{p+8,q} \cong \mathrm{Ciff}^{p,q} \otimes \mathbb{R}(16) \sim \mathrm{Ciff}^{p,q}$

Classification by symmetry

Technicality: Relacing negative Clifford generators with positive:

$$\underline{\mathrm{Ciff}^{q+2,0}} \cong \mathrm{Ciff}^{0,q} \otimes \mathbb{R}(2) \sim \underline{\mathrm{Ciff}^{0,q}}$$

Morita equivalence

$$\boxed{\begin{array}{l} \mathrm{Ciff}^{0,q} \setminus \mathrm{Ciff}^{0,q+1} \\ \sim \mathrm{Ciff}^{q+2,0} \setminus \mathrm{Ciff}^{q+3,0} \end{array}}$$

$p = q + 2$	q	Symmetries	Parameter space R_p
1	-1	Unusual T ($T^2 = 1$)	$O(n)$
2	0	None	$O(2n)/U(n)$
3	1	Standard T ($T^2 = -1$)	$U(2n)/Sp(n)$
4	2	T and Q	$Sp(k+2n)/(Sp(k+n) \times Sp(n))$

- That is, essentially, the classification in dimension $d = 0$.

Dimension shift

- Hamiltonian:

$$\widehat{H} = \frac{i}{2}\int \eta^T\left(\Gamma^\alpha \partial_\alpha + M\right)\eta\, d^d x.$$

real symmetric real skew-symmetric

$$e_j\Gamma^\alpha = -\Gamma^\alpha e_j, \qquad e_j M = -M e_j$$

- Physical requirement:

The spectrum $\varepsilon(\vec{q}) = \text{eigenvalues}\big(-\Gamma^\alpha q_\alpha + M\big)$ is gapped.

- Sufficient condition (equivalent for classificalion purposes):

$$(\Gamma^\alpha)^2 = 1, \qquad M^2 = -1, \qquad \Gamma^\alpha M = -M\Gamma^\alpha.$$

- The symmetry operators $e_j \in \mathrm{Ciff}^{0,q}$ are fixed. Let us also fix Γ^α. For M, we get the Clifford extension problem

$$\mathrm{Ciff}^{d,q} \setminus \mathrm{Ciff}^{d,q+1} \sim \mathrm{Ciff}^{p-d,0} \setminus \mathrm{Ciff}^{p-d+1,0}, \quad \text{where } p = q+2.$$

$$\boxed{p \mapsto p-d}$$

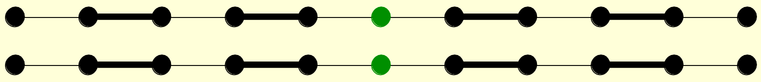
Interactions

- Free fermion phases: $F(\overset{\text{symmetry}}{G}, \overset{\text{dimension}}{d})$ (the present classification)
- Interacting fermion phases: $I(G, d)$ (future classification)
- "Free" is a special case of "interacting":

$$\zeta : F(G, d) \to I(G, d).$$

  - *Is* ζ *surjective?* **No,** there are interacting phases that have no free analogue (e.g. FQHE).
  - *Is* ζ *injective?* A counterexample would be two distinct free phases, X and Y, that can be continuously connected through an interacting phase. **Such an example exists!**
- Nevertheless, in some symmetry settings the free classification is stable, eg. $G = U(1)$, $d = 2$ (IQHE).

The counterexample



Majorana chains: $c_{j,\alpha}$

site number

chain

$$T(c_{j,\alpha}) = (-1)^j c_{j,\alpha}, \qquad \text{(unusual: } T^2 = 1\text{)}$$

- This symmetry prohibits terms like $ic_{j,\alpha}c_{k,\beta}$, where j and k have the same parity. Therefore unpaired modes on parallel chains do not cancel.

- The noniteracting classification predicts an integer invariant (i.e., $F = \mathbb{Z}$).

$$\nu = (\#\text{ of solitons at even } j) - (\#\text{ of solitons at odd } j)$$

- Yet 8 solitons can cancel each other, and the corresponding dimer phases on 8 parallel chains can be continuously connected through an interacting phase! ($I = \mathbb{Z}_8$)

Summary

- Topological phases of noninteracting fermions can be classified using K-theory.
- Most natural symmetries are captured by complex and real Clifford algebras ($2+8$ universality classes).
- Dimension change is described by periodic shift $\pmod 2$ or $\pmod 8$ — Bott periodicity.
- The basic description uses Dirac operators, while a more general theory involves analytic K-homology.
- In some cases (IQHE, Majorana chains, $p_x + ip_y$, TRI insulators in 2d and 3d) the classification is stable to strong interactions.
- That is not true in general; a counterexample is known.