Dynamical Mean-Field Theory for Correlated Topological Phases

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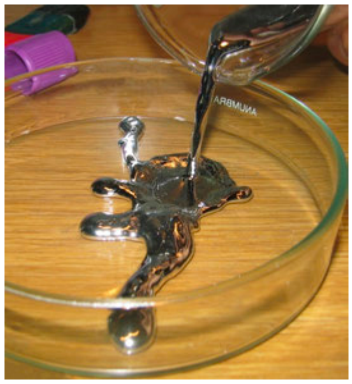
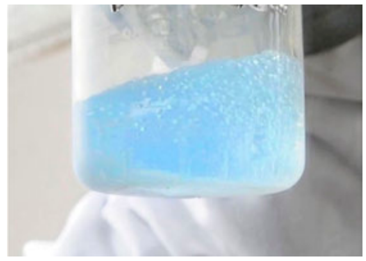
$$A \cong B \quad ?$$

matter





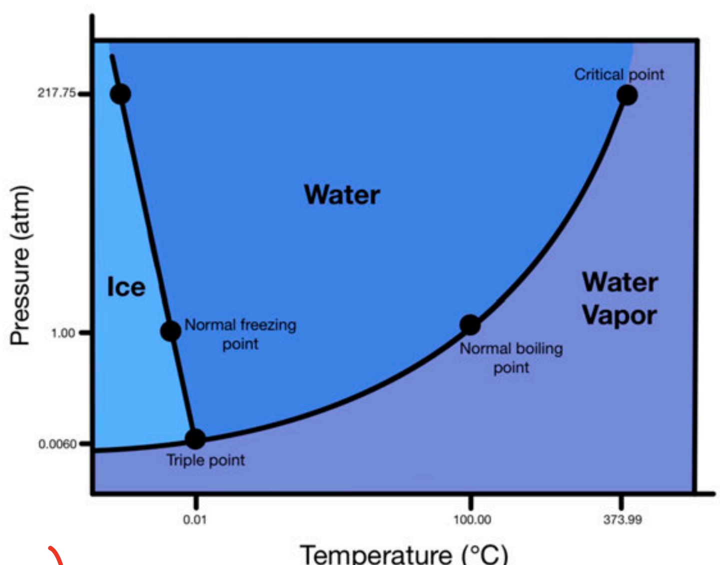
and a way of classification

Group / Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57-71	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89-103	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Periodic Table Key

X Synthetic Elements	X Liquids or melt at close to room temp.	X Solids	X Gases	Alkali Metals	Alkali Earth Metals	Transition Metals	Other Metals	Metalloids	Other Non Metals	Halogens	Noble Gases	Lanthanides & Actinides



another way of classification
(symmetry and symmetry breaking)

many-body models

$$H = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + J \sum_i \vec{s}_i \cdot \vec{S}_i$$

$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} - |g_{\text{eff}}|^2 \sum_{k,k'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$H = \sum_{ij,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$H = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

$$\mathcal{L} = \frac{1}{2} \partial_\mu \hat{n} \cdot \partial^\mu \hat{n}, \quad \hat{n}^2 = 1$$

$$H = \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$H = \sum_k c^\dagger_k \left[\left(m + t \sum_{r=1}^{D} \cos k_r \right) \gamma_D^{(0)} + t \sum_{r=1}^{D} \sin k_r \, \gamma_D^{(r)} \right] c_k$$

classification ?

Classification, mathematically

objects A, B

is A essentially the same as B ?

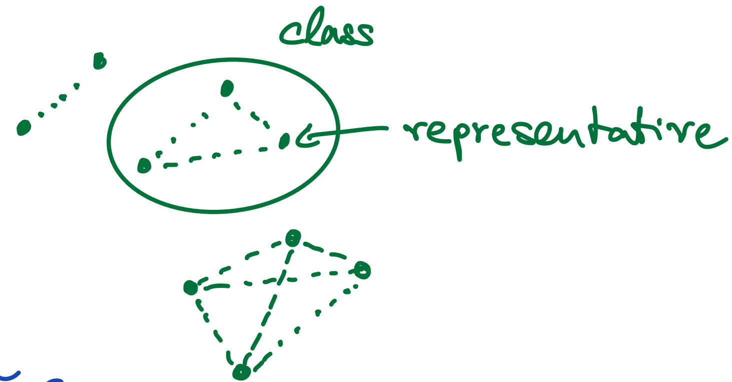
$A \cong B$?

equivalence relation

$A \cong A$

$A \cong B \Rightarrow B \cong A$

$A \cong B, \ B \cong C \Rightarrow A \cong C$



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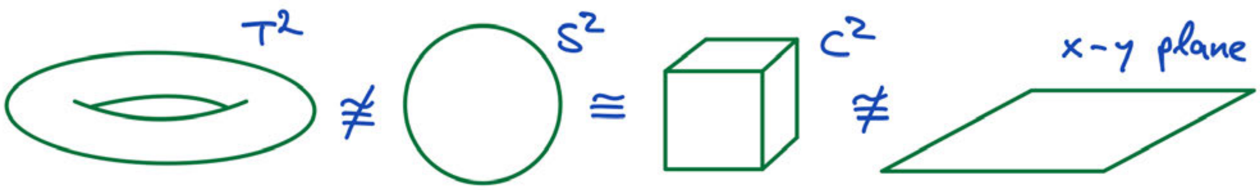
continuity: a powerful equivalence relation in the context of condensed-matter physics

Example from mathematics

$A \cong B$: A can continuously and reversibly be deformed into B

→ topology

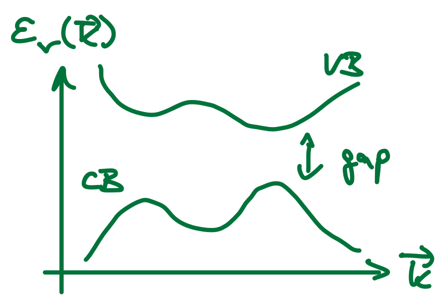


topological invariants:

- preserved under homeomorphisms
  (continuous maps with a continuous inverse)
- here: number of holes
  $\Rightarrow \; S^2 \ncong T^2$
- but: $C^2 \ncong$ x-y plane ?!

Condensed-matter theory

- can we topologically classify band structures?
- the problem is solved for band insulators
  (gapped electronic structure, no correlations)
- can we topologically classify the electronic structure of correlated materials?
- can we topologically classify many-body models?
  unsolved!



the "ten-fold way":

this lecture (part I)

Cartan \ d	0	1	2	3	4	5	6	7	8	
Complex case:										
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
Real case:										
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\cdots$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\cdots$
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\cdots$
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\cdots$
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	$\cdots$
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\cdots$
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\cdots$
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	$\cdots$

nice review:

A. Ludwig, Phys. Scr. T 168, 014001 (2016)

add correlations

this lecture (part II)

Cartan \ d	0	1	2	3	4	5	6	7	8	
Complex case:										
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
Real case:										
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\cdots$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\cdots$
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\cdots$
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\cdots$
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	$\cdots$
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\cdots$
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\cdots$
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	$\cdots$

$d \to \infty$?

see :
- David Krüger & M.P., PRL 126, 196401 (2021)
- poster by David

Plan (for part I)

adiabatic theorem $\longrightarrow$ Berry connection

time dependence of gapped quantum systems

$\downarrow$

gauge transformations

$\downarrow$

Berry phase

toy model: $H = -\frac{1}{2}\vec{R}\,\vec{\sigma}$

topological properties of gapped quantum systems

$\downarrow$

Berry curvature

$\downarrow$

topological invariant $\longleftarrow$ Chern number $\longrightarrow$ Chern insulator

Adiabatic theorem

- parameter-dependent Hamiltonian

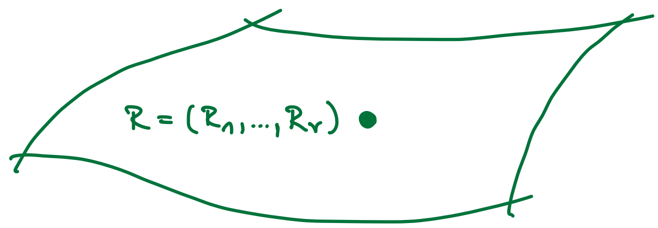
$$H = H(\boldsymbol{R}) = H(R_1, ..., R_r)$$

orthonormal basis at every R:

$$H(\boldsymbol{R})|\Phi_j(\boldsymbol{R})\rangle = E_j(\boldsymbol{R})|\Phi_j(\boldsymbol{R})\rangle$$

ground state $|\Phi_0(R)\rangle$

$\mathcal{M}$: r-dimensional parameter manifold



- we assume:

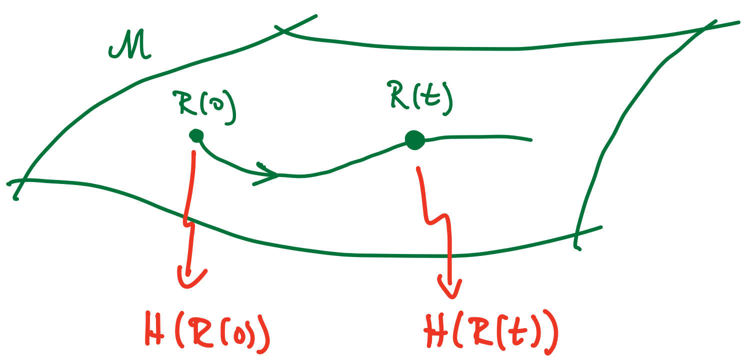
H(R) is gapped on $\mathcal{M}$

$E_0(R) < E_1(R) \quad \forall R$

$E_0(R)$ non-degenerate

gap $\Delta(R) \equiv E_1(R) - E_0(R) > 0$

- let $R = R(t)$ be time-dependent



- given $|\psi(0)\rangle$, what is $|\psi(t)\rangle$?

- $i\partial_t |\Psi(t)\rangle = H(R(t))\,|\Psi(t)\rangle$ (Schrödinger eqn.)

  $|\Psi(0)\rangle = |\Phi_0(R(0))\rangle$ (initial condition)

  formal solution:

  $$|\Psi(t)\rangle = \mathcal{T} \exp\left(-i\int_0^t d\tau \; H(R(\tau))\right) \cdot |\Psi(0)\rangle$$

Theorem: (adiabatic theorem)

If the time evolution of the parameters $R(t)$ is sufficiently slow ($\tau_{typical} \gg 1/\Delta$), then:

$$|\Psi(t)\rangle \propto |\Phi_0(\boldsymbol{R}(t))\rangle$$

i.e.:

$$\boxed{|\Psi(t)\rangle = e^{-i\gamma(t)} |\Phi_0(\boldsymbol{R}(t))\rangle} \qquad (*)$$

- $\gamma(t) = ?$

  idea: insert $(*)$ into Schrödinger's eqn.:

l.h.s.: $i\partial_t |\Psi(t)\rangle = i\partial_t \left(e^{-i\gamma(t)} |\Phi_0(R(t))\rangle \right)$

$$= i(-i)\,\dot{\gamma}(t)\, e^{-i\gamma(t)} |\Phi_0(R(t))\rangle + i\, e^{-i\gamma(t)} \frac{\partial}{\partial R} |\Phi_0(R(t))\rangle \cdot \dot{R}(t)$$

r.h.s.: $H(R(t))\,|\Psi(t)\rangle$

$$= H(R(t)) \left(e^{-i\gamma(t)} |\Phi_0(R(t))\rangle \right)$$

$$= e^{-i\gamma(t)} E_0(R(t)) \, |\Phi_0(R(t))\rangle$$

$\Longrightarrow$

$$\dot{\gamma}(t) \, |\Phi_0(R(t))\rangle + i \frac{\partial}{\partial R} |\Phi_0(R(t))\rangle \cdot \dot{R}(t) = E_0(R(t)) \, |\Phi_0(R(t))\rangle$$

multiply with $\langle \Phi_0(R(t))|$, this yields:

$$\dot{\gamma}(t) + A_0(R) \cdot \dot{R}(t) = E_0(R(t))$$

with

$$\boldsymbol{A}_0(\boldsymbol{R}) = i\langle \Phi_0(\boldsymbol{R})| \frac{\partial}{\partial \boldsymbol{R}} |\Phi_0(\boldsymbol{R})\rangle$$

(Berry connection)

integrate:

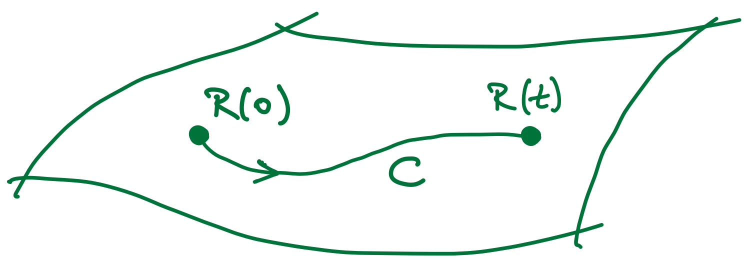
$$\gamma(t) = \gamma(0) + \int_0^t E_0(\boldsymbol{R}(\tau))d\tau - \int_0^t \boldsymbol{A}_0(\boldsymbol{R}(\tau))\dot{\boldsymbol{R}}(\tau)d\tau$$

insert into (*): (and choose $\gamma(0) = 0$)

$$|\Psi(t)\rangle = \exp\left(-i \int_0^t E_0(\boldsymbol{R}(\tau))d\tau\right) \exp\left(i \int_{\mathcal{C},\boldsymbol{R}(0)}^{\boldsymbol{R}(t)} \boldsymbol{A}_0(\boldsymbol{R})d\boldsymbol{R}\right) |\Phi_0(\boldsymbol{R}(t))\rangle$$

"dynamical" phase factor (depends on $R = R(\tau)$)

"geometrical" phase factor (depends on C only)



Gauge transformations

properties of the Berry connection

$$\boldsymbol{A}_0(\boldsymbol{R}) = i\langle\Phi_0(\boldsymbol{R})|\frac{\partial}{\partial\boldsymbol{R}}|\Phi_0(\boldsymbol{R})\rangle$$

- it is time-independent
- it is a property of the ground state, actually of the

  bundle of ground states ← possibly "twisted"?

  $|\Phi_0(R)\rangle$, $R \in \mathcal{M}$?
- is it an observable?

the choice of the phase of $|\Phi_0(R)\rangle$ is arbitrary!

what happens under a gauge transformation?

$$\boxed{|\Phi_0(\boldsymbol{R})\rangle \mapsto e^{i\varphi(\boldsymbol{R})}|\Phi_0(\boldsymbol{R})\rangle}$$

let's compute

$$A_0(R) = i\langle\Phi_0(R)|\frac{\partial}{\partial R}|\Phi_0(R)\rangle$$

$$\mapsto i\, \underbrace{e^{-i\varphi(R)}\langle\Phi_0(R)|}\, \frac{\partial}{\partial R}\left(\underbrace{e^{i\varphi(R)}|\Phi_0(R)\rangle}\right)$$

$\Rightarrow$

$$\boxed{\boldsymbol{A}_0(\boldsymbol{R}) \mapsto \boldsymbol{A}'_0(\boldsymbol{R}) = \boldsymbol{A}_0(\boldsymbol{R}) - \frac{\partial\varphi(\boldsymbol{R})}{\partial\boldsymbol{R}}}$$

the Berry connection depends on the arbitrary choice of $\varphi(R)$!

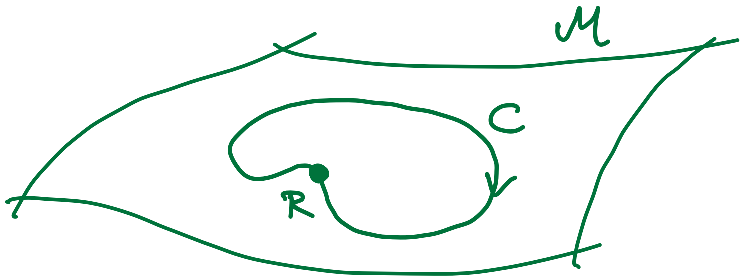
→ $A_0(R)$ is gauge dependent!

→ $\int_C A_0(R)\, dR$ or $e^{i\int_C A_0(R)\, dR}$ is no observable!

M. Berry (1984)

$$\boxed{\gamma_C := \oint_C A_0(R)\, dR}$$

Berry phase



C : <u>closed</u> path in $\mathcal{M}$

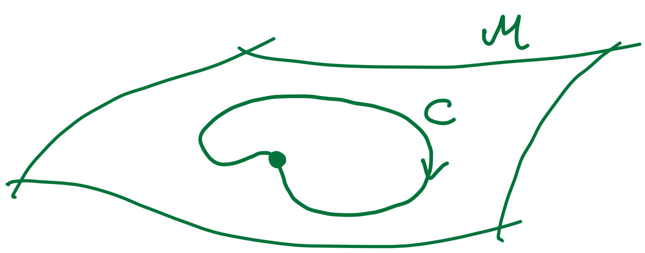
How does γ_C behave under a gauge transformation?

compute:

$$\gamma_C = \oint_C A_0(R)\, dR \longmapsto \oint_C A_0'(R)\, dR$$

$$= \oint_C \left(A_0(R) - \frac{\partial \chi(R)}{\partial R} \right) dR$$

$$= \gamma_C - \underbrace{\oint_C \frac{\partial \chi(R)}{\partial R}\, dR}_{d\chi} \overset{?}{=} \gamma_C \quad \text{gauge invariant?}$$



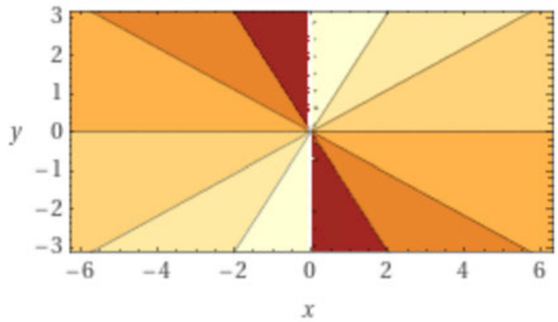
$\gamma_C \mapsto \gamma_C$,

if $\partial\chi/\partial R$ is continuous on $\mathcal{M}$, and if $\mathcal{M}$ is simply connected (loops can be contracted to zero)

Example:

gauge transformation:

$$\boxed{\chi(\vec{R}) = \arctan\left(Y/X\right)}$$



(discontinuous on the $X = 0$ plane)

we have:

$$\frac{\partial \chi(\vec{R})}{\partial \vec{R}} = \frac{1}{X^2+Y^2} \cdot \begin{pmatrix} -Y \\ X \\ 0 \end{pmatrix}$$

(singular on the Z axis)

under this gauge transformation

$$\vec{A}_0(\vec{R}) \longmapsto \vec{A}_0'(\vec{R}) = \vec{A}_0(\vec{R}) - \frac{1}{X^2+Y^2} \cdot \begin{pmatrix} -Y \\ X \\ 0 \end{pmatrix}$$

and in fact, for the circle of radius R around the origin in X–Y plane

$$C = \left\{ \vec{R} = \begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = R \begin{pmatrix} \cos\lambda \\ \sin\lambda \\ 0 \end{pmatrix} \;,\; \lambda = 0, \dots, 2\pi \right\}$$

we get

$$\oint_C \frac{1}{X^2+Y^2} \cdot \begin{pmatrix} -Y \\ X \\ 0 \end{pmatrix} d\vec{R} = \int_0^{2\pi} \frac{1}{R^2} \underbrace{\begin{pmatrix} -R\sin\lambda \\ R\cos\lambda \\ 0 \end{pmatrix} \begin{pmatrix} -R\sin\lambda \\ R\cos\lambda \\ 0 \end{pmatrix}}_{R^2} d\lambda$$

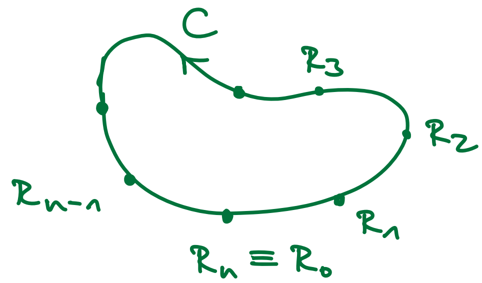
$$= \int_0^{2\pi} \frac{1}{R^2} \cdot R^2 \, d\lambda = 2\pi \neq 0$$

Theorem:

$$\gamma_C = \oint_C A_0(R)\, dR \xmapsto{\text{gauge trsf.}} \gamma_C + 2\pi k \,, \quad k \in \mathbb{Z}$$

Berry phase factor $e^{i\gamma_C}$ is gauge invariant

"Proof":



$$e^{i\gamma_C} = \exp\left(i \oint_C A_0(R)\, dR \right)$$

$$= \lim_{n\to\infty} \exp\left(i A_0(R_n)\,\Delta R_n + \dots + i A_0(R_1)\,\Delta R_1 \right)$$

$\leftarrow$ Riemann sum

$$= \lim_{n\to\infty} \exp\left(i A_0(R_n)\,\Delta R_n \right) \cdots \exp\left(i A_0(R_1)\,\Delta R_1 \right)$$

$$= \lim_{n\to\infty} \left[\left(1 + i A_0(R_n)\,\Delta R_n\right) \cdot \dots \cdot \left(1 + i A_0(R_1)\,\Delta R_1\right) \right]$$

(Volterra product integral)

k-th factor:

$$1 + i A_0(R_k)\,\Delta R_k = 1 + i \cdot i \left\langle \Phi_0(R_k) \middle| \frac{\partial}{\partial \vec{R}} \middle| \Phi_0(R_k) \right\rangle \cdot \Delta R_k$$

$$\overset{(n\to\infty)}{=} 1 - \langle \Phi_0(R_k) | \Big(|\Phi_0(R_k)\rangle - |\Phi_0(R_k - \Delta R_k)\rangle \Big)$$

$$= \langle \Phi_0(R_k) | \Phi_0(R_k - \Delta R_k) \rangle$$

$$= \langle \Phi_0(R_k) | \Phi_0(R_{k-1}) \rangle$$

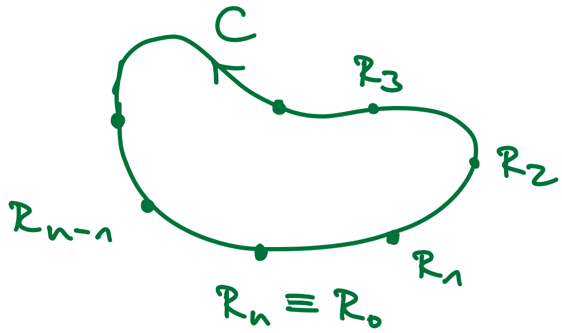
insert:

C closed ($R_n \equiv R_0$)

$$e^{i\gamma_C} = \lim_{n\to\infty} \left[\langle \Phi_0(R_n) | \Phi_0(R_{n-1}) \rangle \cdots \langle \Phi_0(R_1) | \Phi_0(R_0) \rangle \right]$$

$$= \lim_{n\to\infty} \operatorname{tr} \left[|\Phi_0(R_n)\rangle\langle\Phi_0(R_n)| \cdots |\Phi_0(R_1)\rangle\langle\Phi(R_1)| \right]$$

manifestly gauge invariant!



Toy model

$$H = -\frac{1}{2} \boldsymbol{R} \boldsymbol{\tau}$$

$\vec{R} \in \mathcal{M} = \mathbb{R}^3 \setminus \{0\}$

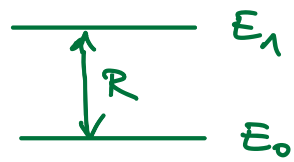
$\begin{pmatrix} \tau_x \\ \tau_y \\ \tau_z \end{pmatrix}$ Pauli matrices

note: <u>any</u> Hamiltonian in a 2-dimensional Hilbert space is a linear combination of the τ's (aside from a trivial offset $\sim \mathbb{1}$)

we can solve the problem:

$E_0(\vec{R}) = -\frac{1}{2} R$

$E_1(\vec{R}) = +\frac{1}{2} R$

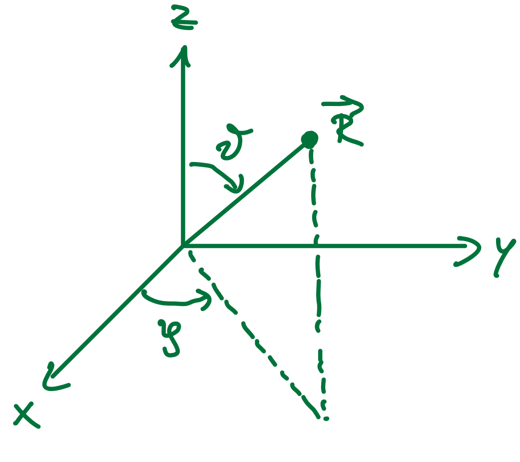


(Zeeman splitting)

$\vec{R}$-dependent ground state:

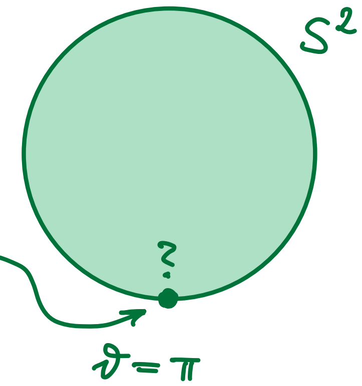
$$\boxed{|\Phi_0(\vec{R})\rangle = |\Phi_0(\vartheta, \varphi)\rangle = \begin{pmatrix} \cos \vartheta/2 \\ e^{i\varphi} \sin \vartheta/2 \end{pmatrix}}$$

$$\vec{R} = R \begin{pmatrix} \cos\varphi \, \sin\vartheta \\ \sin\varphi \, \sin\vartheta \\ \cos\vartheta \end{pmatrix}$$



- there is a problem at the south pole:

$$|\Phi_0(\vec{R})\rangle = \begin{pmatrix} \cos\vartheta/2 \\ e^{i\varphi}\sin\vartheta/2 \end{pmatrix} \in S^2$$



there is a problem here

$(\vartheta,\varphi) \mapsto \vec{R} \mapsto |\Phi_0\rangle$

is discontinuous!

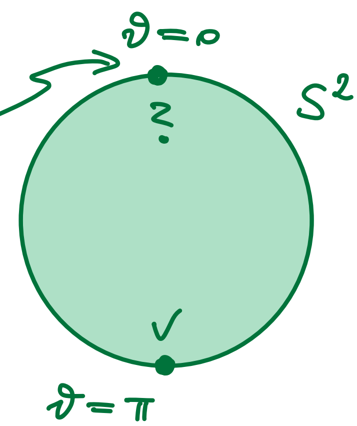
- the problem at the south pole can be fixed:

by a gauge transformation

$$|\Phi_0(\vec{R})\rangle \mapsto e^{-i\varphi}|\Phi_0(\vec{R})\rangle$$

in the new gauge:

$$|\Phi_0'(\vec{R})\rangle = \begin{pmatrix} e^{-i\varphi}\cos\vartheta/2 \\ \sin\vartheta/2 \end{pmatrix} \in S^2$$



now we have a problem here!

but then pops up at the north pole!

note:

the gauge transformation itself,

$$\varphi(\vec{R}) = \varphi(X,Y,Z) = \varphi = \arctan(Y/X),$$

and

$$|\Phi_0(\vec{R})\rangle \mapsto e^{-i\arctan(Y/X)}\cdot|\Phi_0(\vec{R})\rangle$$

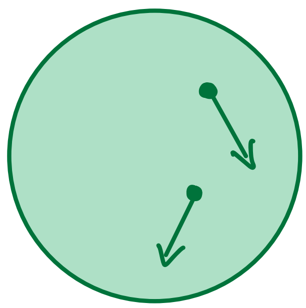
are discontinuous on the $X=0$ plane

- the "problem" is persistent – it is a topological feature!

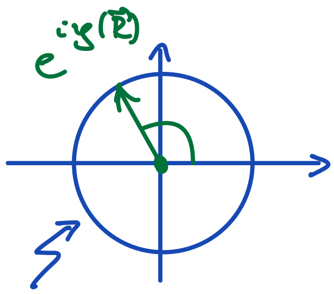
choosing a gauge means to attach a phase factor

$$e^{i\gamma(\vec{R})} \in U(1) \cong S^1$$

to each point on S^2:



← this is a hairy ball!

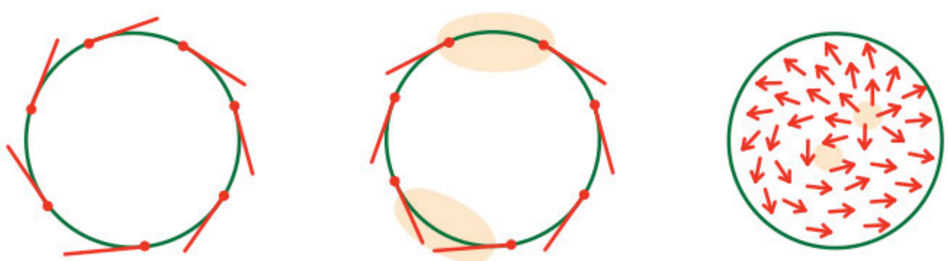


unit circle

the arrow direction specifies $e^{i\gamma(\vec{R})}$

Theorem (the hairy-ball theorem)

There is no everywhere non-vanishing and continuous tangent vector field on an n-sphere, if n is even.



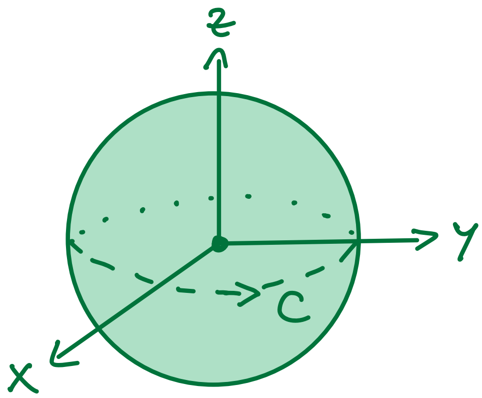
S^1: ✓ $\quad$ S^1 with two twirls $\quad$ S^2 with (already) two twirls

$\Rightarrow$ on S^2 there is no globally smooth gauge!

- the feature shows up in the Berry phase as well

$$\gamma_c = \oint_C \vec{A}_0(\vec{R})\, d\vec{R} = ?$$

C = equator



$$\vec{A}_0(\vec{R}) = i \langle \Phi_0(\vec{R}) | \frac{\partial}{\partial \vec{R}} | \Phi_0(\vec{R}) \rangle$$

continuous along the equator
(in any of the above two gauges)

its φ-component:

$$\vec{A}_0(\vartheta,\varphi) \cdot R\vec{e}_\varphi = i \langle \Phi_0(\vartheta,\varphi) | \frac{\partial}{\partial \varphi} | \Phi_0(\vartheta,\varphi) \rangle = -\frac{1}{2}$$

$$|\Phi_0(\vec{R})\rangle = |\Phi_0(\vartheta,\varphi)\rangle = \begin{pmatrix} \cos\vartheta/2 \\ e^{i\varphi} \sin\vartheta/2 \end{pmatrix}$$

(first gauge)

$$\frac{\partial}{\partial \vec{R}} = \vec{e}_\varphi \frac{1}{R\sin\vartheta} \frac{\partial}{\partial\varphi} + \vec{e}_\vartheta (\cdots) + \vec{e}_R (\cdots)$$

$\vartheta = \pi/2$, $\sin\vartheta = 1$

$$\gamma_c = \oint_C \vec{A}_0(\vec{R})\, d\vec{R} = \int_0^{2\pi} \underbrace{\vec{A}_0(\vec{R}) \cdot R\vec{e}_\varphi}_{-1/2}\, d\varphi = -\pi$$

in the second gauge:

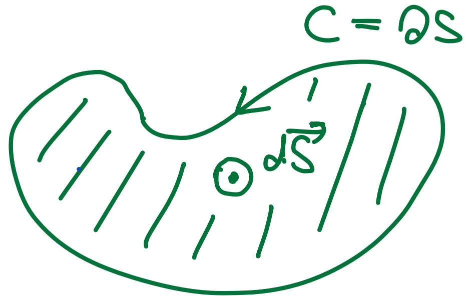
$$\gamma_c' = \oint_C \vec{A}_0'(\vec{R})\, d\vec{R} = +\pi$$

note: $e^{i\gamma_c}$ is gauge invariant!

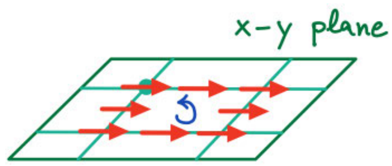
Berry curvature

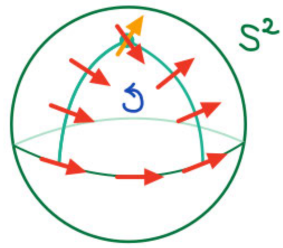
$$\gamma_C = \oint_C \vec{A}_0(\vec{R})\, d\vec{R} \overset{\text{Stokes theorem}}{=} \int_S \vec{\Omega}_0(\vec{R})\, d\vec{S}$$

Berry phase — Berry connection — Berry curvature



Berry phase $\downarrow$ to what degree does parallel transport fail to preserve geometrical data? $\longrightarrow$ failure requires a finite (Berry) curvature





definition:

$$\boxed{\vec{\Omega}_0(\vec{R}) = \partial_{\vec{R}} \times \vec{A}_0(\vec{R})}$$

- the Berry curvature is gauge invariant!

$$\vec{\Omega}_0(\vec{R}) \mapsto \vec{\Omega}_0'(\vec{R}) = \partial_{\vec{R}} \times \vec{A}_0'(\vec{R})$$
$$= \partial_{\vec{R}} \times \left(\vec{A}_0(\vec{R}) - \partial_{\vec{R}}\, \chi(\vec{R}) \right)$$
$$= \vec{\Omega}_0(\vec{R})$$

- the Berry curvature is divergence-free:

$$\partial_{\vec{R}} \cdot \vec{\Omega}_0(\vec{R}) = \partial_{\vec{R}} \cdot \partial_{\vec{R}} \times \vec{A}_0(\vec{R}) = 0$$

- vice versa,

$$\partial_{\vec R}\, \vec\Omega_0(\vec R) = 0 \quad \Rightarrow \quad \vec\Omega_0(\vec R) = \partial_{\vec R} \times \vec A_0(\vec R)$$

for some $\vec A_0(\vec R)$ <u>locally</u>

<u>globally</u>, on the entire parameter manifold $\mathcal{M}$,

Poincaré's lemma ensures that a representation as a curl is possible for a <u>contractible</u> parameter manifold

↳ can be continuously shrunk to a point in that manifold

contractible:

not contractible:

$\mathbb{R}^3 \setminus \{0\}$

- is not contractible
- a representation $\vec\Omega_0(\vec R) = \partial_{\vec R} \times \vec A_0(\vec R)$ might not exist globally

- compute $\vec\Omega_0(\vec R)$ for the toy model $H(\vec R) = -\frac{1}{2}\vec R \vec\tau$

$$\Omega_{0,\alpha}(\boldsymbol{R}) = \frac{1}{2}\sum_{\beta\gamma} \varepsilon_{\alpha\beta\gamma}\Omega_{0,\beta\gamma}(\boldsymbol{R})$$

antisymmetric real 3×3 matrix

$$\Omega_{0,\beta\gamma}(\boldsymbol{R}) \overset{\text{def}}{=} \partial_\beta A_{0,\gamma}(\boldsymbol{R}) - \partial_\gamma A_{0,\beta}(\boldsymbol{R}) \overset{\text{def}}{=} i\Big(\langle\partial_\beta\Phi_0(\boldsymbol{R})|\partial_\gamma\Phi_0(\boldsymbol{R})\rangle - \langle\partial_\gamma\Phi_0(\boldsymbol{R})|\partial_\beta\Phi_0(\boldsymbol{R})\rangle\Big)$$

$$= -2\,\mathrm{Im}\langle\partial_\beta\Phi_0(\boldsymbol{R})|\partial_\gamma\Phi_0(\boldsymbol{R})\rangle = -2\,\mathrm{Im}\sum_{j\neq 0}\langle\partial_\beta\Phi_0(\boldsymbol{R})|\Phi_j(\boldsymbol{R})\rangle\langle\Phi_j(\boldsymbol{R})|\partial_\gamma\Phi_0(\boldsymbol{R})\rangle\,.$$

with identity

$$\langle\Phi_j(\boldsymbol{R})|\partial_\gamma\Phi_0(\boldsymbol{R})\rangle = \langle\Phi_j(\boldsymbol{R})|\partial_\gamma H(\boldsymbol{R})|\Phi_0(\boldsymbol{R})\rangle/(E_0(\boldsymbol{R}) - E_j(\boldsymbol{R}))$$

$$\partial_\beta H(\boldsymbol{R}) = -\tau_\beta/2$$

$$\Omega_{0,\beta\gamma}(\boldsymbol{R}) = -2\,\mathrm{Im}\sum_{j\neq 0}\frac{\langle\Phi_0(\boldsymbol{R})|\partial_\beta H(\boldsymbol{R})|\Phi_j(\boldsymbol{R})\rangle\langle\Phi_j(\boldsymbol{R})|\partial_\gamma H(\boldsymbol{R})|\Phi_0(\boldsymbol{R})\rangle}{(E_0(\boldsymbol{R}) - E_j(\boldsymbol{R}))^2}$$

$$(E_0(\boldsymbol{R}) - E_1(\boldsymbol{R}))^2 = R^2$$

$$\Omega_{0,\beta\gamma}(\boldsymbol{R}) = -\frac{1}{2}\,\mathrm{Im}\frac{\langle\Phi_0(\boldsymbol{R})|\tau_\beta|\Phi_1(\boldsymbol{R})\rangle\langle\Phi_1(\boldsymbol{R})|\tau_\gamma|\Phi_0(\boldsymbol{R})\rangle}{R^2}$$

rewrite as vector again

$$\boldsymbol{\Omega}_0(\boldsymbol{R}) = \frac{1}{2}\sum_{\alpha\beta\gamma}\varepsilon_{\alpha\beta\gamma}\Omega_{0,\beta\gamma}(\boldsymbol{R})\boldsymbol{e}_\alpha = -\frac{1}{4}\,\mathrm{Im}\frac{\langle\Phi_0(\boldsymbol{R})|\boldsymbol{\tau}|\Phi_1(\boldsymbol{R})\rangle \times \langle\Phi_1(\boldsymbol{R})|\boldsymbol{\tau}|\Phi_0(\boldsymbol{R})\rangle}{R^2}$$

compute matrix elements:

$$\langle\Phi_0(\boldsymbol{R})|\boldsymbol{\tau}|\Phi_1(\boldsymbol{R})\rangle = e^{i\phi}(1,0)\,\boldsymbol{\tau}\begin{pmatrix}0\\1\end{pmatrix} = e^{i\phi}\begin{pmatrix}1\\-i\\0\end{pmatrix}$$

- $$\boxed{\boldsymbol{\Omega}_0(\boldsymbol{R}) = -\frac{1}{2}\frac{\boldsymbol{R}}{R^3}}$$

interesting!

- looks like the magnetic field of a magnetic monopole

- $\vec{\Omega}_0(\vec{R})$ is singular, where the magnetic charge sits

we have

$\operatorname{div}\vec{B} = 0$, i.e. there is no magnetic charge

if we had

$\operatorname{div}\vec{B} = \mu_0\rho_m$ (and $\operatorname{rot}\vec{B} = 0$)

then a magnetic point charge

$\rho_m(\vec{r}) = q_m \cdot \delta(\vec{r})$

would produce a monopole field:

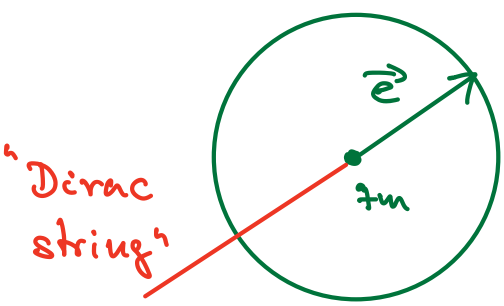
$\vec{B}(\vec{r}) = \frac{\mu_0}{4\pi} q_m \frac{\vec{r}}{r^3}$

- how would the vector potential $\vec{A}_0(\vec{R})$ look like?

Dirac (1931):

$$\boxed{\boldsymbol{A}_0(\boldsymbol{R}) = -\frac{1}{2}\frac{1}{R^2}\frac{\boldsymbol{e}\times\boldsymbol{R}}{1+\boldsymbol{e}\boldsymbol{R}/R}}$$

$$\Rightarrow \quad \partial_{\vec{R}} \times \vec{A}_0(\vec{R}) = -\frac{1}{2}\frac{\vec{R}}{R^3} = \vec{\Omega}_0(\vec{R})$$



- $\vec{e}$ (with $|\vec{e}| = 1$) is arbitrary.
a gauge transformation implies $\vec{e} \mapsto \vec{e}\,'$
(this shifts the singularity but does not remove it)

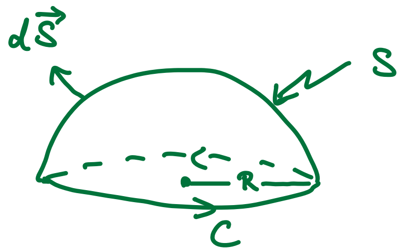
- there is no globally smooth potential.

$\vec{A}_0(\vec{R})$ is singular, if

$$\vec{e} \cdot \frac{\vec{R}}{R} = -1$$

- $\gamma_c = \oint_C \vec{A}_0(\vec{R})\, d\vec{R} \overset{\text{Stokes}}{=} \int_S \vec{\Omega}_0(\vec{R})\, d\vec{S}$

γ_c is the flux of the magnetic field through a surface bounded by C

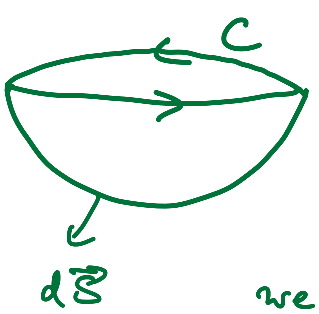


(oriented equator)

$$\gamma_c = \int_S \left(-\frac{1}{2}\frac{\vec{R}}{R^3}\right) d\vec{S} \qquad \frac{\vec{R}}{R}\, dS$$

$$= -\frac{1}{2} \cdot \frac{1}{R^2} \cdot \int_S dS = -\frac{1}{2} \cdot 2\pi = -\pi \quad \checkmark$$

- same calculation, but with the lower hemisphere



$$\oint_C \vec{A}_0'(\vec{R})\, d\vec{R} = -\int_{S_{lower}} \vec{\Omega}_0(\vec{R})\, d\vec{S}$$

we must choose a gauge where the potential is smooth on the lower hemisphere

"left-hand rule"

we again get $\int_{S_{lower}} \vec{\Omega}_0(\vec{R})\, d\vec{S} = -\pi \quad \checkmark$

The Chern theorem

- quantum system with parameter-dependent Hamiltonian $H(\vec{R})$ $\quad \vec{R} \in \mathcal{M} \subset \mathbb{R}^3$
- non-degenerate ground state $\forall \vec{R} \in \mathcal{M}$
- S closed surface in $\mathcal{M}$

$$\Rightarrow \quad \boxed{C = \frac{1}{2\pi} \oint_S \vec{\Omega}_0(\vec{R})\, d\vec{S} \in \mathbb{Z}}$$

definition of the Chern number

Chern theorem: C is quantized!

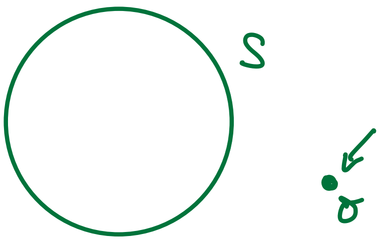
- there is a generalization to $\mathbb{R}^n$
- here $\mathcal{M} = \mathbb{R}^3 \setminus \{0\}$ $\quad$ ($\Leftrightarrow$ toy model)
- if $\mathcal{M}$ was contractible (e.g. $\mathbb{R}^3$), $\operatorname{div} \vec{\Omega}_0(\vec{R}) = 0$ would imply $\vec{\Omega}_0(\vec{R}) = \nabla_{\vec{R}} \times \vec{A}_0(\vec{R})$ globally and thus $C = 0$:

$$\oint_S \vec{\Omega}_0(\vec{R})\, d\vec{S} \overset{\text{Stokes}}{=} \int_{\partial S} \vec{A}_0(\vec{R})\, d\vec{R} = 0$$

$\partial S = \emptyset$!

- C depends on our choice for S !
- a "non-trivial topology" ($C \neq 0$) <u>requires</u> a non-trivial parameter manifold (not just $\mathbb{R}^3$),

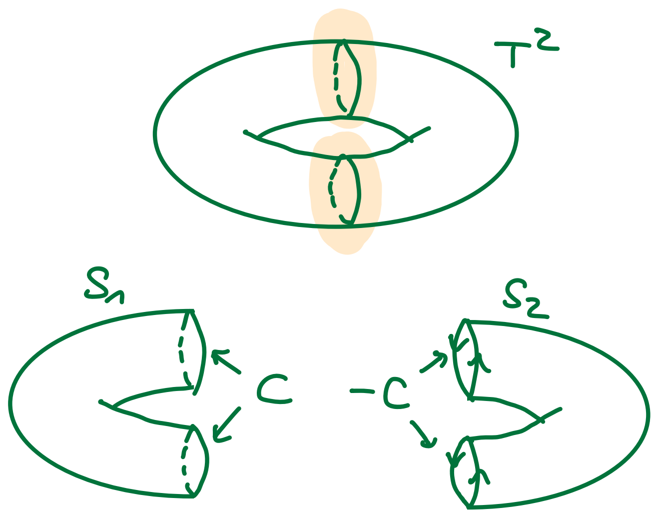
but this is not sufficient



$\mathcal{M} = \mathbb{R}^3 \setminus \{0\}$

$\Rightarrow \quad C = 0$

Proof of the Chern theorem



- write the closed surface as

$$S = S_1 \cup S_2$$

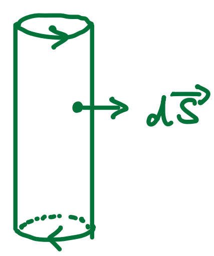
boundary of S_1 : $\partial S_1 = C$

boundary of S_2 : $\partial S_2 = -C$

- such that

$$\vec{\Omega}_0(\vec{R}) = \partial_{\vec{R}} \times \vec{A}_{0,1}(\vec{R}) \quad \text{on } S_1$$

$$\vec{\Omega}_0(\vec{R}) = \partial_{\vec{R}} \times \vec{A}_{0,2}(\vec{R}) \quad \text{on } S_2$$



- on an environment of C

$$\partial_{\vec{R}} \times \left(\vec{A}_{0,1}(\vec{R}) - \vec{A}_{0,2}(\vec{R}) \right) = 0$$

$$\Rightarrow \quad \vec{A}_{0,1}(\vec{R}) - \vec{A}_{0,2}(\vec{R}) \quad \text{is a gradient field}$$

$$\Rightarrow \quad \vec{A}_{0,1}(\vec{R}) \xleftrightarrow[\text{transf.}]{\text{gauge}} \vec{A}_{0,2}(\vec{R})$$

$$\Rightarrow \quad e^{i\gamma_{c,1}} = e^{i\gamma_{c,2}}$$

$$\Rightarrow \quad \oint_C \vec{A}_{0,1}(\vec{R})\, d\vec{R} - \oint_C \vec{A}_{0,2}(\vec{R})\, d\vec{R} = 2\pi k \; , \; k \in \mathbb{Z}$$

- Stokes theorem

$$\int_{S_1} \vec{\Omega}_0(\vec{R})\, d\vec{S}_1 = \oint_C \vec{A}_{0,1}(\vec{R})\cdot d\vec{R}$$

$$\int_{S_2} \vec{\Omega}_0(\vec{R})\, d\vec{S}_2 = \oint_{-C} \vec{A}_{0,2}(\vec{R})\cdot d\vec{R} = -\oint_C \vec{A}_{0,2}(\vec{R})\, d\vec{R}$$

- conclusion:

$$\oint_S \vec{\Omega}_0(\vec{R})\, d\vec{S} = \int_{S_1} \vec{\Omega}_0(\vec{R})\, d\vec{S}_1 + \int_{S_2} \vec{\Omega}_0(\vec{R})\, d\vec{S}_2$$

$$= \oint_C \vec{A}_{0,1}(\vec{R})\cdot d\vec{R} - \oint_C \vec{A}_{0,2}(\vec{R})\, d\vec{R}$$

$$= 2\pi \cdot k \quad \text{with } k \in \mathbb{Z}$$

✓

---

for the toy model:

$$C = \frac{1}{2\pi} \oint_S \vec{\Omega}_0(\vec{R})\, d\vec{S} = \frac{1}{2\pi}\left(-\frac{1}{2}\right) \oint_S \frac{\vec{R}}{R^3}\cdot\frac{\vec{R}}{R}\, d\vec{S}$$

$$= -\frac{1}{4\pi}\frac{1}{R^2}\oint_S dS = -1$$

if S is the surface of a ball with radius R

or for any continuous deformation S' of S

(as long as there is no gap closure during the deformation)

Remark:

- extension to arbitrary even $D = 2n$:

$$C_n = \frac{i^n}{(2\pi)^n} \frac{1}{n!} \int_S \mathrm{tr}(\Omega^n) \qquad \Omega = dA + A^2$$

C_n: n-th Chern number

S: 2n-dimensional closed manifold

Remark:

- the Chern number is assigned to a

  bundle $\{|\Phi_0(R)\rangle\}$ of ground states

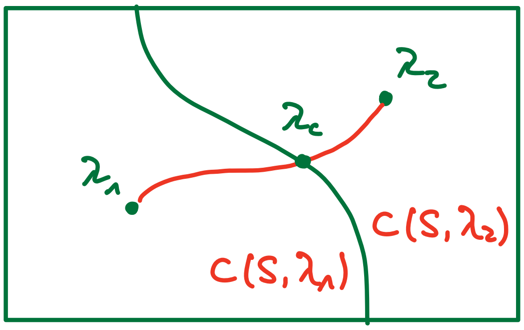
  of Hamiltonians $H(R)$, $R \in S$

- $H = H(R, \lambda) \longrightarrow \boxed{C = C(S, \lambda)}$

  $R \in S$ further control parameters

- if $C(S,\lambda_1) \neq C(S,\lambda_2)$, then

$$\{|\Phi_0(R,\lambda_1)\rangle\} \xleftrightarrow[\text{deformation}]{\text{no continuous}} \{|\Phi_0(R,\lambda_2)\rangle\}$$



critical λ_c:

- gap closure at one (or several) points $k \in S$
- topological phase transition

Application to a generic insulator

tight-binding model of independent fermions on a lattice

$D=2: \vec{k} = \begin{pmatrix} k_x \\ k_y \end{pmatrix} \in 1BZ$

$$H = \sum_{i,i'=1}^{\overset{\#\text{ sites}}{L}} \sum_{\alpha,\alpha'=1}^{\overset{n=2\text{ orbitals}}{n}} t_{i\alpha,i'\alpha'} \, c^{\dagger}_{i\alpha} c_{i'\alpha'} \overset{\text{Fourier trsf.}}{=} \sum_{\vec{k}\in 1BZ} \sum_{\alpha\alpha'} t_{\alpha\alpha'}(\vec{k}) \, c^{\dagger}_{\vec{k}\alpha} c_{\vec{k}\alpha'}$$

$\{\underline{t}(\vec{k})\}$: bundle of 2×2 Bloch Hamiltonians on $S = T^2 \cong 1BZ$

note:

- all Bloch Hamiltonians $\underline{t}(\vec{k})$ derive from one and the same Hamiltonian H
- $S = 1BZ$ is an intrinsic system property ($\sim$ geometry) S is given a priori, no choice necessary !
- $C(S,\lambda) = C(\lambda)$ is a material property, depends on control parameters only

Expansion into a basis of hermitian 2×2 matrices

$$\underline{t}(\vec{k}) = d_0(\vec{k})\,\mathbb{1} + d_1(\vec{k})\,\underline{\tau}_x + d_2(\vec{k})\,\underline{\tau}_y + d_3(\vec{k})\,\underline{\tau}_z$$

$$\underline{t}(\vec{k}) = d_0(\vec{k})\,\mathbb{1} + \vec{d}(\vec{k})\cdot\vec{\underline{\tau}}$$

$\vec{\underline{\tau}}$: Pauli matrices

$\Rightarrow$

$$\varepsilon_{\pm}(\vec{k}) = d_0(\vec{k}) \pm |\vec{d}(\vec{k})|$$

Qi – Wu – Zhang (QWZ) model

Qi, Wu, Zhang, PRB (2006)

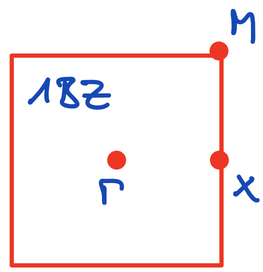
$\underline{h}(\vec{k}) = \vec{d}(\vec{k}) \cdot \underline{\vec{\sigma}}$ with

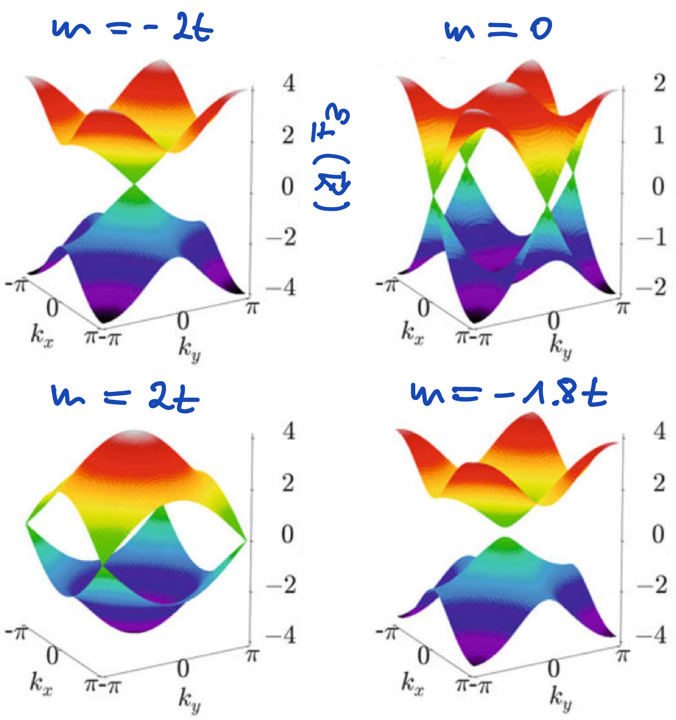
$$d_0(\vec{k}) = 0\,, \qquad \vec{d}(\vec{k}) = \begin{pmatrix} t \sin k_x \\ t \sin k_y \\ m + t\cos k_x + t \cos k_y \end{pmatrix}$$

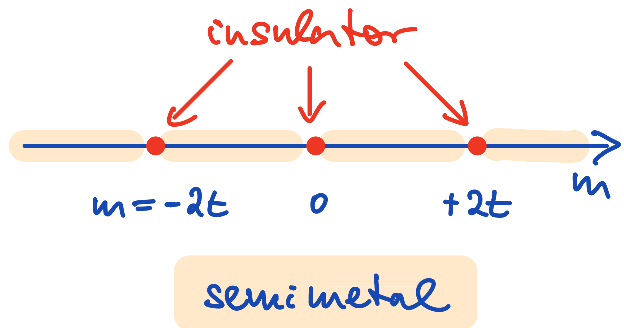
two bands:

$$\varepsilon_\pm(\vec{k}) = \pm\sqrt{t^2(\sin^2 k_x + \sin^2 k_y) + (m + t\cos k_x + t\cos k_y)^2}$$

the gap closes at	if
$\vec{k} = \Gamma = (0,0)$	$m = -2t$
$\vec{k} = X = (\pi,0)\,,\,(0,\pi)$	$m = 0$
$\vec{k} = M = (\pm\pi, \pm\pi)$	$m = +2t$







Asbóth, Oroszlány, Pályi (Springer, 2006)

Topological classification

(compute the Chern number of the QWZ model for all control parameters, i.e. for m)

QWZ model	toy model
$\underline{\underline{H}}(\vec{k}) = \vec{d}(\vec{k}) \cdot \underline{\underline{\vec{\sigma}}}$	$\underline{\underline{H}}(\vec{R}) = -\frac{1}{2}\vec{R} \cdot \underline{\underline{\vec{\sigma}}}$

$$\Rightarrow \quad \vec{\Omega}_0(\vec{d}) = \frac{1}{2}\frac{\vec{d}}{d^3}$$

- the physical parameter manifold is the 1BZ

we have a smooth map (if $m \neq m_{critical}$)

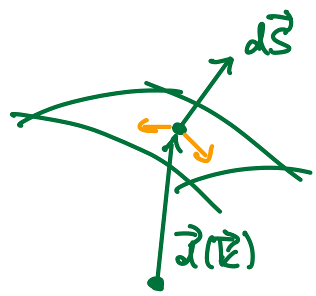
$$\vec{d}: 1BZ \longrightarrow \mathbb{R}^3 \setminus \{0\}$$
$$\vec{k} \longmapsto \vec{d}(\vec{k})$$

the image of the 1BZ under $\vec{d}$,

$$D := \{\vec{d}(\vec{k}) \in \mathbb{R}^3 \setminus \{0\} \mid \vec{k} = (k_x, k_y) \in 1BZ\},$$

is

- 2-dimensional
- closed
- with infinitesimal surface element

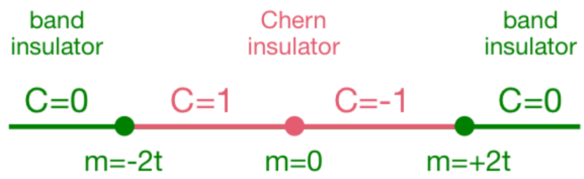


$$d\vec{S} = \frac{\partial \vec{d}(\vec{k})}{\partial k_x} \times \frac{\partial \vec{d}(\vec{k})}{\partial k_y}\, dk_x\, dk_y \quad \perp \quad D \quad \text{at } \vec{d}(\vec{k})$$

$$\Rightarrow \quad C = \frac{1}{2\pi} \iint \frac{1}{2}\frac{\vec{d}(\vec{k})}{d(\vec{k})^3} \cdot \frac{\partial \vec{d}(\vec{k})}{\partial k_x} \times \frac{\partial \vec{d}(\vec{k})}{\partial k_y}\, dk_x\, dk_y$$

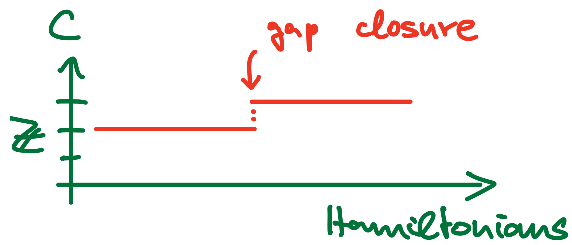
Wolfram Alpha

topological phase diagram:



One may continuously deform the Hamiltonian

- $C \in \mathbb{Z} \Rightarrow C$ cannot change (unless there is a gap closure)



Example

treat $d(\vec{k}) = |\vec{d}(\vec{k})|$ as a control parameter

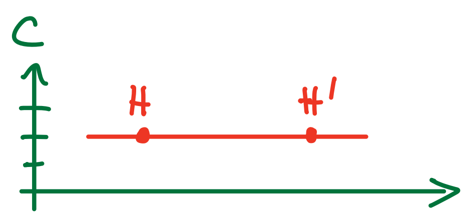
deformation:

$$d(\vec{k}) \longmapsto d'(\vec{k}) = 1$$

there is no gap closure: $\Delta(\vec{k}) = 2\, d(\vec{k}) > 0$

$$\Rightarrow \quad H(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\underline{\sigma}} \cong \frac{\vec{d}(\vec{k})}{d(\vec{k})} \cdot \vec{\underline{\sigma}} = \vec{d}'(\vec{k}) \cdot \vec{\underline{\sigma}} = H'(\vec{k})$$

"essentially the same"



we have

$$0 = \frac{\partial\, \vec{d}'(\vec{k})^2}{\partial k_x} = \frac{\partial \vec{d}'(\vec{k})}{\partial k_x} \cdot \vec{d}'(\vec{k}) \,, \quad \frac{\partial \vec{d}'(\vec{k})}{\partial k_x} \perp \vec{d}'(\vec{k})$$

(and the same with $\partial/\partial k_y$)

and thus

$$\vec{d}'(\vec{k}) \cdot d\vec{S} = \vec{d}'(\vec{k}) \cdot \frac{\partial \vec{d}'(\vec{k})}{\partial k_x} \times \frac{\partial \vec{d}'(\vec{k})}{\partial k_y}\, dk_x dk_y = \pm\, d'(\vec{k})\, dS = \pm\, dS$$

$$\Rightarrow \quad C = \pm \frac{1}{4\pi} \oint_D dS$$

D is the image of the 1BZ under $\vec{d}'$

D must cover the entire S^2 (once or several times)

C is the wrapping number

(how often does T^2 wrap around S^2 ?)

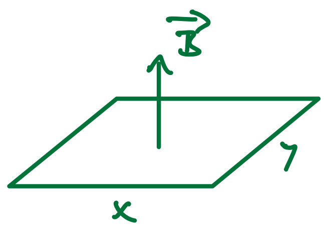
Is a topological invariant directly observable experimentally?

No !

exception:

quantum Hall effect (QHE) in, e.g., GaAs heterostructures

(inverse) transverse Hall resistivity:



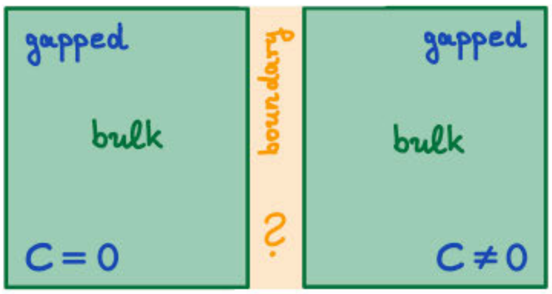
$$\frac{1}{R_{xy}} = \nu \cdot \frac{e^2}{h}$$

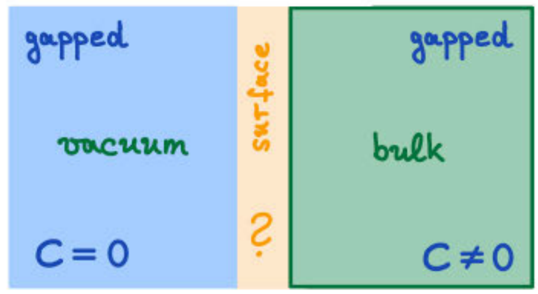
$\nu \in \mathbb{Z}$, "Hall plateaus"!

ν is the first Chern number

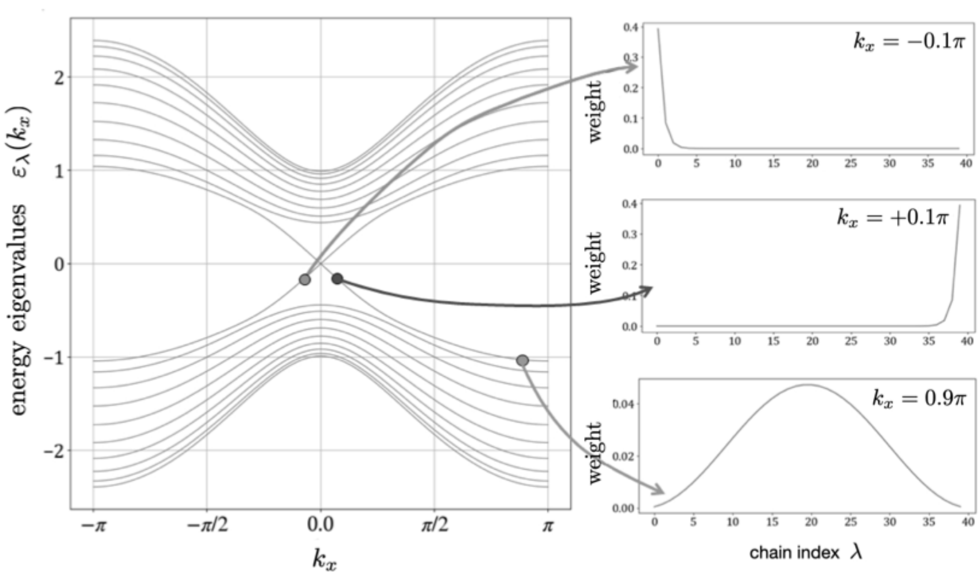
$\rightarrow$ new standard for electrical resistivity!

Bulk - boundary correspondence





Example:



calculation for the QWZ model in a ribbon geometry

Part II

Our Goal ?

Can we topologically classify all interacting electron models ? ✗

Can we topologically classify all interacting lattice electron models ? ✗

Can we topologically classify all lattice-electron models with local interactions on infinite-dimensional lattices ? ✗

Can we topologically classify, in infinite dimensions, Hubbard-type lattice models derived from noninteracting prototypes of the tenfold way? ?

Can we topologically classify at least one of the prototype band models of the tenfold way, plus Hubbard-U, on an infinite-dimensional lattice ? ✓

Topological Hamiltonian

noninteracting system, M orbitals, dimension D

$$1\mathrm{BZ} = T^D \ni k \mapsto \boldsymbol{\epsilon}(k) \in GL(M, \mathbb{R})$$

equivalently classification can be based on the map

$$k \rightarrow \boldsymbol{G}^{(0)}(k,\omega) = \frac{1}{\omega - \boldsymbol{\epsilon}(k)}$$

interacting system: classification in terms of

$$(k,\omega) \mapsto \boldsymbol{G}(k,\omega) = \frac{1}{\omega - \boldsymbol{\epsilon}(k) - \boldsymbol{\Sigma}(k,\omega)}$$

e.g. for D=2: $N_2 = \frac{1}{24\pi^2}\int dk_0 d^2k \mathrm{Tr}[\epsilon^{\mu\nu\rho} G\partial_\mu G^{-1} G\partial_\nu G^{-1} G\partial_\rho G^{-1}]$

Volovik, Zh. Eksp. Teor. Fiz.(1988)
Ishikawa and Matsuyama, ZPC (1986)

smooth interpolation

$$\boldsymbol{G}(k,\omega,\lambda) := \frac{1-\lambda}{\omega - \boldsymbol{\epsilon}(k) - \boldsymbol{\Sigma}(k,\omega)} + \frac{\lambda}{\omega - \boldsymbol{\epsilon}(k) - \boldsymbol{\Sigma}(k,\omega=0)}$$

Wang, Zhang, PRX (2012)

… if the self-energy is local

Thunström, Held, arXiv (2019)
Savrasov, Haule, Kotliar, PRL (2006)

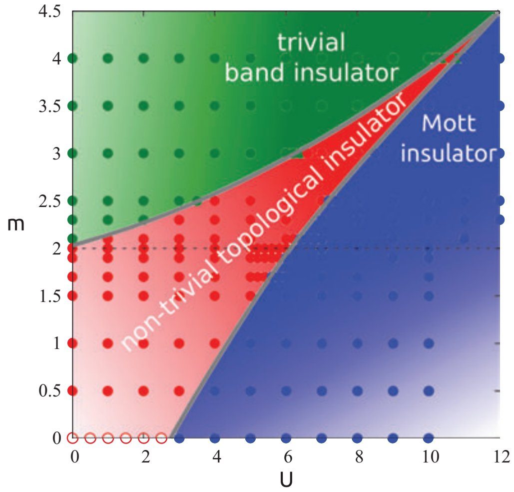
topological Hamiltonian

$$\boldsymbol{H}_{\mathrm{top}}(k) = \boldsymbol{\epsilon}(k) + \boldsymbol{\Sigma}(\omega = 0)$$

DMFT applied to TI's + U in D=2 or D=3

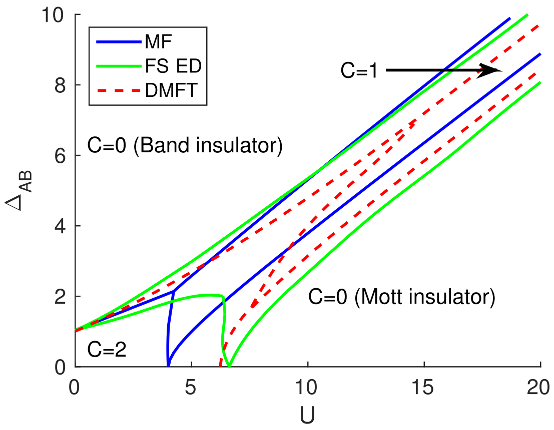
BHZ model + U

Budich, Trauzettel, Sangiovanni, PRB (2013)



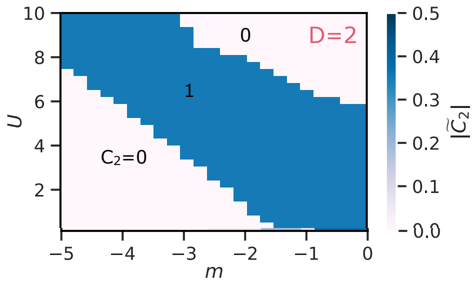
Haldane model + U

Vanhala, Siro, Liang, Troyer,
Harju, Törmä , PRL (2016)



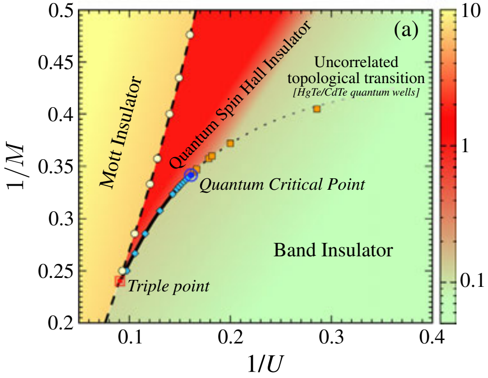
QWZ model + U

Krüger, Potthoff, PRL (2021)



BHZ model + U

Amaricci, Budich, Capone,
Trauzettel, Sangiovanni, PRL (2015)



Hofstadter butterfly + U

Markov, Rohringer, Rubtsov, PRB (2019)

DFT + U for SmB_6

Thunström, Held, PRB (2021)

Qi-Wu-Zhang (QWZ) model

Cartan \ d	0	1	2	3	4	5	6	7	8	
Complex case:										
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
Real case:										
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\cdots$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\cdots$
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\cdots$
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\cdots$
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	$\cdots$
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\cdots$
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\cdots$
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	$\cdots$

D=2 square lattice, two-orbitals, broken TRS, made spinful

$$H_0 = \sum_k \sum_{\alpha,\beta=1}^{M} \sum_{\sigma=\uparrow,\downarrow} \epsilon_{\alpha\beta}(k) c^\dagger_{k\alpha\sigma} c_{k\beta\sigma} \qquad (M=2)$$

$$\boldsymbol{\epsilon}(k) = d(k)\cdot\boldsymbol{\tau} \qquad d(k) = \begin{pmatrix} t\sin k_x \\ t\sin k_y \\ m + t\cos k_x + t\cos k_y \end{pmatrix} \qquad \boldsymbol{\tau} = \begin{pmatrix} \tau_x \\ \tau_y \\ \tau_z \end{pmatrix}$$

Qi, Wu, Zhang, PRB (2006)

two bands:

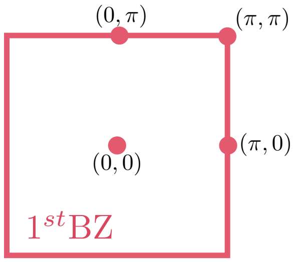
$$\epsilon_\pm(k) = \pm\sqrt{t^2(\sin^2 k_x + \sin^2 k_y) + (m + t\cos k_x + t\cos k_y)^2}$$

topological invariant:

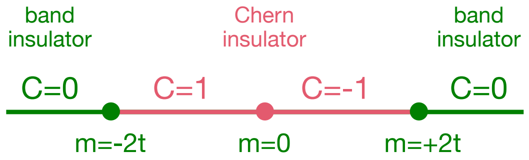
$$C = \frac{1}{2\pi}\oint_{1\mathrm{BZ}} d^2k\, F(k)$$

gap closes at: if:

$$\begin{array}{lll} k_x = 0,\ k_y = 0 & \text{and} & m = -2t \\ k_x = 0,\ k_y = \pi & \text{and} & m = 0 \\ k_x = \pi,\ k_y = 0 & \text{and} & m = 0 \\ k_x = \pi,\ k_y = \pi & \text{and} & m = +2t \end{array}$$



topological phase diagram:



Qi-Wu-Zhang (QWZ) model

Cartan \ d	0	1	2	3	4	5	6	7	8	
Complex case:										
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	$\cdots$
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\cdots$
Real case:										
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	$\cdots$
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\cdots$
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\cdots$
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\cdots$
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	$\cdots$
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\cdots$
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	$\cdots$
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	$\cdots$

D=2 square lattice, two-orbitals, broken TRS, made spinful

$$H_0 = \sum_k \sum_{\alpha,\beta=1}^{M} \sum_{\sigma=\uparrow,\downarrow} \epsilon_{\alpha\beta}(k) c^\dagger_{k\alpha\sigma} c_{k\beta\sigma} \qquad (M=2)$$

$$\boldsymbol{\epsilon}(k) = d(k)\cdot\boldsymbol{\tau} \qquad d(k) = \begin{pmatrix} t\sin k_x \\ t\sin k_y \\ m + t\cos k_x + t\cos k_y \end{pmatrix} \qquad \boldsymbol{\tau} = \begin{pmatrix} \tau_x \\ \tau_y \\ \tau_z \end{pmatrix}$$

Qi, Wu, Zhang, PRB (2006)

can be written as (D=2)

$$\boldsymbol{\epsilon}(k) = \left(m + t\sum_{r=1}^{D}\cos k_r\right)\boldsymbol{\gamma}_D^{(0)} + t\sum_{r=1}^{D}\sin k_r \boldsymbol{\gamma}_D^{(r)}$$

and with

$$\boldsymbol{\gamma}_D^{(1)} = \boldsymbol{\tau}_x \qquad \boldsymbol{\gamma}_D^{(2)} = \boldsymbol{\tau}_y \qquad \boldsymbol{\gamma}_D^{(0)} = \boldsymbol{\tau}_z = -i\boldsymbol{\tau}_x\boldsymbol{\tau}_y$$

and

$$\{\boldsymbol{\gamma}_D^{(1)},\boldsymbol{\gamma}_D^{(2)}\} = \{\boldsymbol{\gamma}_D^{(2)},\boldsymbol{\gamma}_D^{(0)}\} = \{\boldsymbol{\gamma}_D^{(0)},\boldsymbol{\gamma}_D^{(1)}\} = 0$$

$$(\boldsymbol{\gamma}_D^{(1)})^2 = (\boldsymbol{\gamma}_D^{(2)})^2 = (\boldsymbol{\gamma}_D^{(0)})^2 = 1$$

QWZ model on the hypercubic lattice (even D)

Bloch Hamiltonian

$$\boldsymbol{\epsilon}(k) = \left(m + t\sum_{r=1}^{D}\cos k_r\right)\boldsymbol{\gamma}_D^{(0)} + t\sum_{r=1}^{D}\sin k_r \boldsymbol{\gamma}_D^{(r)}$$

with generators of Clifford algebra

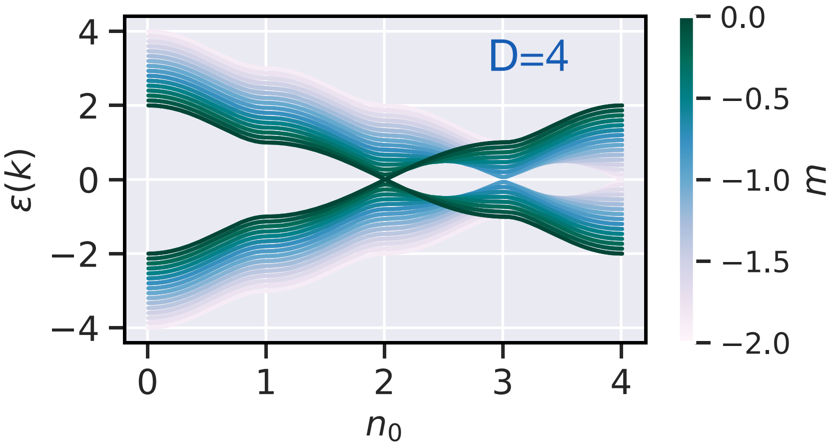
$$\{\boldsymbol{\gamma}_D^{(\mu)}, \boldsymbol{\gamma}_D^{(\nu)}\} = 2\delta^{(\mu\nu)} \text{ for } \mu,\nu = 0,1,...,D$$

$$\boldsymbol{\gamma}_D^{(0)} = (-i)^{D/2}\boldsymbol{\gamma}_D^{(1)}\cdots\boldsymbol{\gamma}_D^{(D)}$$

band dispersions

$$\boldsymbol{\epsilon}(k)^2 = \left(\sum_{\mu=0}^{D} d_\mu(k)\boldsymbol{\gamma}_D^{(\mu)}\right)^2 = \sum_{\mu\mu'} d_\mu(k)d_{\mu'}(k)\boldsymbol{\gamma}_D^{(\mu)}\boldsymbol{\gamma}_D^{(\mu')} = \left(d_0(k)^2 + \sum_{r=1}^{D} d_r(k)^2\right)\mathbf{1}$$

$$\epsilon(k) = \pm\left((m + t\sum_r \cos k_r)^2 + \sum_r t^2\sin^2 k_r\right)^{1/2}$$



gap closure for $m = (D - 2n_0)t$

at $\binom{D}{n_0}$ HSPs $k_{n_0} = (\underbrace{0,\ldots,0}_{n_0},\pi,\ldots,\pi)$ in the 1BZ

$D \to \infty$ limit and scaling of the hopping

free Green's function of orbital α

$$G^{(0)}_{\alpha\alpha}(k,\omega) = \left[\frac{\omega + \sum_\mu d_\mu(k)\gamma^\mu_D}{\omega^2 - \sum_\mu d_\mu(k)^2}\right]_{\alpha\alpha} = \sum_{n=0}^{\infty} \frac{M^{(n)}_\alpha(k)}{\omega^{n+1}}$$

A and B orbitals

$$\gamma^{(0)}_D = \mathrm{diag}(+1, -1, ...)$$

moments of the local DOS of orbital α

$$M^{(n)}_\alpha = \frac{1}{L}\sum_k M^{(n)}_\alpha(k) = \int d\omega\, \omega^k \rho_\alpha(\omega)$$

$$M^{(0)}_\alpha = 1$$

$$M^{(1)}_\alpha = m\gamma^{(0)}_{\alpha\alpha} = \pm m$$

$$M^{(2)}_\alpha = t^2 D + m^2 = {t^*}^2 + m^2$$

with the usual scaling

$$t = t^*/\sqrt{D} \qquad t^* = 1$$

band edges

$$\epsilon_{\max,\min} = \pm(|m| + \sqrt{D}t^*) \mapsto \pm\infty$$

band closures at

$$m = \left(\sqrt{D} - 2\frac{n_0}{\sqrt{D}}\right)t^* \qquad (n_0 = 0, ..., D)$$

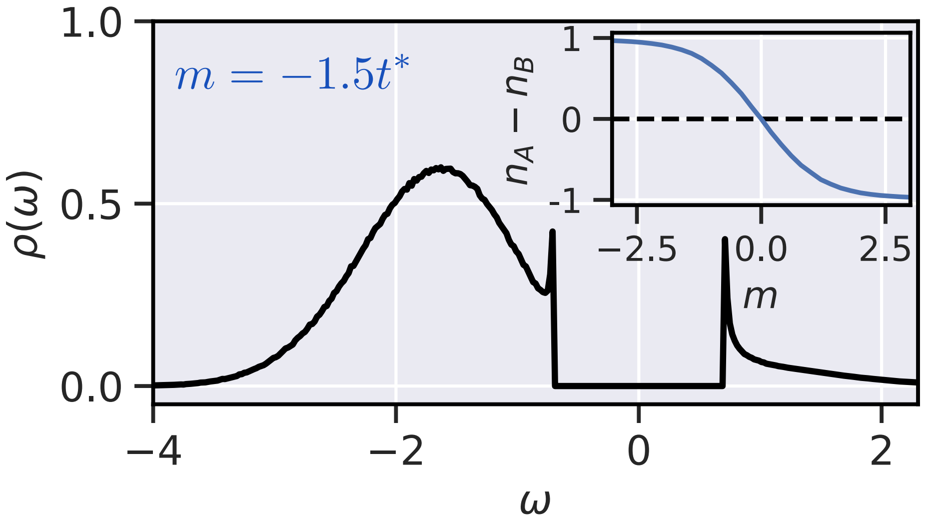
$$D = 2: \quad m = \sqrt{2}t^*, 0, -\sqrt{2}t^*$$

$$D = 4: \quad m = -2t^*, -t^*, 0, t^*, 2t^*$$

$$D = 6: \quad m = \sqrt{6}t^*, \frac{2}{3}\sqrt{6}t^*, \frac{1}{3}\sqrt{6}t^*, 0, -\frac{1}{3}\sqrt{6}t^*, -\frac{2}{3}\sqrt{6}t^*, -\sqrt{6}t^*$$

$$\vdots$$

DOS in the $D \to \infty$ limit



local DOS of orbital α in the limit $D \to \infty$

$$\rho_\alpha(\omega) = \frac{1}{2}\frac{1}{t^*\sqrt{\pi}}\Theta(|\omega| - \frac{1}{\sqrt{2}}t^*)\,\mathrm{sign}\,\omega \sum_{s=\pm}\left(\frac{\omega}{\sqrt{\omega^2 - \frac{1}{2}t^{*2}}} + s z_\alpha\right)\exp\left(-\frac{\left(s\sqrt{\omega^2 - \frac{1}{2}t^{*2}} - m\right)^2}{t^{*2}}\right)$$

there is a finite gap $\Delta = \sqrt{2}t^*$ independent of m!

Irreps of Clifford algebra

Bloch Hamiltonian

$$\boldsymbol{\epsilon}(k) = \left(m + t \sum_{r=1}^{D} \cos k_r \right) \boldsymbol{\gamma}_D^{(0)} + t \sum_{r=1}^{D} \sin k_r \boldsymbol{\gamma}_D^{(r)}$$

with generators of Clifford algebra

$$\{\boldsymbol{\gamma}_D^{(\mu)}, \boldsymbol{\gamma}_D^{(\nu)}\} = 2\delta^{(\mu\nu)} \text{ for } \mu, \nu = 0, 1, ..., D$$

Theorem

- for even D, there is a **unique** irrep of the complex Clifford algebra
- $\mathbb{C}l_{D+2} \cong \mathrm{Mat}(2, \mathbb{C}) \otimes \mathbb{C}l_D$
- dimension of the representation: M= $2^{D/2}$

Prodan, Schulz-Baldes (2016)
"Bulk and Boundary Invariant for Complex Topological Insulators"

explicit iterative construction

$$\begin{aligned}
\boldsymbol{\gamma}_{D+2}^{(r)} &= \boldsymbol{\tau}_x \otimes \boldsymbol{\gamma}_D^{(r)}, \text{ for } r = 1, ..., D \\
\boldsymbol{\gamma}_{D+2}^{(D+1)} &= \boldsymbol{\tau}_x \otimes \boldsymbol{\gamma}_D^{(0)}, \ \boldsymbol{\gamma}_{D+2}^{(D+2)} = \boldsymbol{\tau}_y \otimes \mathbf{1} \\
\boldsymbol{\gamma}_{D+2}^{(0)} &= \boldsymbol{\tau}_z \otimes \mathbf{1},
\end{aligned}$$

immediate consequences

- number of orbitals $M = 2^{D/2}$ (diverges for $D \to \infty$)
- A- and B-orbitals (m: strength of staggered orbital field)
- degenerate band structure

Chern number

$$C_D = \frac{1}{(D/2)!}\frac{i^{D/2}}{(2\pi)^{D/2}}\int_{1\mathrm{BZ}_D} \mathrm{tr}\, F^{D/2}$$

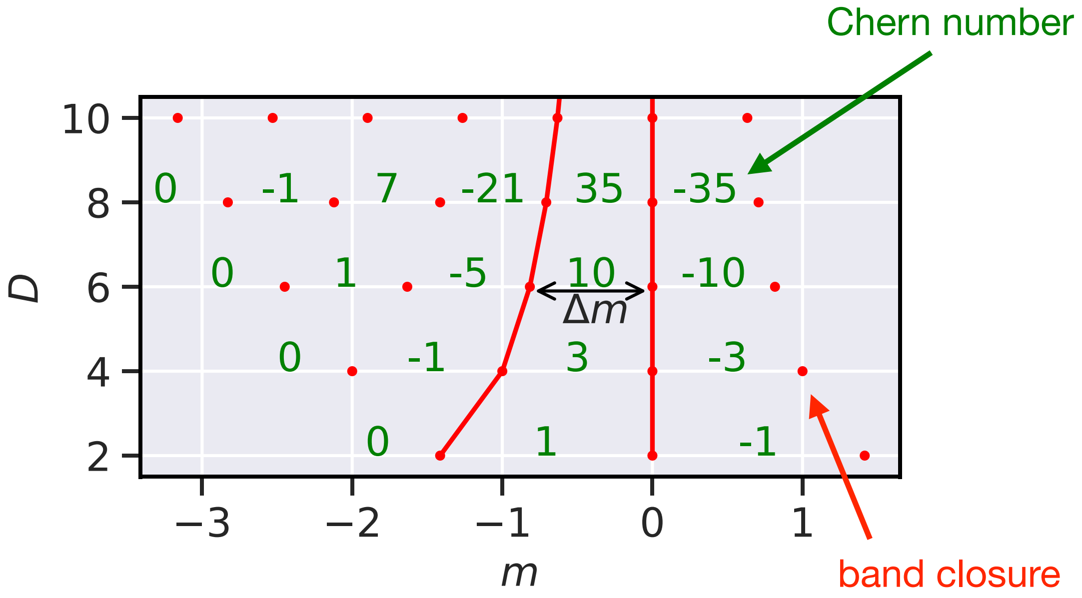
$$F = dA + A^2$$
$$A_{\alpha\beta}(k) = \langle u_\alpha(k)|\partial_k|u_\beta(k)\rangle\, dk$$

K-theory yields: Prodan, Schulz-Baldes (2016)

$$C_D(n_0) = (-1)^{n_0+\frac{D}{2}}\binom{D-1}{n_0}$$

interpretation

- (D-1)-dim. (1000…) surface hosts $\binom{D-1}{n_0}$ gapless edge states
- Weyl nodes at surface-projected HSP's k_{n_0} in the (D-1)-dim surface BZ
- sign: chirality of the of the Weyl points



$$m = \left(\sqrt{D} - 2\frac{n_0}{\sqrt{D}}\right)t^*$$

with increasing lattice dimension:

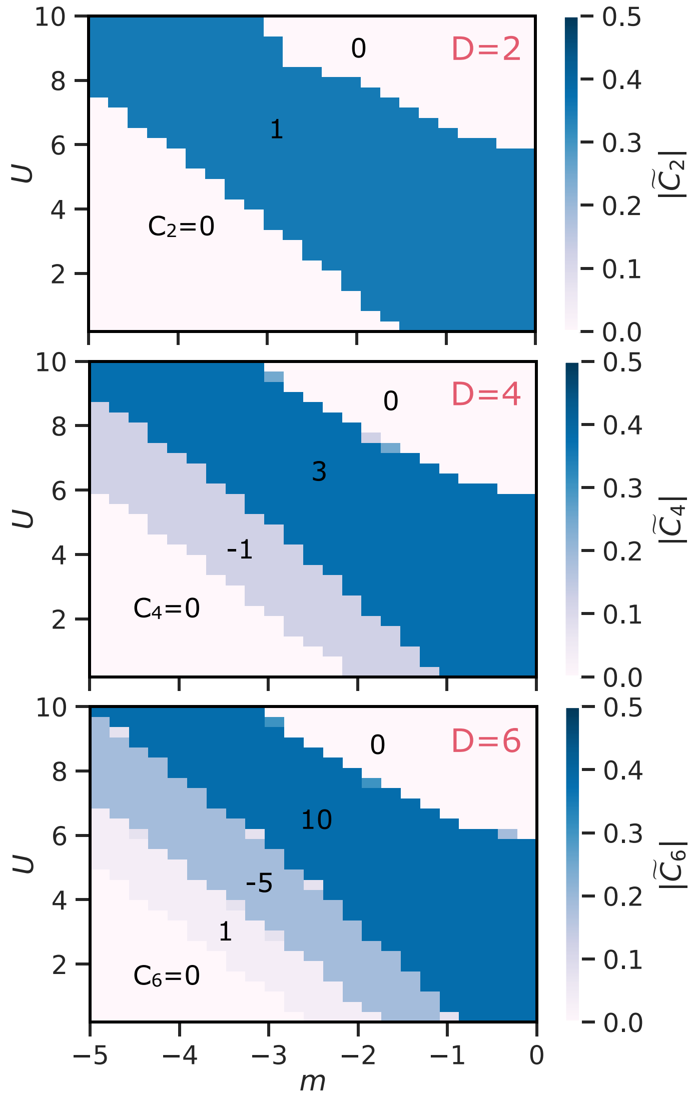
- more and more topological phases
- with increasing Chern numbers
- in an ever narrower m-range $\Delta m = 2t^*/\sqrt{D}$

$$\lim_{D\to\infty} C_D\ ?$$

DMFT of QWZ+U

topological phase diagrams for even finite D at half-filling

- trivial band insulator, trivial Mott insulator
- nontrivial intermediate phases
- more phases with increasing D
- phase diagram symmetric $m \leftrightarrow -m$
- at m=0: transition from an interacting Chern insulator to trivial Mott insulator
- strong A-B orbital polarization: $\Sigma_A \to U\,, \Sigma_B \to 0$ for $m \to \infty$
- $U_c(m) \sim |m|$ for $m \to \pm\infty$



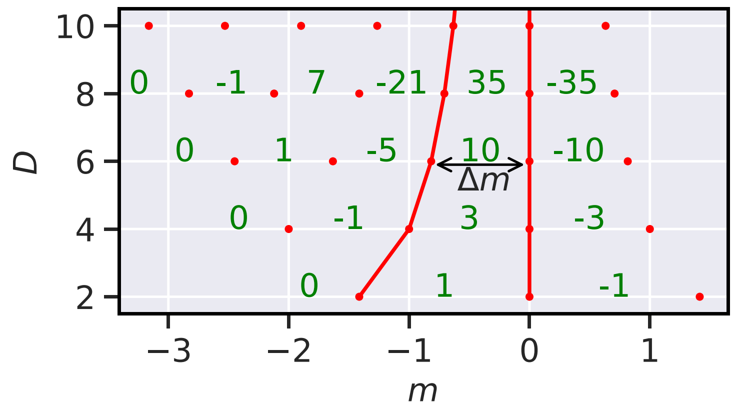
topological Hamiltonian

$$\mu \to \mu + \Sigma_+(\omega = 0)$$

$$m \to m + \Sigma_-(\omega = 0)$$

$$\Sigma_\pm = \frac{1}{2}(\Sigma_A \pm \Sigma_B)$$

Chern density



Chern number

$$C_D(n_0) = (-1)^{n_0 + \frac{D}{2}} \binom{D-1}{n_0}$$

sum rule

$$\sum_{n_0=0}^{D-1} \frac{1}{2^{D-1}} |C_D(n_0)| = 1$$

define:

Moivre-Laplace theorem

$$c(n_0) = \frac{1}{2^{D-1}} \binom{D-1}{n_0} \overset{D\to\infty}{=} \sqrt{\frac{2}{\pi D}} \exp\left(-2\frac{[(D/2)-n_0]^2}{D}\right)$$

$$= \sqrt{\frac{2}{\pi D}} \exp\left(-\frac{1}{2}\frac{m^2}{t^{*2}}\right) = \underbrace{\frac{2t^*}{\sqrt{D}}} \frac{1}{t^*\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{m^2}{t^{*2}}\right) \equiv c(m)dm$$

band closure condition

$$m = \left(\sqrt{D} - 2\frac{n_0}{\sqrt{D}}\right) t^*$$

continuum limit

$$\Delta m = 2t^*/\sqrt{D} \to dm$$

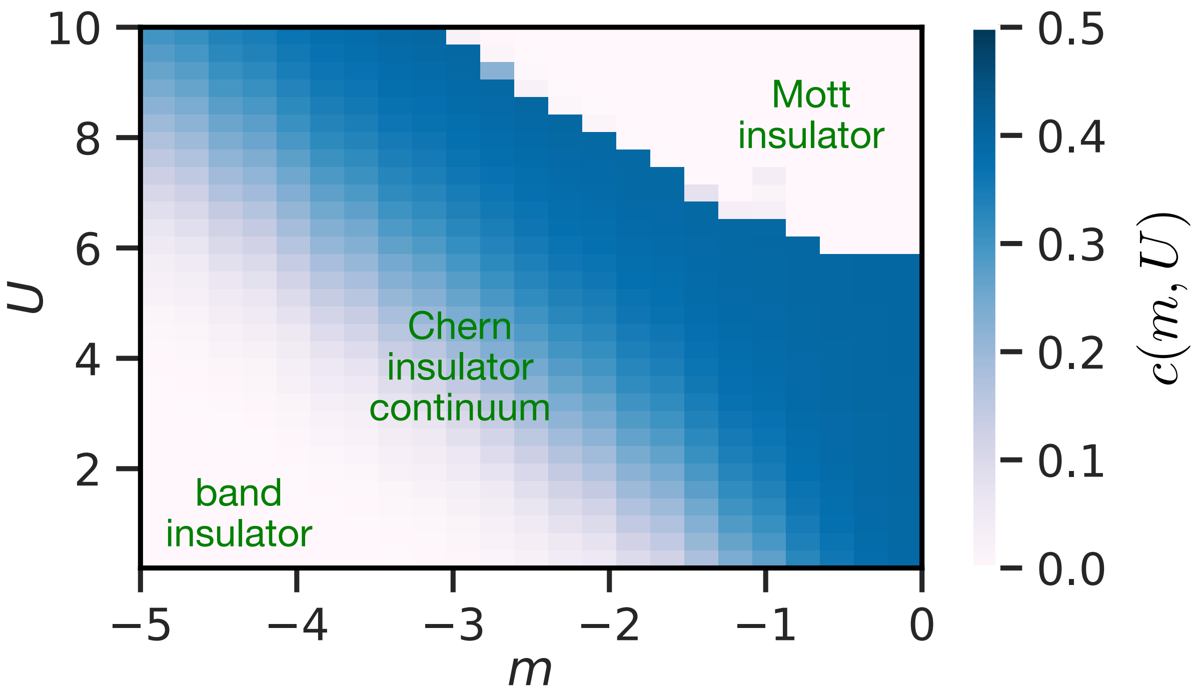
every m is critical !

Chern density

$$c(m) = \frac{1}{t^*\sqrt{2\pi}} e^{-\frac{1}{2}\frac{m^2}{t^{*2}}}$$

$$\int_{-\infty}^{\infty} c(m)dm = 1$$

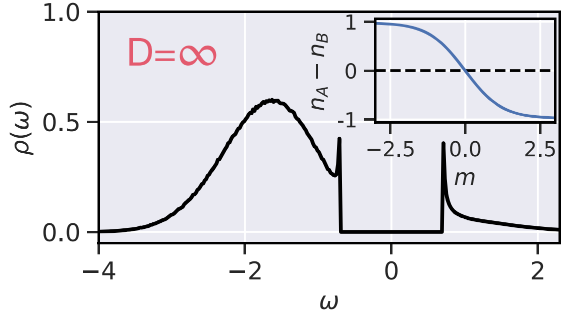
Phase diagram of the $D \to \infty$ QWZ+U model



- on iso-Chern lines: topologically equivalent systems
- continuum of topologically different phases on paths crossing iso-Cherns

Electronic structure

$$\Delta = \sqrt{2}t^*$$



for $m = \left(\sqrt{D} - 2\frac{n_0}{\sqrt{D}}\right)t^*$ the Bloch Hamiltonian

$$\epsilon(k) = \left(m + t\sum_{r=1}^{D}\cos k_r\right)\gamma_D^{(0)} + t\sum_{r=1}^{D}\sin k_r \gamma_D^{(r)}$$

close to one of the $\binom{D}{n_0}$ equivalent HSPs $k_{n_0} = (\underbrace{0, \ldots, 0}_{n_0}, \pi, \ldots, \pi)$ in the 1BZ

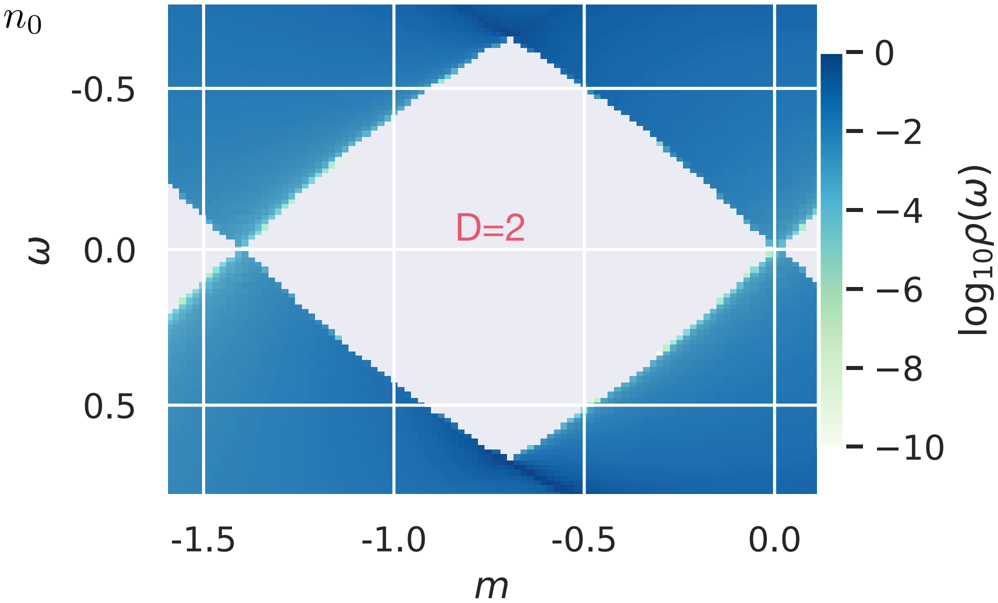
leads to a Dirac-cone dispersion

$$\epsilon_\pm(k) = \pm\frac{t^*}{\sqrt{D}}\sqrt{\sum_{r=1}^{D}(k_r - k_{n_0,r})^2}$$

local DOS at low frequencies

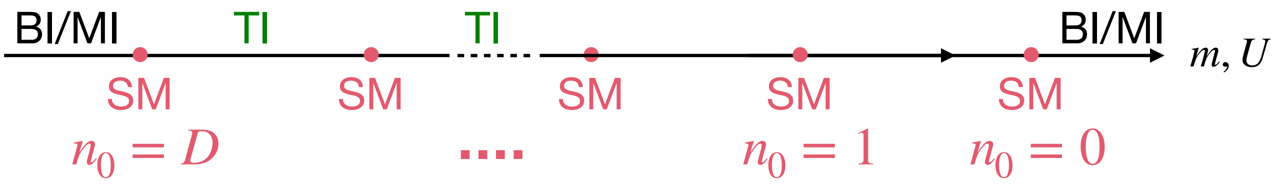
$$\boxed{\rho_\alpha(\omega) = \underbrace{c(D, n_0)}_{\uparrow}|\omega|^{D-1}/t^{*D}}$$

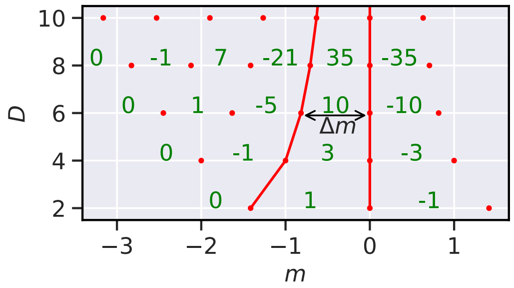
c(D,n₀) $\rightarrow 0$ for $D \rightarrow \infty$ exponentially fast



Semimetal vs. topological insulator

finite dimension D:





$$m = \left(\sqrt{D} - 2\frac{n_0}{\sqrt{D}}\right) t^*$$

$$k_{n_0} = (\underbrace{0, \ldots, 0}_{n_0}, \pi, \ldots, \pi)$$

infinite dimensions:

- Chern density c(m,U) varies continuously $\quad \Delta m = 2t^*/\sqrt{D} \rightarrow dm$
- distinction between SM and TI not meaningful
- there is no “band closure at isolated k-points in the 1BZ”

Dirac cone: $\quad \epsilon_\pm(k) = \pm t^* \sqrt{\frac{1}{D}\sum_{r=1}^{D}(k_r - k_{n_0,r})^2} = \pm t^* \|k - k_{n_0}\|$

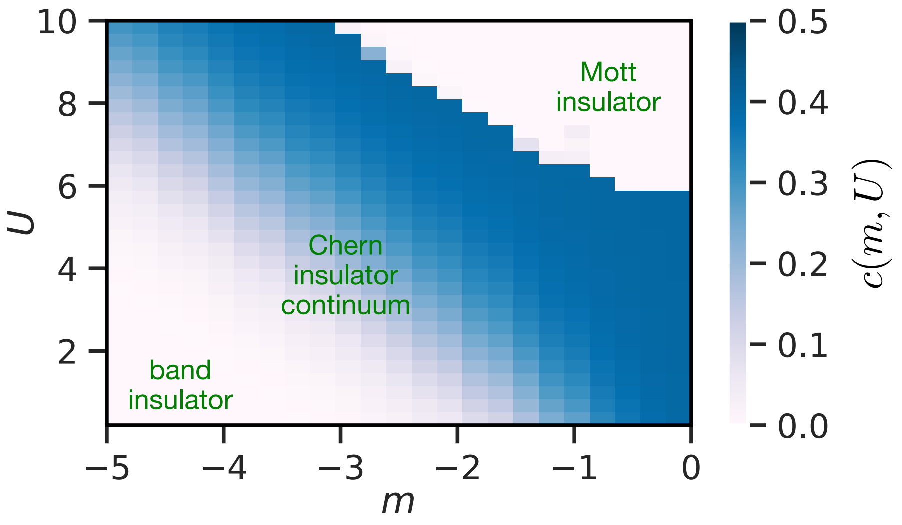
here $\quad \|k\|^2 = \lim_{D\to\infty} \frac{1}{D}\sum_{r=1}^{D} k_r^2$

but $\quad \|k\| = 0 \not\Rightarrow k = 0 \qquad \|\cdot\|$ is a semi-norm

Conclusions

What survives $D \to \infty$?

- local correlations effects
- nontrivial topological classification
- the overall structure of the finite-D phase diagrams
- DMFT solves the problem exactly



D. Krüger, M.P., PRL (2021)

What does not ?

- distinction between semi-metal / insulator states
- arguments based on the discreteness of the topological invariant
- Chern density is positive: chirality of edge modes ?
- there is not *the* $D \to \infty$ limit (only even D considered)

To do

Can we topologically classify all interacting electron models ?

Can we topologically classify all interacting lattice electron models ?

Can we topologically classify all lattice-electron models with local interactions on infinite-dimensional lattices ?

Can we topologically classify, in infinite dimensions, Hubbard-type lattice models derived from noninteracting prototypes of the tenfold way?

Can we topologically classify at least one of the prototype band models of the tenfold way, plus Hubbard-U, on an infinite-dimensional lattice ?

Example for a classification of mathematical structures

group : set G, operation $\circ : G \times G \to G$

postulates
$$a \circ (b \circ c) = (a \circ b) \circ c$$
$$a \circ e = e \circ a = a$$
$$a \circ a^{-1} = a^{-1} \circ a = e$$

G_1, G_2 are isomorphic, $G_1 \cong G_2$,

if there is a bijective map $\varphi : G_1 \to G_2$, s.t.

$$\boxed{\varphi(a \circ b) = \varphi(a) \circ \varphi(b)}$$

Classification of all simple finite groups

(milestone of group theory ?)

proof : $O(10^3)$ pages, $O(10^2)$ authors
1955 – 2004

group

finite

simple

series: $\mathbb{Z}_n$ (n prime) A_n ($n \geq 5$)   Lie-type groups   26 sporadic groups

Mathieu group M_{11}, $11 = \max_{M_{11}} \{|g|\}$

$|M_{11}| = 2^4 3^2 5\, 11 = 7920$

smallest

2
3
:
25

largest

Fischer monster group (friendly giant)

rotations in a 196883-dimensional space, order: 54-digit number

matrix groups over finite fields $\mathbb{F}$, char $\mathbb{F}$ $= \min\{p \mid \overbrace{1+1+\cdots+1}^{p \text{ times}} = 0\}$ ← prime

Chevalley

twisted Chevalley

Tits group ← "27th sporadic group", order $\approx 10^7$

presentation: $\langle a, b \mid a^2 = b^3 = (ab)^{13} = [a,b]^5 =$
$= [a, bab]^4 = ((ab)^4 ab^{-1})^6 = e \rangle$