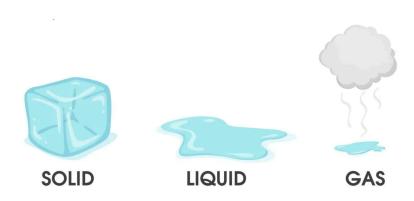
The Curious Symmetry Breaking of O(n) Quantum Spin Chains

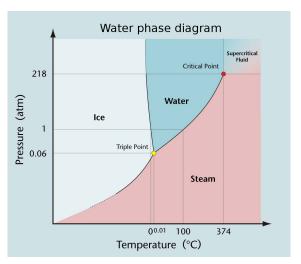
Michael Ragone

...or, what I did during grad school.

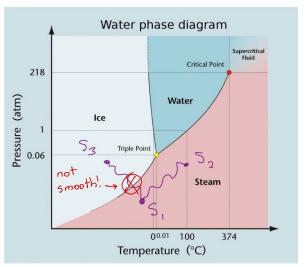
March 12, 2024

Phases of matter





What is a phase?



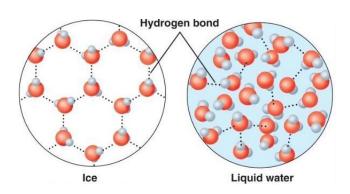
"Two systems are in the same phase if we can find a smooth path connecting them."

Phases and invariants

- How do we distinguish phases?
- One approach: find invariants preserved along paths.
- The "does it have a well-defined volume?" invariant.
 - Water and ice have a well-defined volume.
 - Steam does not.
- This cannot distinguish water from ice.
- By finding more invariants, we can distinguish more phases!

Phases and invariants

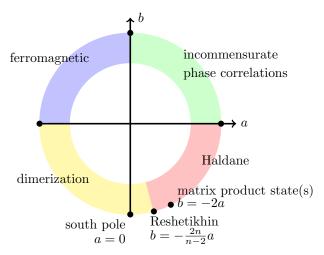
Rich source of invariants: symmetry properties.



Time-averaged density $\rho(x), x \in \mathbb{R}^3$:

- Liquid: $\rho(x) = \rho(x+v), v \in \mathbb{R}^3$. Continuous symmetry.
- Not so for ice! Only has discrete lattice symmetry.

Another phase diagram



Our goal: better understand (and prove the distinctness of) the "Haldane" and "dimerized" phases.

Classical analogy for setup

Suppose we have a particle which moves on the space $[a, b] \subseteq \mathbb{R}$. We want to describe a collection of experiments which measures its position.

- Observable: Position function A(x) = x.
 - This lives in an algebra, 1 say $\mathcal{A} = C([a, b])$, with some topological structure, say $\|\cdot\|_{\infty}$.
- State: ω is integration against a probability density $\rho(x)dx$, representing the position of a particle taken over many experiments.
- The expected position of the distribution $\rho(x)dx$ is

$$\omega(A) = \int_{[a,b]} x \, \rho(x) dx.$$

Experiment = pairing of observable $A \in \mathcal{A}$ and state $\omega \in \mathcal{A}^*$.

¹Vector space + multiplication

Finite Quantum spin chains

- Work on finite chains $[a, b] \subseteq \mathbb{Z}$.
- Each site $x \in \mathbb{Z}$ has a Hilbert space $\mathcal{H}_x = \mathbb{C}^n$. Combining sites is tensor product:

$$\mathcal{H}_{[a,b]} = \mathcal{H}_a \otimes \mathcal{H}_{a+1} \otimes \cdots \otimes \mathcal{H}_b.$$

Bases are easy to find. For example, if \mathcal{H}_1 has orthonormal basis

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
, then $\mathcal{H}_1 \otimes \mathcal{H}_2$ has orthonormal basis

$$|00\rangle$$
, $|01\rangle$, $|10\rangle$, $|11\rangle$,

where $|ij\rangle = |i\rangle \otimes |j\rangle$.

• So, $\dim(\mathcal{H}_{[1,\ell]}) = n^{\ell}$.

Finite Quantum spin chains

- Observables: $\mathcal{A}_{[a,b]} = \mathcal{B}(\mathcal{H}_{[a,b]})$ with operator norm $\|\cdot\|_{\infty}$.
 - $\mathcal{A}_{[1,\ell]}$ is just $n^{\ell} \times n^{\ell}$ complex matrices $M_{n^{\ell}}(\mathbb{C})$.
 - Note: this is a noncommutative algebra!
- States: positive, normalized linear functionals $\omega: \mathcal{A}_{[a,b]} \to \mathbb{C}$.
 - Since dim($\mathcal{H}_{[a,b]}$) finite, Riesz representation theorem applied to the inner product $\langle A, B \rangle = \text{Tr} A^* B$ on $\mathcal{A}_{[a,b]}$ says there is a $\rho \in \mathcal{A}_{[a,b]}$ such that

$$\omega(A) = \text{Tr}\rho A.$$

- $\rho = \rho^* \ge 0$ is positive $\rho \ge 0$, and ρ is normalized $\text{Tr}\rho = 1$. In this sense ρ is a quantum analogue of a probability density function.
- Pure states: density matrices are rank-1 orthogonal projections $\rho = |\psi\rangle\langle\psi|$ onto the subspace spanned by $|\psi\rangle \in \mathcal{H}_{[a,b]}$.

Quantum spin chain setting

- The "energy" (and thus the dynamics) of the system is dictated by a Hamiltonian $H_{[a,b]} = H^*_{[a,b]} \in \mathcal{A}_{[a,b]}$.
- Locality: a particle at site $x \in \mathbb{Z}$ should not interact too strongly with spatially distant $y \in \mathbb{Z}$.
- Nearest neighbor Hamiltonian: $H_{\ell} \in \mathcal{A}_{[1,\ell]}$

$$H_{\ell} := \sum_{x=1}^{\ell-1} h_{x,x+1},$$

where $h_{x,x+1}$ is a copy of $h = h^* \in M_n(\mathbb{C}) \otimes M_n(\mathbb{C})$ acting on sites x, x + 1.

• We will study ground states. Pure ground states correspond to lowest eigenvalue eigenvectors $H_{[1,\ell]} |\psi\rangle = \lambda |\psi\rangle$.

Example: Just Transverse Fields

- Qubit chain: each site is $\mathcal{H}_x = \mathbb{C}^2$, so Hilbert space is $\mathcal{H}_{[1,\ell]} = \mathbb{C}^{2^\ell}$.
- On-site orthonormal basis: $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \in \mathbb{C}^2.$
- Hamiltonian:

$$H_{[1,\ell]} = \sum_{x=1}^{\ell} Z_x,$$

where $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. How to find ground state? Easy here, since $[Z_x, Z_y] = 0$ so each term is simultaneously diagonalizable.

$$H_{[1,\ell]}|11...1\rangle = (Z_1 + Z_2 + \cdots + Z_\ell)|11...1\rangle = -\ell|11...1\rangle.$$

Example: The Heisenberg Chain

- Qubit chain: each site is $\mathcal{H}_x = \mathbb{C}^2$, so Hilbert space is $\mathcal{H}_{[1,\ell]} = \mathbb{C}^{2^\ell}$.
- Hamiltonian:

$$H_{[1,\ell]} = \sum_{x=1}^{\ell-1} - \mathtt{SWAP}_{x,x+1},$$

where SWAP_{x,x+1} $|u v\rangle = |v u\rangle$.

• To find ground states, we diagonalize $H_{[1,\ell]}$. Let's start with $\ell=2$, $\mathcal{H}_{[1,\ell]}=\mathbb{C}^4$,

$$\begin{split} \operatorname{SWAP}|00\rangle &= |00\rangle \\ \operatorname{SWAP}\left(|01\rangle + |10\rangle\right) &= |01\rangle + |10\rangle \\ \operatorname{SWAP}\left(|11\rangle\right) &= |11\rangle \\ \operatorname{SWAP}\left(|01\rangle - |10\rangle\right) &= -\left(|01\rangle - |10\rangle\right). \end{split}$$

Example: The Heisenberg Chain

• In other words: in the basis $\underbrace{|00\rangle, |10\rangle + |01\rangle, |11\rangle}_{sym}, \underbrace{|01\rangle - |10\rangle}_{antisym},$

$$\mathtt{SWAP} = P_{sym} - P_{antisym} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

So: -SWAP has pure ground states whose vectors are in the range of P_{sym} .

- Not hard to see that ground state vectors of $H_{[1,\ell]}$ are the symmetric tensors $\operatorname{Sym}^{\ell}(\mathbb{C}^2) \subseteq (\mathbb{C}^2)^{\otimes \ell}$.
- The ground state vector for the interaction h = SWAP is just $|01\rangle |10\rangle$, which is *entangled*, i.e. cannot be expressed as 1 simple tensor.

Symmetry and Symmetry Breaking

- Symmetry is often given as a unitary representation (cts. group homomorphism $G \to \mathcal{B}(\mathcal{H}_{[1,\ell]})$) of a Lie group.
- Ex: the Heisenberg Chain is invariant under tensor rep of SU(2):

$$[U^{\otimes \ell}, H_{[1,\ell]}] = 0, \qquad \text{for all } U \in SU(2).$$

ullet Question: do the ground states of H also possess this symmetry?

Symmetry and Symmetry Breaking

Simultaneous Block-Diagonalization Lemma: Let $U: G \to \mathcal{B}(\mathcal{H}_{[1,\ell]})$ a rep of G and $H = H^*$ such that

$$[U_g, H] = 0$$
 for all $g \in G$.

Then, for any eigenvector $|\psi\rangle$ with eigenvalue λ , $U_g |\psi\rangle$ is also an eigenvector of H with eigenvalue λ . Proof:

$$H(U_g | \psi \rangle) = U_g H | \psi \rangle = U_g \lambda | \psi \rangle = \lambda (U_g | \psi \rangle).$$

Consequence: The ground state space is invariant under G.

• If every pure ground state $|\psi\rangle$ is invariant under symmetry, i.e. $U_g |\psi\rangle = |\psi\rangle$ for all $g \in G$, we say the symmetry is *unbroken*.

Symmetry and Symmetry Breaking

- What else might happen?
- Ex: The ground state space $\operatorname{Sym}^2(\mathbb{C}^2)$ of the 2-site Heisenberg chain is invariant under $U \otimes U$, $U \in SU(2)$. But

$$U = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \in SU(2)$$
 and

$$U \otimes U |00\rangle = (U |0\rangle) \otimes (U |0\rangle) = |11\rangle.$$

H is invariant under an SU(2) symmetry, but its ground states aren't. The SU(2) symmetry is broken.

- Let's introduce the phase diagram.
- Just like the water example, symmetry breaking can be used to distinguish phases.

A phase diagram: O(n)-invariant spin chains

- On-site Hilbert space: $\mathcal{H}_x = \mathbb{C}^n$.
- The tensor representation of O(n), the orthogonal group, on $\mathbb{C}^n \otimes \mathbb{C}^n$ is given by $R \mapsto R \otimes R$.
- MAT 261 (Lie Groups) \implies the irrep decomposition² is

$$\mathbb{C}^n \otimes \mathbb{C}^n \cong \underbrace{M_2 \oplus \mathbb{C} |\xi\rangle}_{sym} \oplus \underbrace{\bigwedge^2(\mathbb{C}^n)}_{antisym},$$

where
$$|\xi\rangle = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} |ii\rangle$$
.

• We can then parameterize orthogonally invariant n.n. interactions, i.e. those with

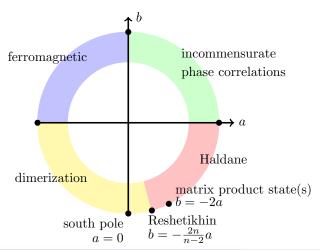
$$(R \otimes R)h_{x,x+1}(R^{-1} \otimes R^{-1}) = h_{x,x+1}.$$

 $^{^2}$... except n=4.

A phase diagram: O(n)-invariant spin chains

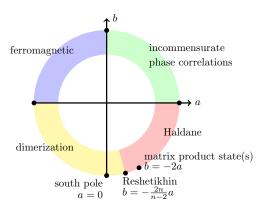
Up to a shift in ground state energy, every such interaction is given by

$$h = a \operatorname{SWAP} + b \left| \xi \right\rangle \left\langle \xi \right| + \mathbb{1}, \qquad a, b \in \mathbb{R}.$$



Phases as equivalence classes

"Two model Hamiltonians H_0, H_1 are in the same gapped phase if we can find a smooth path of gapped Hamiltonians connecting them."



How do we distinguish the Haldane phase from the dimerized phase?

Dimerization at the south pole

- Dimerization is a type of symmetry breaking where translation invariance of H is broken by a pair of 2-periodic ground state.
- Physically, dimerization happens when Hamiltonian encourages strong entanglement + "monogamy of entanglement".
- This is what happens at the south pole point: $Q = |\xi\rangle \langle \xi|$, and

$$H_{[1,\ell]} = \sum_{x=1}^{\ell-1} -Q_{x,x+1}.$$

- $-Q_{x,x+1}$ rewards entanglement across sites x, x+1. But particles can only entangle strongly with one neighbor.
- Björnberg et.al. 2021 proved there are two 2-periodic ground states ω_{\pm} such that:
 - Entanglement structure "alternates"
 - ω_+ and ω_- distinguishable by 2-site observable

The odd n case

- When n is odd, Tu et. al. 2008 showed the matrix product state (MPS) point has only one translation-invariant ground state.
- So: translation symmetry is unbroken in the Haldane phase, but broken in the dimerized phase.

Theorem (Bachmann, Mickalakis, Nachtergaele, Sims 2012)

Two Hamiltonians H_0 , H_1 connected by a smooth path of uniformly gapped Hamiltonians must have the same number of pure ground states.

• When n is odd, these phases are distinct.

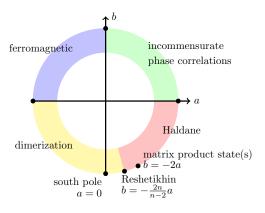
The even n case

- When n is even, the MPS point has a pair of 2-periodic ground states ω_{\pm} . So dimension is not enough.
 - Will later see this is not dimerization. Physical mechanism is very different!

• Our lesson from water: studying symmetry properties can help us distinguish these phases. We have a natural G = O(n) symmetry.

G-symmetric phases as equivalence classes

"Two G-symmetric Hamiltonians H_0 , H_1 are in the same G-gapped phase³ if we can find a smooth path of G-symmetric gapped Hamiltonians connecting them."



 $^{^3}$ aka $symmetry\mbox{-}protected\ topological\ (SPT)\ phase$

G-symmetric phases as equivalence classes

- Let G be a compact Lie group (this includes finite groups). Let H_0, H_1 be G-symmetric gapped Hamiltonians. Then let s = 0, 1 and define $S(s) \subseteq A^*$ to be ground state space of H_s .
- Just like simultaneous block diagonalization: S(s) is invariant under G.
 - If every $\omega \in \mathcal{S}(s)$ is invariant under G, i.e. $g \cdot \omega = \omega$ for all $g \in G$, then G-symmetry is unbroken.
 - If there exists an $\omega \in \mathcal{S}(s)$ where $g \cdot \omega \neq \omega$, then G-symmetry is broken.

Theorem (Bachmann, Nachtergaele 2014)

Two G-symmetric Hamiltonians H_0, H_1 connected by a smooth path of uniformly gapped G-symmetric Hamiltonians have that $S(0) \cong S(1)$ as G-representations.

O(n)-to-SO(n) symmetry breaking

• It was proven in Björnberg 2021 that the south pole ground states $\widetilde{\omega}_+, \widetilde{\omega}_-$ are both invariant under O(n): for all $R \in O(n)$ and $A_1 \otimes \cdots \otimes A_\ell \in \mathcal{A}_{[1,\ell]}$,

$$\widetilde{\omega}_{+}(RA_{1}R^{-1}\otimes\cdots\otimes RA_{\ell}R^{-1}) = \widetilde{\omega}_{+}(A_{1}\otimes\cdots\otimes A_{\ell})$$
$$\widetilde{\omega}_{-}(RA_{1}R^{-1}\otimes\cdots\otimes RA_{\ell}R^{-1}) = \widetilde{\omega}_{-}(A_{1}\otimes\cdots\otimes A_{\ell}).$$

O(n)-to-SO(n) symmetry breaking

Theorem (Nachtergaele, R)

The MPS ground states ω_+, ω_- are invariant under SO(n), but swapped under O(n), i.e. for any $R \in O(n)$ with det(R) = -1,

$$\omega_+(RA_1R^{-1}\otimes\cdots\otimes RA_\ell R^{-1})=\omega_-(A_1\otimes\cdots\otimes A_\ell).$$

Symmetry is broken! These two points support different irreps of O(n) and so these are different O(n)-symmetric phases.

Corollary

The south pole point and the MPS occupy distinct O(n) gapped phases.

The MPS point: it ain't dimerization

- Two key features of dimerization:
 - Entanglement structure "alternates".
 - ω_{+} and ω_{-} are distinguishable by a 2-site observable.
- It was believed that the even n MPS ground states were dimerized. But we found something surprising.

The MPS point: it ain't dimerization

Theorem (Nachtergaele, R)

- \bullet ω_{+} and ω_{-} have identical entanglement structure.
- ② $\omega_+ \neq \omega_-$, but ω_+ and ω_- are indistinguishable by any observable with support k < n/2, i.e. for any $A_1 \otimes \cdots \otimes A_k \in \mathcal{A}_{[1,k]}$,

$$\omega_+(A_1\otimes\cdots\otimes A_k)=\omega_-(A_1\otimes\cdots\otimes A_k).$$

So: if $n \ge 6$, then every 2-local observable has identical expectation:

$$\omega_+(A_1 \otimes A_2) = \omega_-(A_1 \otimes A_2)$$
 for all $A_1, A_2 \in M_n(\mathbb{C})$.

Let's talk a little representation theory.

Building the MPSs

The interaction $h = SWAP - 2|\xi\rangle\langle\xi| + 1 \ge 0$ is frustration free, i.e.

$$\ker \sum_{x=1}^{\ell-1} h_{x,x+1} = \bigcap_{x=1}^{\ell-1} \ker h_{x,x+1} \neq \{0\}.$$

Finite chain ground states are given by MPSs.

The rank-n Clifford algebra C_n

The rank-n Clifford algebra is the associative algebra generated by the operators $\gamma_1, \ldots, \gamma_n$ subject to

$$\gamma_i \gamma_j + \gamma_j \gamma_i = 2\delta_{ij} \mathbb{1}, \qquad \gamma_i^* = \gamma_i, \qquad i, j = 1, \dots, n.$$

- Finite dimensional matrix algebra
- n even: center is just 1, so $\mathcal{C}_n = M_{2^{n/2}}(\mathbb{C})$.

Matrix Product States

When n even, $\mathcal{B} = \mathcal{C}_n$. Define MPS by $\psi : \mathcal{B} \to (\mathbb{C}^n)^{\otimes \ell}$

$$\psi(B) = \sum_{i_1,\dots,i_\ell=1}^n \operatorname{Tr} \left(B \gamma_{i_\ell} \dots \gamma_{i_1} \right) | i_1,\dots,i_\ell \rangle.$$

• Let's get some intuition for n=4.

Let's explicitly compute the MPSs on $\ell = 2$ sites for n = 4. Recall that since $h = \text{SWAP} - 2|\xi\rangle\langle\xi| + 1$, the ground state space is \mathcal{G}_2

$$\mathcal{G}_2 = \bigwedge^2 \mathbb{C}^4 \oplus \mathbb{C} \ket{\xi} \bra{\xi}.$$

Clifford algebra basis $\mathcal{B} = \mathcal{C}_4$:

A useful lemma

Lemma

$$Tr\gamma_I\gamma_J=0$$
 whenever $I\neq J$.

Proof.

(Idea)

$$2\mathrm{Tr}\gamma_1=\mathrm{Tr}\gamma_1(\gamma_2\gamma_2+\gamma_2\gamma_2)=\mathrm{Tr}\gamma_2(\gamma_1\gamma_2+\gamma_2\gamma_1)=0.$$



Calculate some MPSs, with $D = \text{Tr } \mathbb{1}$.

$$\frac{1}{D}\psi(\mathbb{1}) = \frac{1}{D} \sum_{i_1, i_2} \operatorname{Tr} \left(\mathbb{1} \gamma_{i_2} \gamma_{i_1} \right) | i_1, i_2 \rangle$$

$$= \frac{1}{D}\psi(\gamma_1) = \frac{1}{D} \sum_{i_1, i_2} \operatorname{Tr} \left(\gamma_1 \gamma_{i_2} \gamma_{i_1} \right) | i_1, i_2 \rangle$$

$$= \frac{1}{D}\psi(\gamma_1 \gamma_2) = \frac{1}{D} \sum_{i_1, i_2} \operatorname{Tr} \left(\gamma_1 \gamma_2 \gamma_{i_2} \gamma_{i_1} \right) | i_1, i_2 \rangle$$

$$= \frac{1}{D}\psi(\gamma_0) = \frac{1}{D} \sum_{i_1, i_2} \operatorname{Tr} \left(\gamma_0 \gamma_{i_2} \gamma_{i_1} \right) | i_1, i_2 \rangle$$

Finite chain ground states

Check: every $\psi(B)$ is a ground state of H.

Finite chains as SO(n) representations

• The Lie algebra $\mathfrak{so}(n)$ embeds into the Clifford algebra in a natural way. Let $L_{i,j} = |i\rangle \langle j| - |j\rangle \langle i|$, $1 \leq i < j \leq n$. Then the map $\pi : L_{i,j} \mapsto \frac{1}{2} \gamma_i \gamma_j$ is a Lie algebra homomorphism $\pi : \mathfrak{g} \to \mathcal{C}_n$:

$$\frac{1}{4}[\gamma_i \gamma_j, \gamma_r \gamma_s] = \delta_{jr} \gamma_i \gamma_s - \delta_{ir} \gamma_j \gamma_s + \delta_{is} \gamma_j \gamma_r - \delta_{js} \gamma_i \gamma_r. \tag{1}$$

Since $C_n \cong M_{2^{n/2}}(\mathbb{C})$, this defines a Lie algebra representation on $\mathbb{C}^{2^{n/2}}$ called the *spin* representation.

- Exponentiates to unitary representation $\Pi: Spin(n) \to \mathcal{U}(\mathbb{C}^{2^{n/2}})$, where we recall $Spin(n)/\{\pm 1\} \cong SO(n)$.
 - If $\Pi(1) = \Pi(-1)$, this descends to a representation of SO(n).
 - If $\Pi(1) \neq \Pi(-1)$, only get a *projective* representation of SO(n), i.e.

$$\Pi(w)\Pi(v) = \alpha(w,v)\Pi(wv), \qquad w,v \in SO(n),$$

where $\alpha: SO(n) \times SO(n) \to U(1)$ is a phase.

Finite chains as SO(n) representations

• Turns out, this is what we need to understand the symmetry of our MPSs:

$$w^{\otimes \ell}\psi(B) = \psi(\Pi(w)B\Pi(w)^{-1}), \qquad B \in \mathcal{B}, w \in SO(n),$$
 (2)

where we use that $Spin(n)/\{\pm 1\} \cong SO(n)$.

- This has a nice tensor network representation.
- Thermodynamic limiting states inherit this symmetry! So if we rotate the full chain,

$$\dots w \otimes w \otimes w \otimes w \otimes \dots$$

then ω is invariant under this.

• This reaction to symmetry will shed light on the states and give yet another index.

Finite chains as SO(n) representations

Define $\psi_{\ell}: \mathcal{B} \to (\mathbb{C}^n)^{\otimes \ell}$, and write $\mathcal{G}_{\ell} = \{\psi_{\ell}(B): B \in \mathcal{B}\}.$

Theorem (Nachtergaele, R)

Let $\ell \geq n$ and let $V = \mathbb{C}^n$. Then the representation \mathcal{G}_{ℓ} of SO(n) decomposes as

$$\mathcal{G}_{\ell} = \begin{cases} \bigwedge^{1} V \oplus \bigwedge^{3} V \oplus \cdots \oplus \bigwedge^{n-1} V & \text{if } \ell \text{ is odd.} \\ \bigwedge^{0} V \oplus \bigwedge^{2} V \oplus \cdots \oplus \bigwedge^{n} V & \text{if } \ell \text{ is even.} \end{cases}$$

This is an irrep decomposition, except for $\bigwedge^{n/2}V \cong U_+ \oplus U_-$.

In some sense, the U_+ and U_- are the only things distinguishing the two infinite volume ground states ω_+ and ω_- , and they only appear when the chain is long enough $\ell \geq n/2$.

• This is a representation-theoretic symptom of the "short chain indistinguishability"!

Another index

- We can extract yet another invariant of G-gapped phases⁴.
- If we cut the lattice $\mathbb{Z} = \mathbb{Z}_{(-\infty,0]} \cup \mathbb{Z}_{[1,\infty)}$, we expose some degrees of freedom of the state.
- If we then rotate the half-chain, this gives another representation of Spin(n). This is a type of bulk-boundary correspondence.
- For our MPS, this is exactly $\Pi!$
- We can assign a (Borel) group cohomology index $h \in H^2(SO(n), U(1))$ to any projective rep.
 - Can show $H^2(SO(n), U(1)) \cong \mathbb{Z}_2$. There is only trivial and nontrivial projective.
- Chen-Gu-Liu-Wen 2013, Ogata 2020: SPT index h is invariant within a G-gapped phase.

⁴aka SPT index

SPT indices

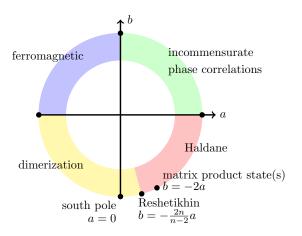
Theorem (Nachtergaele, \mathbf{R})

The south pole point has a pair of trivial SPT indices, and the MPS point has a pair of nontrivial SPT points.

Corollary

The south pole point and the MPS point occupy distinct SO(n) gapped phases.

Who knows what else is hiding in this O(n)-chain phase diagram?



Maybe **your** PhD!