dedicated to the memory of Ian Affleck (1952 - 2024)

Haldane conjecture valence-bond picture SPT phases and all that in quantum spin chains

Hal Tasaki

The 3rd public ExU Online Colloquium / February 6th, 2025, UTC 8:00-

"quantum phases of matter"

quantum mechanics is surprising, in all directions

Part 1

Haldane gap, valence-bond picture, and SPT phases

Part 2

$S=1$ antiferromagnetic Heisenberg chain is topologically nontrivial if gapped

- elementary index theorem
- main theorem

Part 1
Haldane gap, valence-bond picture, and SPT phases

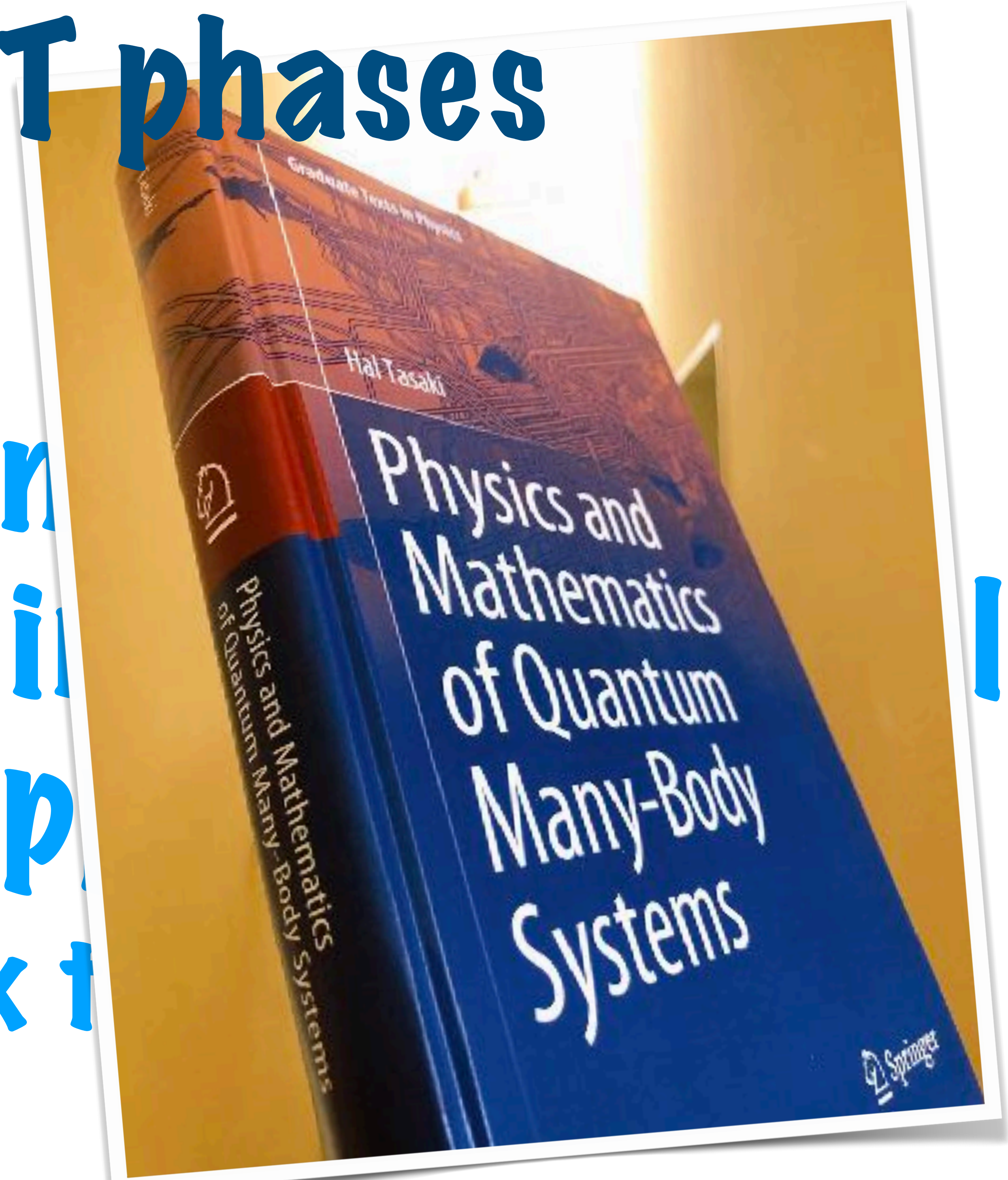
Part 2

$S = 1$ antiferrom

Heisenberg chai lly

nontrivial if gap

- elementary index t
- main theorem

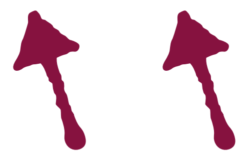


ground states of two-spin systems

classical spin $\boldsymbol{S} = (S^{\mathrm{x}}, S^{\mathrm{y}}, S^{\mathrm{z}}) \in \mathbb{R}^3 \qquad |\boldsymbol{S}| = S$

ferromagnetic interaction

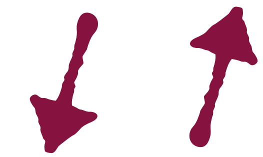
$$E = -\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$$



infinitely many g.s.

antiferromagnetic interaction

$$E = \boldsymbol{S}_1 \cdot \boldsymbol{S}_2$$



infinitely many g.s.

quantum spin (operators) $\hat{\boldsymbol{S}} = (\hat{S}^{\mathrm{x}}, \hat{S}^{\mathrm{y}}, \hat{S}^{\mathrm{z}})$

$$[\hat{S}^{\mathrm{x}}, \hat{S}^{\mathrm{y}}] = \mathrm{i}\hat{S}^{\mathrm{z}}, \ldots \qquad \hat{\boldsymbol{S}}^2 = S(S+1) \qquad S = \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots$$

ferromagnetic interaction

$$\hat{H} = -\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2$$

$|\uparrow\rangle|\uparrow\rangle$

$|\downarrow\rangle|\downarrow\rangle$

$\{|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle\}/\sqrt{2}$

spin triplet

infinitely many g.s.

antiferromagnetic interaction

$$\hat{H} = \hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2$$

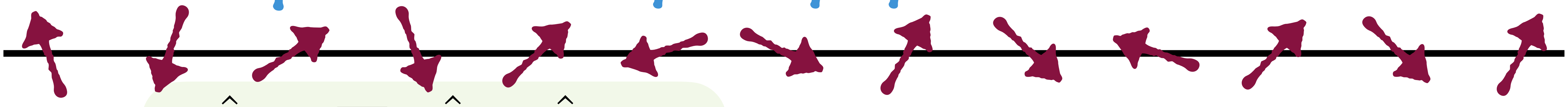
$$\{|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\}/\sqrt{2}$$

spin singlet

unique rotationally invariant ground state

quantum antiferromagnetic Heisenberg chain

one of the most standard and realistic models of quantum many-body systems



$$\hat{H} = \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} \qquad (\hat{\boldsymbol{S}}_j)^2 = S(S+1)$$

the only parameter is the spin $S = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$

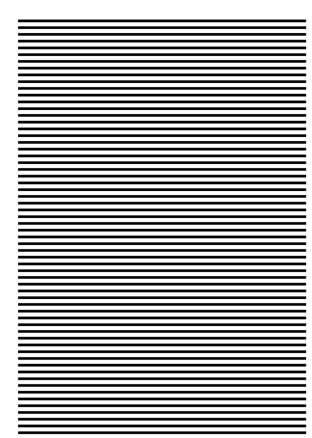
what are the ground state and low energy excitations?

Haldane's discovery Haldane 1981, 1983, 1983

Bethe ansatz for $S = \frac{1}{2}$

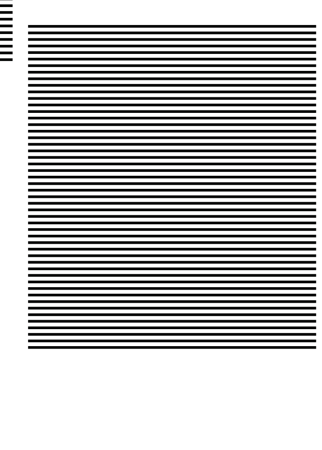
half-odd integer S

unique gapless ground state



integer S

unique **gapped** ground state



unique ground state accompanied by a nonzero energy gap above the g.s. energy

Photo: A. Mahmoud

F. Duncan M. Haldane

Prize share: 1/4

$S=1$ quantum spin chains

single spin $\hat{\boldsymbol{S}}=(\hat{S}^{\mathrm{x}},\hat{S}^{\mathrm{y}},\hat{S}^{\mathrm{z}})$ **acts on** $\mathbb{C}^3$

standard basis $\{|+\rangle,|0\rangle,|-\rangle\}$

$$|+\rangle=\begin{pmatrix}1\\0\\0\end{pmatrix},\quad |0\rangle=\begin{pmatrix}0\\1\\0\end{pmatrix},\quad |-\rangle=\begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$\hat{S}^{\mathrm{z}}|0\rangle=0,\qquad \hat{S}^{\mathrm{z}}|\pm\rangle=\pm|\pm\rangle$$

$$\hat{S}^{\mathrm{x}}=\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix},\quad \hat{S}^{\mathrm{y}}=\frac{1}{\sqrt{2}}\begin{pmatrix}0&-\mathrm{i}&0\\\mathrm{i}&0&-\mathrm{i}\\0&\mathrm{i}&0\end{pmatrix},\quad \hat{S}^{\mathrm{z}}=\frac{1}{\sqrt{2}}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}$$

spin chain $\hat{\boldsymbol{S}}_j$ **copy of** $\hat{\boldsymbol{S}}$ **on** $j\in\mathbb{Z}$

antiferromagnetic Heisenberg chain

$$\hat{H}_{\mathrm{Heis}}=\sum_j \hat{\boldsymbol{S}}_j\cdot\hat{\boldsymbol{S}}_{j+1}$$

expected to have a unique gapped g.s.

trivial model with a unique gapped g.s.

$$\hat{H}_{\mathrm{tr}}=\sum_j(\hat{S}^{\mathrm{z}}_j)^2\qquad |\Phi^{\mathrm{GS}}_{\mathrm{tr}}\rangle=\bigotimes_j|0\rangle_j$$

$$E^{\mathrm{GS}}_{\mathrm{tr}}=0\qquad E^{\mathrm{1st}}_{\mathrm{tr}}=1$$

interpolating model: a phase transition

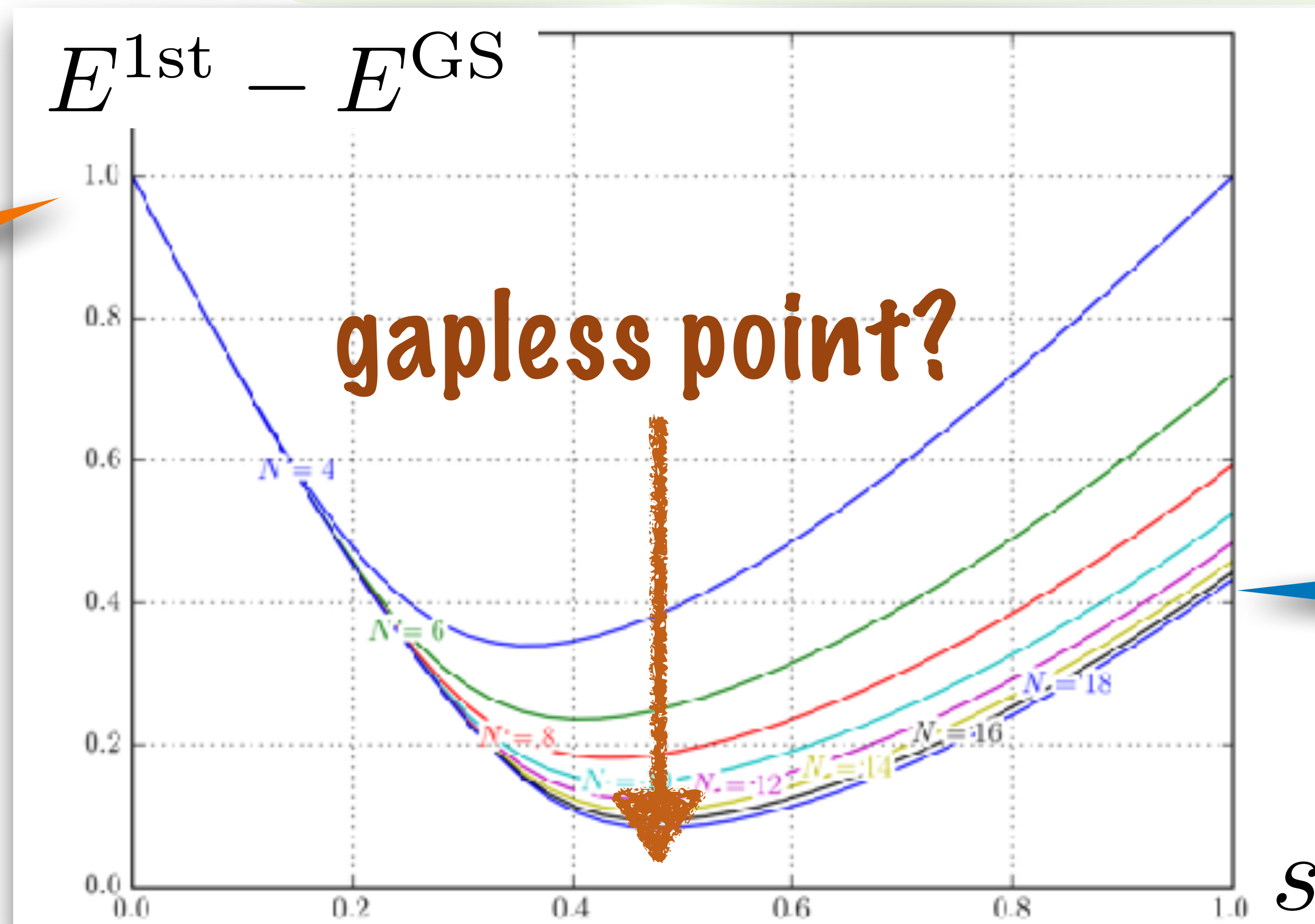
AF Heisenberg chain $\hat{H}_{\mathrm{Heis}} = \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}$ unique gapped g.s.

trivial model $\hat{H}_{\mathrm{tr}} = \sum_j (\hat{S}_j^{\mathrm{z}})^2$ unique gapped g.s. $\bigotimes_j |0\rangle_j$

interpolating model $\hat{H}^{(s)} = \sum_j \{s\,\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + (1-s)(\hat{S}_j^{\mathrm{z}})^2\}$

$s \in [0,1]$

energy gap



trivial gap

Haldane gap

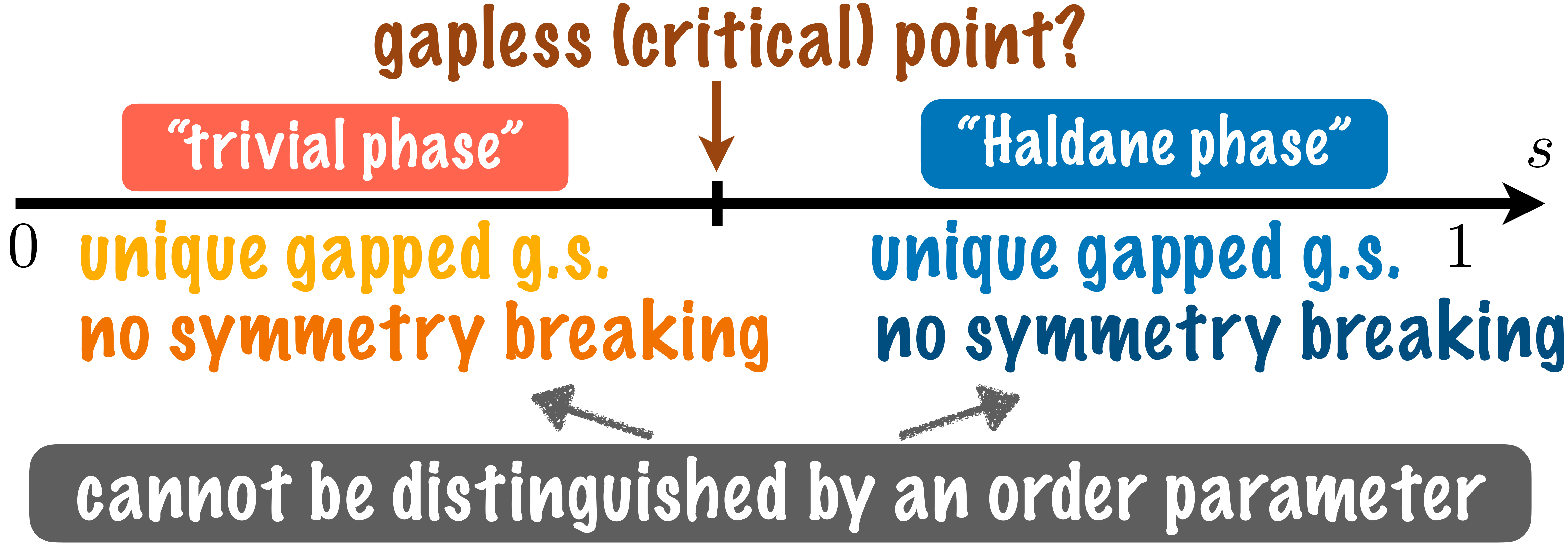
plot by Emil Aagaard

is there a phase transition between the two models?

but there are no broken symmetries!!??

Haldane phase?

$$\hat{H}^{(s)} = \sum_j \{ s\, \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + (1-s)(\hat{S}^{\mathrm{z}}_j)^2 \} \quad s \in [0,1]$$



valence-bond picture

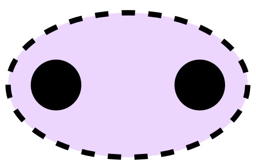
Affleck, Kennedy, Lieb, Tasaki 1987

g.s. of $\hat{H}_{\rm Heis}$ resembles the VBS (valence-bond solid) state

$|\Phi_{\rm VBS}\rangle \propto$ 

• a spin with $S = 1/2$

 $= \frac{1}{\sqrt{2}}\{|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\}$ spin singlet

 symmetrization of two $S = 1/2$'s ($S = 1$)

$$|\sigma\rangle|\sigma'\rangle \to \frac{1}{2}\{|\sigma\rangle|\sigma'\rangle + |\sigma'\rangle|\sigma\rangle\}$$

spin triplet

$\sigma, \sigma' = \uparrow, \downarrow$

a prototypical example of a matrix product state (MPS)

exponential decaying correlation function

$$\langle\Phi_{\rm VBS}|\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j'}|\Phi_{\rm VBS}\rangle \propto (-3)^{-|j-j'|}$$

frustration free

$|\Phi_{\rm VBS}\rangle$ **is the unique gapped g.s. of the artificial Hamiltonian**

$$\hat{H}_{\rm AKLT} = \sum_j \{\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + \tfrac{1}{3}(\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1})^2\}$$

exotic properties of the VBS model

expansion in the standard basis

$|\Phi_{\rm VBS}\rangle \propto$ 

$$= \sum |\cdots +0-+0-+-0+0-+0-00+-+0-+0-\cdots\rangle$$

alternating + and −

hidden antiferromagnetic order

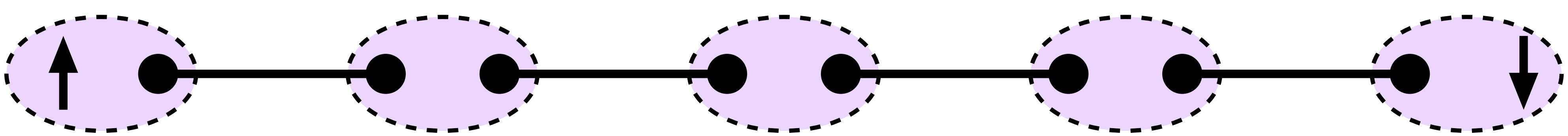
non-local string order paramter

$$\mathcal{O}_{\rm string} = -\lim_{j'-j\uparrow\infty} \langle\Phi_{\rm VBS}|\hat{S}^{\rm z}_j \, e^{{\rm i}\pi\sum_{k=j+1}^{j'-1}\hat{S}^{\rm z}_k} \, \hat{S}^{\rm z}_{j'}|\Phi_{\rm VBS}\rangle > 0$$

den Nijs, Rommelse 1989

ground states on the open chain

$$\hat{H}_{\rm AKLT} = \sum_{j=-L}^{L-1}\{\hat{\boldsymbol{S}}_j\cdot\hat{\boldsymbol{S}}_{j+1} + \tfrac{1}{3}(\hat{\boldsymbol{S}}_j\cdot\hat{\boldsymbol{S}}_{j+1})^2\}$$



four-fold degenerate ground states

emergent $S = 1/2$ gapless modes at the edges

Haldane phase

"exotic" properties of the VBS model turned out to be universal features that characterize the "Haldane phase"

$$\hat{H}^{(s)} = \sum_j \{ s\, \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + (1-s)(\hat{S}_j^{\mathrm{z}})^2 \} \qquad s \in [0,1]$$

gapless (critical) point?

"trivial phase" — "Haldane phase" — s

0 — unique gapped g.s., no symmetry breaking

1 — unique gapped g.s., no symmetry breaking

cannot be distinguished by an order parameter

nothing weird

hidden antiferromagnetic order

den Nijs, Rommelse 1989

emergent $S = 1/2$ at edges

Kennedy 1990

Hagiwara, Katsumata, Affleck, Halperin, Renard 1990

duality transformation

$$\hat{U}_{\mathrm{KT}} = \prod_{j<k} \exp[\mathrm{i}\pi \hat{S}^{\mathrm{z}}_j \hat{S}^{\mathrm{x}}_k]$$

Kennedy, Tasaki 1992, Oshikawa 1992

antiferromagnetic model with continuous $U(1)$ symmetry

$$\hat{H}^{(s)} = s \sum_{j=-L}^{L-1} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + (1-s) \sum_{j=-L}^{L} (\hat{S}^{\mathrm{z}}_j)^2$$

$s \in [0,1]$

0 — unique gapped g.s. / no symmetry breaking | unique gapped g.s. / no symmetry breaking — 1

$\hat{U}_{\mathrm{KT}}$

0 — unique gapped g.s. / no symmetry breaking | four degenerate g.s. / full symmetry breaking — 1

ferromagnetic model with discrete $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry

$$\hat{U}_{\mathrm{KT}} \hat{H}^{(s)} \hat{U}_{\mathrm{KT}} = s \sum_{j=-L}^{L-1} \{ -\hat{S}^{\mathrm{x}}_j \hat{S}^{\mathrm{x}}_{j+1} + \hat{S}^{\mathrm{y}}_j e^{\mathrm{i}\pi(\hat{S}^{\mathrm{z}}_j + \hat{S}^{\mathrm{x}}_{j+1})} \hat{S}^{\mathrm{y}}_{j+1} - \hat{S}^{\mathrm{z}}_j \hat{S}^{\mathrm{z}}_{j+1} \} + (1-s) \sum_{j=-L}^{L} (\hat{S}^{\mathrm{z}}_j)^2$$

duality and hidden symmetry breaking

$$\hat{U}_{\mathrm{KT}} = \prod_{j<k} \exp[\mathrm{i}\pi \hat{S}^{\mathrm{z}}_j \hat{S}^{\mathrm{x}}_k]$$

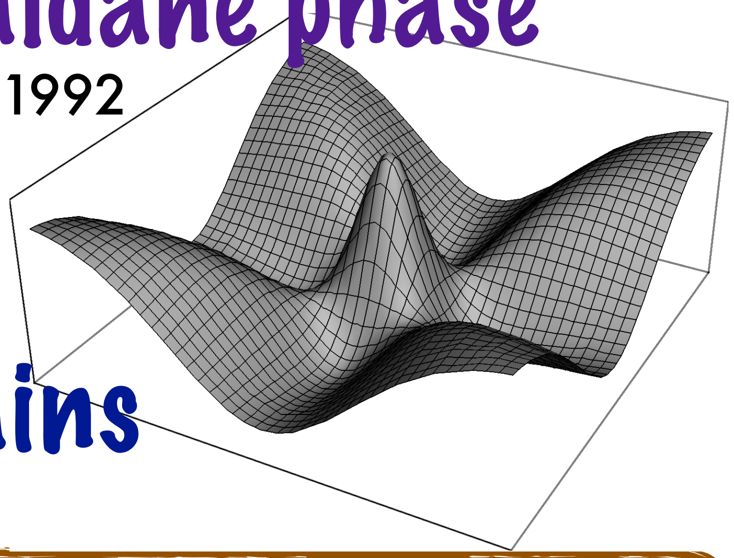
Kennedy, Tasaki 1992, Oshikawa 1992

Haldane phase $\xrightarrow{\hat{U}_{\mathrm{KT}}}$ ferromagnetic phase with full spontaneous breakdown of the discrete $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry

rigorous (only) for $\hat{H}_{\mathrm{AKLT}}$

the picture of the hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry breaking explains all the "exotic" properties of the Haldane phase

Kennedy, Tasaki 1992



- the existence of a gap
- the hidden antiferromagnetic order
- four-fold (near) degeneracy in open chains

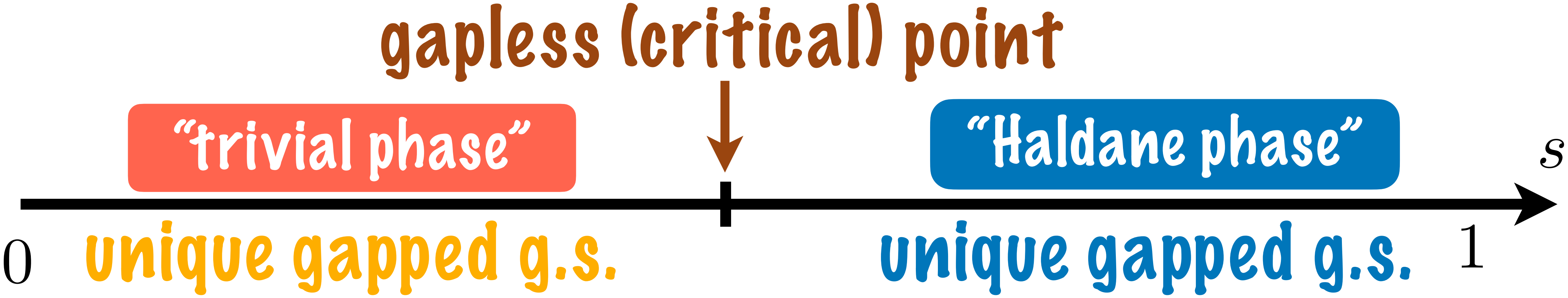
still, the existence of a phase transition even in the model

$$\hat{H}'^{(s)} = s\hat{H}_{\mathrm{AKLT}} + (1-s)\sum_j (\hat{S}^{\mathrm{z}}_j)^2 \qquad s \in [0,1]$$

could NOT be proved...

symmetry protected topological (SPT) phases

$$\hat{H}^{(s)} = \sum_j \{ s\, \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + (1-s)(\hat{S}^{\mathrm{z}}_j)^2 \} \quad s \in [0,1]$$



unique gapped g.s.
no symmetry breaking

unique gapped g.s.
no symmetry breaking

distinct SPT phases

Gu,Wen 2009

there is always a phase transition if the interpolating Hamiltonians have one of the following symmetries

- time-reversal symmetry
- $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry (π rotations about x, y, z axes)
- bond-centered inversion symmetry
- $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry (π rotation about z axis + site-centered inversion)

Pollmann, Turner, Berg, Oshikawa 2010, 2012

Fuji, Pollmann, Oshikawa 2015

symmetry protected topological (SPT) phases

$\hat{H}^{(s)} = \sum_j \{ s\, \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}$

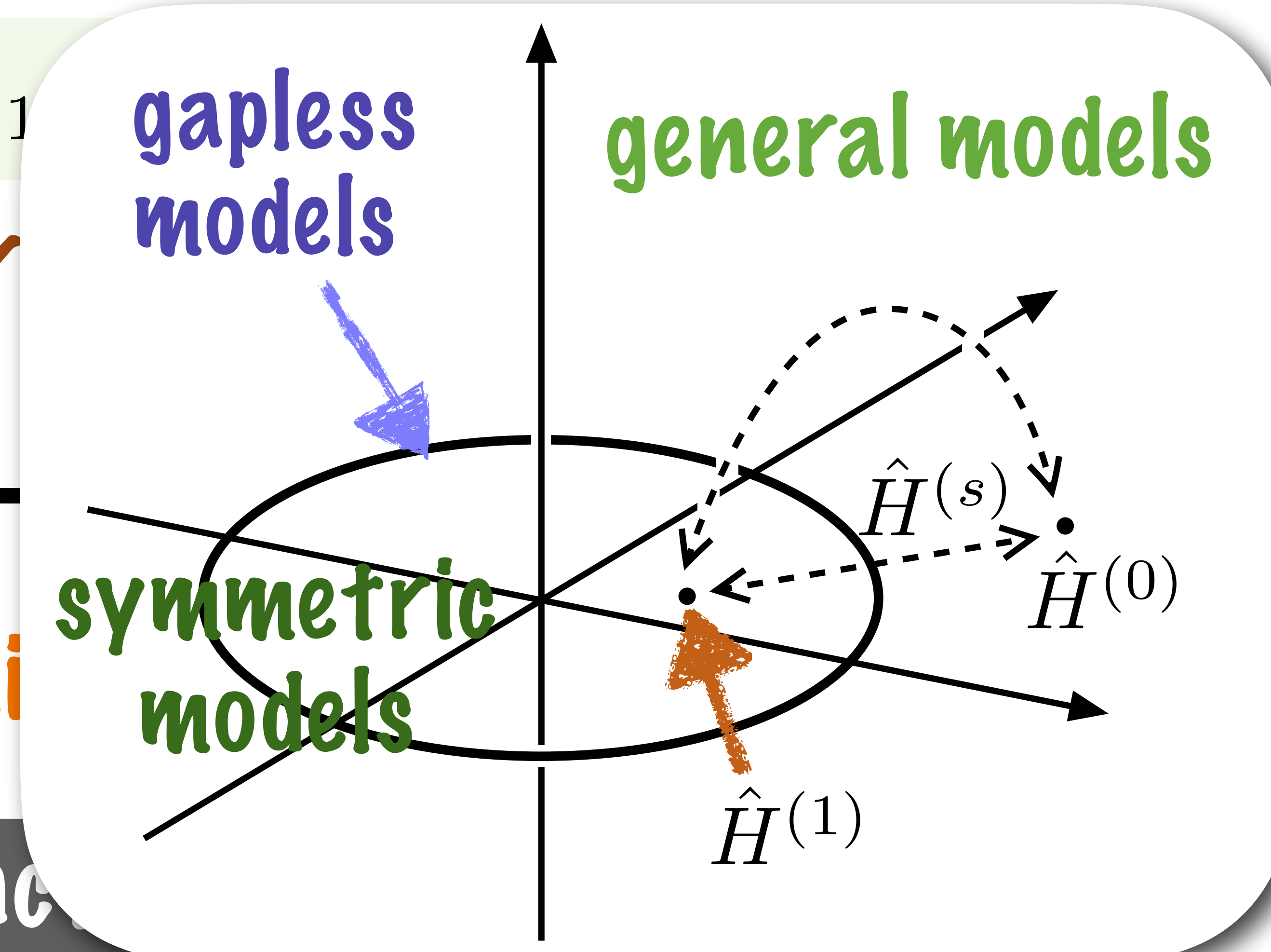
gapless (cr

"trivial phase"

0 unique gapped g.s.

no symmetry breaki

distinc



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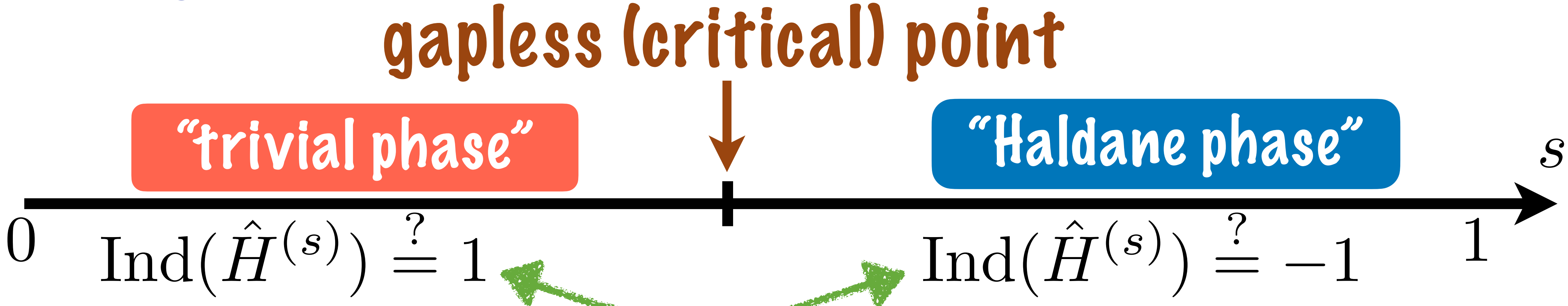
Pollmann, Turner, Berg, Oshikawa 2010, 2012

- $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry (π rotation about z axis + site-centered inversion)

Fuji, Pollmann, Oshikawa 2015

topological indices



the two phases should be distinguished by a “topological index” $\mathrm{Ind} \in \mathrm{H}^2(G, \mathrm{U}(1))$ (G is the symmetry group)

“topological” index is defined for a unique gapped ground state on the infinite chain, and is invariant under a smooth modification of the model with symmetry G

matrix product states Pollmann, Turner, Berg, Oshikawa 2010, 2012

$U(1)$ invariant unique gapped ground states Tasaki 2018

general unique gapped ground states Ogata 2020

calculations showed $\mathrm{Ind}(\hat{H}_{\mathrm{tr}}) = 1$ $\qquad \hat{H}_{\mathrm{tr}} = \hat{H}^{(0)}$

$\mathrm{Ind}(\hat{H}_{\mathrm{AKLT}}) = -1$

summary of part 1: Haldane gap and SPT phases - before the summer of 2024

- ☑ general picture of SPT phases
- ☑ well-defined indices and index theorem
- ☑ VBS model provides a rigorous example of the Haldane gap and topologically nontrivial ground state

$$\hat{H}_{\mathrm{AKLT}} = \sum_j \{\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + \tfrac{1}{3}(\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1})^2\}$$

$|\Phi_{\mathrm{VBS}}\rangle \propto$ 

the existence of a g.s. phase transition in the model

$$\hat{H'}^{(s)} = s\hat{H}_{\mathrm{AKLT}} + (1-s)\sum_j (\hat{S}_j^{\mathrm{z}})^2 \qquad s \in [0,1]$$

was rigorously established Tasaki 2018, Ogata 2020

nothing rigorous was proved about the antiferromagnetic Heisenberg chain!

Part 1
Haldane gap, valence-bond picture, and SPT phases

Part 2
$S=1$ antiferromagnetic Heisenberg chain is topologically nontrivial if gapped

- elementary index theorem
- main theorem

the goal of part 2

two conjectures about the $S = 1$ antiferromagnetic Heisenberg chain

$$\hat{H}_{\text{Heis}} = \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}$$

"Haldane conjecture" (probably very difficult)

(1) it has a unique gapped ground state

(2) it belongs to a nontrivial SPT phase

we assume (1) and rigorously justify (2)

proof is elementary!

- standard Lieb-Mattis-type technique
- elementary index theorem by Tasaki

Hal Tasaki, *Ground state of the antiferromagnetic Heisenberg chain is topologically nontrivial if gapped*, Phys. Rev. Lett, coming soon (2025). arXiv:2407.17041

Part 1

Haldane gap, valence-bond picture, and SPT phases

Part 2

$S = 1$ antiferromagnetic Heisenberg chain is topologically nontrivial if gapped

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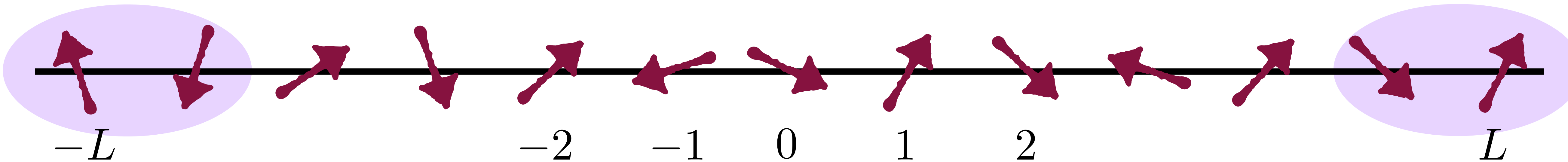
index theorem for $U(1)$ invariant chains

Tasaki 2018, 2025

$S=1$ system on a finite chain $\{-L,\ldots,L\}$



short-ranged Hamiltonian

$$\hat{H}_L=\sum_{j=-L}^{L}\hat{h}_j+\Delta\hat{H}_L$$

$U(1)$ invariant

$$e^{\mathrm{i}\theta\hat{S}^{\mathrm{z}}_{\mathrm{tot}}}\hat{H}_L e^{-\mathrm{i}\theta\hat{S}^{\mathrm{z}}_{\mathrm{tot}}}=\hat{H}_L \qquad \hat{S}^{\mathrm{z}}_{\mathrm{tot}}=\sum_{j=-L}^{L}\hat{S}^{\mathrm{z}}_j$$

invariant under site-centered inversion

$$\hat{U}_{\mathrm{si}}^{\dagger}\hat{H}_L\hat{U}_{\mathrm{si}}=\hat{H}_L \qquad \hat{U}_{\mathrm{si}}\bigotimes_{j=-L}^{L}|\sigma_j\rangle_j=\bigotimes_{j=-L}^{L}|\sigma_{-j}\rangle_j$$

unique gapped ground state $|\Phi_L^{\mathrm{GS}}\rangle$

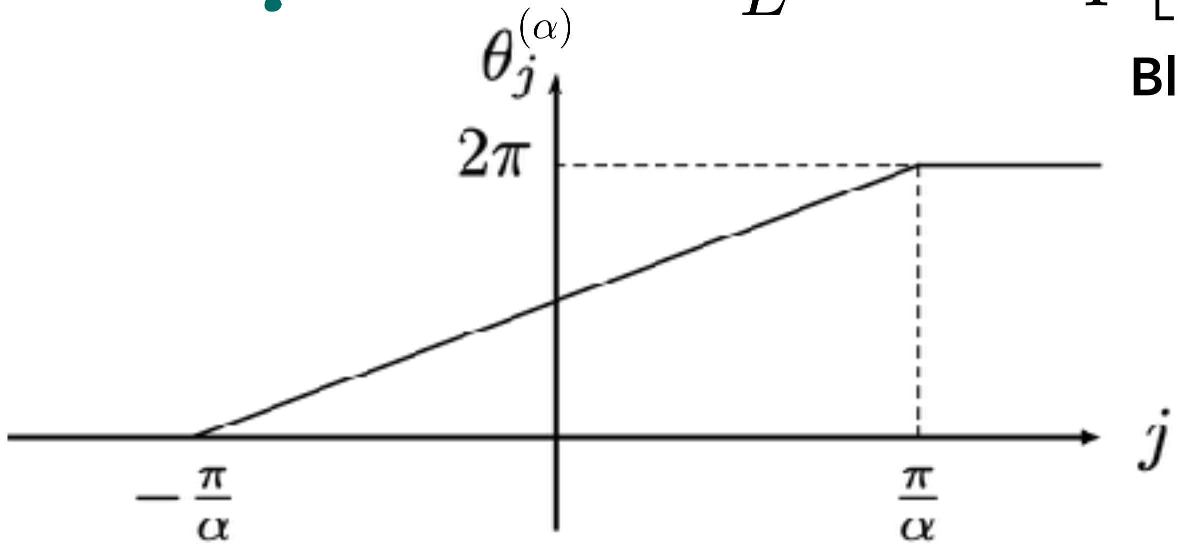
$$E_L^{\mathrm{1st}}-E_L^{\mathrm{GS}}\geq\Delta E>0 \text{ for any } L\geq L_0$$

Theorem: there is a well-defined index $\mathrm{ind}(\hat{H})\in\{1,-1\}$ that is invariant under a continuous modification of the g.s.

the index and simple examples

twist operator $\hat{U}_L^{(\alpha)} = \exp\left[-\mathrm{i}\sum_{j=-L}^{L}\theta_j^{(\alpha)}\hat{S}_j^{\mathrm{z}}\right]$

Bloch 1940's, Lieb, Schultz, Mattis 1961, Affleck Lieb 1986



$$\theta_j^{(\alpha)} = \begin{cases} 0, & j \le -\frac{\pi}{\alpha}; \\ \pi + \alpha j, & -\frac{\pi}{\alpha} \le j \le \frac{\pi}{\alpha}; \\ 2\pi, & j \ge \frac{\pi}{\alpha}, \end{cases}$$

$\alpha > 0$

$$e^{-\mathrm{i}2\pi\hat{S}_j^{\mathrm{z}}} = \hat{1}$$

$$\mathrm{Ind}(\hat{H}) = \lim_{\alpha\downarrow 0}\lim_{L\uparrow\infty}\langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle \in \{1, -1\}$$

trivial model $\hat{H}_{\mathrm{tr}} = \sum_j(\hat{S}_{\mathrm{z}})^2$ $\quad |\Phi_{\mathrm{tr}}^{\mathrm{GS}}\rangle = \bigotimes_j |0\rangle_j$

$\langle\Phi_{\mathrm{tr}}^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_{\mathrm{tr}}^{\mathrm{GS}}\rangle = 1$ $\quad \mathrm{Ind}(\hat{H}_{\mathrm{tr}}) = 1$

VBS state $\langle\Phi_{\mathrm{VBS}}|\hat{U}_L^{(\alpha)}|\Phi_{\mathrm{VBS}}\rangle \simeq -1$ $\quad \mathrm{Ind}(\hat{H}_{\mathrm{AKLT}}) = -1$

Nakamura, Todo 2002

this proves the existence of a g.s. phase transition in the model $\hat{H'}^{(s)} = s\hat{H}_{\mathrm{AKLT}} + (1-s)\hat{H}_{\mathrm{tr}}$ $\quad s \in [0,1]$

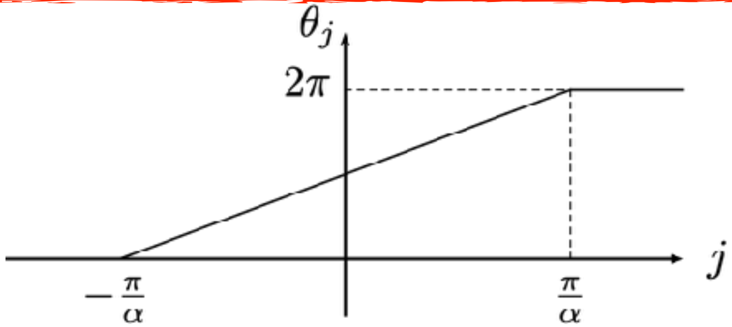
Tasaki 2018

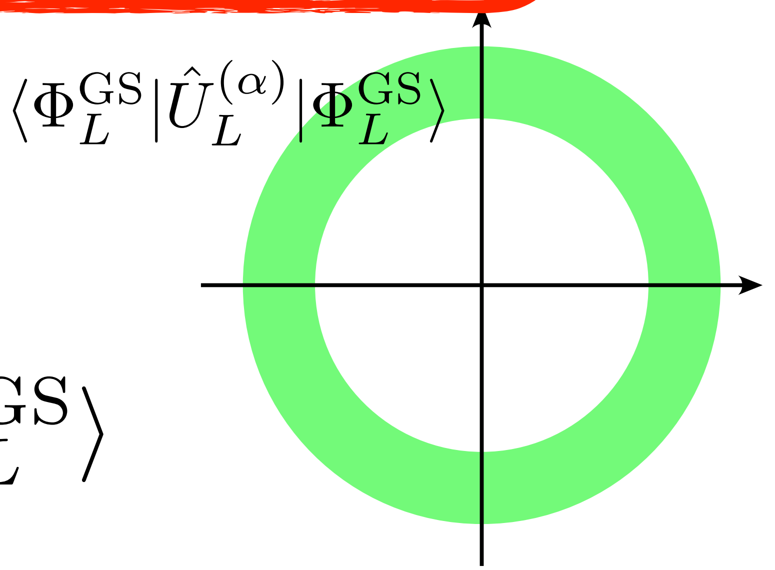
proof of the index theorem 1/3

Lemma: $U(1)$ **invariance + unique gapped g.s. imply**

$$\sqrt{1-\frac{C}{\Delta E}\alpha} \le \left|\langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle\right| \le 1 \text{ for any } L \ge L_0$$

Lieb-Schultz-Mattis type variational estimate





$$|\Psi_L^{(\alpha)}\rangle = \hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle = e^{-\mathrm{i}\sum_{j=-L}^{L}\theta_j^{(\alpha)}\hat{S}_j^{\mathrm{z}}}|\Phi_L^{\mathrm{GS}}\rangle$$

for $U(1)$ invariant Hamiltonian

$$\langle\Psi_L^{(\alpha)}|\hat{H}_L|\Psi_L^{(\alpha)}\rangle - E_L^{\mathrm{GS}} \le C\,\alpha \qquad C > 0$$

because energy increase per bond $\propto \alpha^2$
the length of the twisted range $\propto \alpha^{-1}$

if $\hat{H}_L$ has a unique gapped g.s. $|\Psi_L^{(\alpha)}\rangle$ must be close to $|\Phi_L^{\mathrm{GS}}\rangle$

$$\left|\langle\Phi_L^{\mathrm{GS}}|\Psi_L^{(\alpha)}\rangle\right|^2 \ge 1-\frac{C}{\Delta E}\alpha \qquad \langle\Phi_L^{\mathrm{GS}}|\Psi_L^{(\alpha)}\rangle = \langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle$$

proof of the index theorem 2/3

Lemma: invariance under site-centered inversion implies

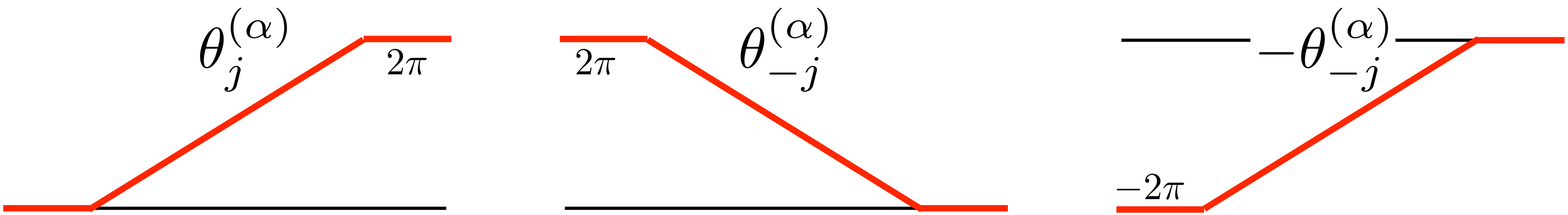
$$\langle \Phi_L^{\mathrm{GS}} | \hat{U}_L^{(\alpha)} | \Phi_L^{\mathrm{GS}} \rangle \in \mathbb{R}$$

inversion of the twist operator

$$\hat{U}_L^{(\alpha)} = e^{-\mathrm{i}\sum_{j=-L}^{L} \theta_j^{(\alpha)} \hat{S}_j^{\mathrm{z}}}$$

$$\hat{U}_{\mathrm{si}}^{\dagger} \hat{U}_L^{(\alpha)} \hat{U}_{\mathrm{si}} = e^{-\mathrm{i}\sum_{j=-L}^{L} \theta_{-j}^{(\alpha)} \hat{S}_j^{\mathrm{z}}} = e^{+\mathrm{i}\sum_{j=-L}^{L} (2\pi - \theta_{-j}^{(\alpha)}) \hat{S}_j^{\mathrm{z}}} = (\hat{U}_L^{(\alpha)})^{\dagger}$$

$$(2\pi - \theta_{-j}^{(\alpha)}) = \theta_j^{(\alpha)}$$



invariance of the Hamiltonian $\hat{U}_{\mathrm{si}}^{\dagger} \hat{H}_L \hat{U}_{\mathrm{si}} = \hat{H}_L$

the unique g.s. must be invariant $\hat{U}_{\mathrm{si}} | \Phi_L^{\mathrm{GS}} \rangle = \pm | \Phi_L^{\mathrm{GS}} \rangle$

$$\langle \Phi_L^{\mathrm{GS}} | \hat{U}_L^{(\alpha)} | \Phi_L^{\mathrm{GS}} \rangle = \langle \Phi_L^{\mathrm{GS}} | \hat{U}_{\mathrm{si}}^{\dagger} \hat{U}_L^{(\alpha)} \hat{U}_{\mathrm{si}} | \Phi_L^{\mathrm{GS}} \rangle = \langle \Phi_L^{\mathrm{GS}} | \hat{U}_L^{(\alpha)} | \Phi_L^{\mathrm{GS}} \rangle^*$$

proof of the index theorem 3/3

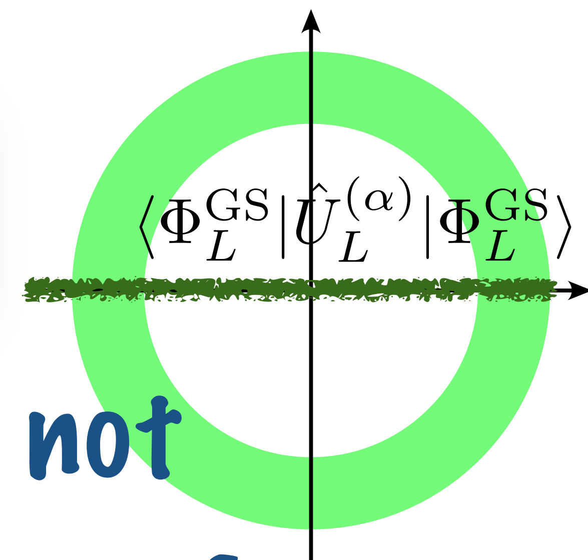
Lemma: $U(1)$ **invariance + unique gapped g.s. implies**

$$\sqrt{1-\frac{C}{\Delta E}\alpha} \le \left|\langle\Phi_L^{\rm GS}|\hat{U}_L^{(\alpha)}|\Phi_L^{\rm GS}\rangle\right| \le 1 \text{ for any } L \ge L_0$$

Lemma: invariance under site-centered inversion implies

$$\langle\Phi_L^{\rm GS}|\hat{U}_L^{(\alpha)}|\Phi_L^{\rm GS}\rangle \in \mathbb{R}$$

$$\mathrm{Ind}(\hat{H}) = \mathrm{sign}\lim_{L\uparrow\infty}\langle\Phi_L^{\rm GS}|\hat{U}_L^{(\alpha)}|\Phi_L^{\rm GS}\rangle \in \{1,-1\}$$



for a fixed $\alpha \in (0, \frac{\Delta E}{C})$, $\lim_{L\uparrow\infty}\langle\Phi_L^{\rm GS}|\hat{U}_L^{(\alpha)}|\Phi_L^{\rm GS}\rangle$ does not change the sign when the g.s. is continuously modified

the index is a topological invariant!

we also see

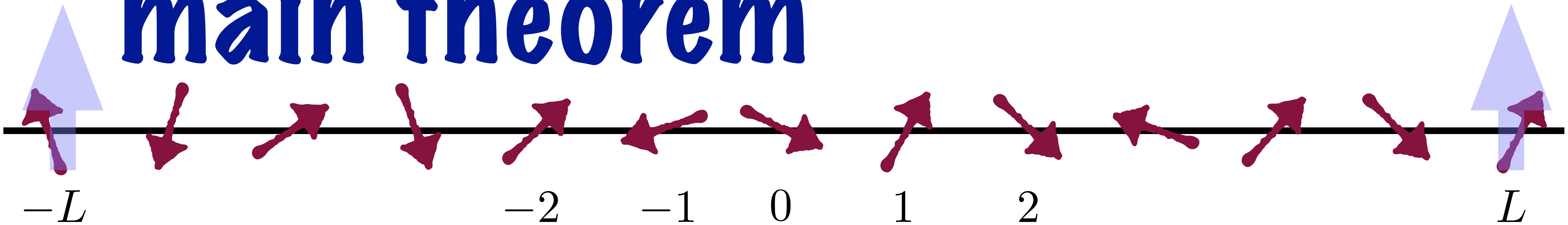
$$\mathrm{Ind}(\hat{H}) = \lim_{\alpha\downarrow 0}\lim_{L\uparrow\infty}\langle\Phi_L^{\rm GS}|\hat{U}_L^{(\alpha)}|\Phi_L^{\rm GS}\rangle \in \{1,-1\}$$

Part 1
Haldane gap, valence-bond picture, and SPT phases

Part 2
$S=1$ antiferromagnetic Heisenberg chain is topologically nontrivial if gapped

- elementary index theorem
- main theorem

main theorem



AF Heisenberg model on the finite open chain $\{-L, \cdots, L\}$

$$\hat{H}_L^{\mathrm{Heis}} = \sum_{j=-L}^{L-1} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} - h(\hat{S}^{\mathrm{z}}_{-L} + \hat{S}^{\mathrm{z}}_{L})$$

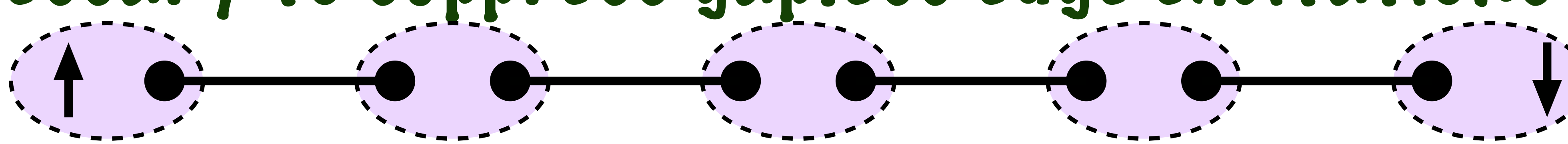
E_L^{GS}, E_L^{1st} the ground state and the 1st excited energies

highly nontrivial and unproven

assumption: there are constants $h > 0$, $\Delta E > 0$, and L_0 such that $E_L^{\mathrm{1st}} - E_L^{\mathrm{GS}} \geq \Delta E$ for any $L \geq L_0$

expected hold with $\Delta E \simeq 0.41$ and $h \gtrsim 1$

$h \gtrsim 1$ is necessary to suppress gapless edge excitations



Theorem: $\mathrm{Ind}(\hat{H}_{\mathrm{Heis}})$ is well-defined and equals -1

proof of the main theorem 1/2

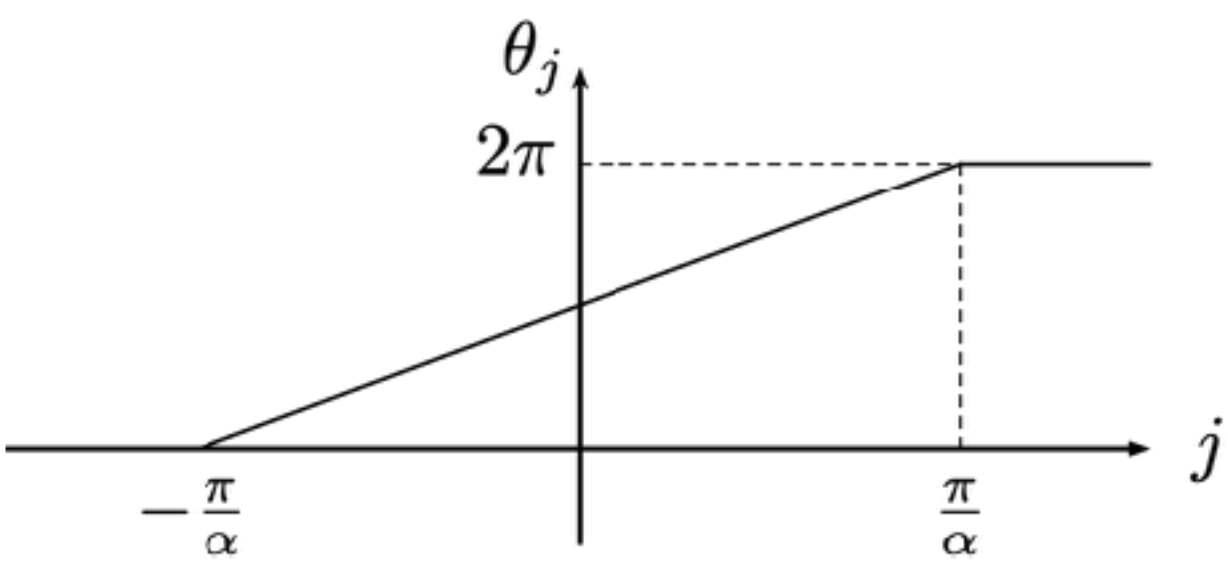
$$\hat{H}_L^{\text{Heis}} = \sum_{j=-L}^{L-1} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} - h(\hat{S}^{\text{z}}_{-L} + \hat{S}^{\text{z}}_L)$$

Lemma: $\hat{H}_L^{\text{Heis}}$ **has a unique ground state** $|\Phi_L^{\text{GS}}\rangle$
it satisfies $\left(\sum_{j=-L}^{L} \hat{S}_j^{\text{z}}\right)|\Phi_L^{\text{GS}}\rangle = |\Phi_L^{\text{GS}}\rangle$

proof: standard Perron-Frobenius argument as in the proof of the Lieb-Mattis theorem

$$\hat{U}_L^{(\alpha)} = e^{-\mathrm{i}\sum_{j=-L}^{L} \theta_j^{(\alpha)} \hat{S}_j^{\text{z}}}$$

$$\theta_j^{(\alpha)} = \begin{cases} 0, & j \le -\frac{\pi}{\alpha}; \\ \pi + \alpha j, & -\frac{\pi}{\alpha} \le j \le \frac{\pi}{\alpha}; \\ 2\pi, & j \ge \frac{\pi}{\alpha}, \end{cases}$$



$$\lim_{\alpha\downarrow 0}\langle\Phi_L^{\text{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\text{GS}}\rangle = \langle\Phi_L^{\text{GS}}|e^{\mathrm{i}\pi\sum_{j=-L}^{L}\hat{S}_j^{\text{z}}}|\Phi_L^{\text{GS}}\rangle = e^{\mathrm{i}\pi} = -1$$

proof of the main theorem 2/2

$$\lim_{\alpha\downarrow 0}\langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle = -1$$

Lemma: $U(1)$ invariance + unique gapped g.s. implies

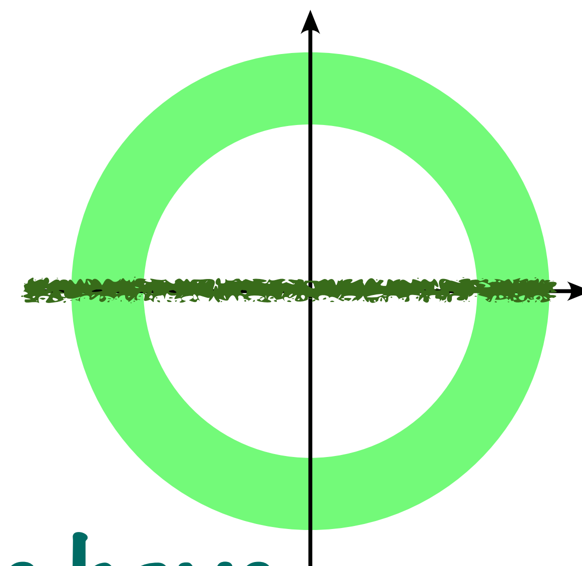
$\sqrt{1-\frac{C}{\Delta E}\alpha} \le \left|\langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle\right| \le 1$ for any $L \ge L_0$

Lemma: invariance under site-centered inversion implies

$$\langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle \in \mathbb{R}$$

$$-1 \le \langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle \le -\sqrt{1-\frac{C}{\Delta E}\alpha}$$

for any $\alpha > 0$ and $L \ge L_0$



letting $L \uparrow \infty$ with sufficiently small $\alpha > 0$, we have

$$\mathrm{Ind}(\hat{H}_{\mathrm{Heis}}) = \lim_{\alpha\downarrow 0}\lim_{L\uparrow\infty}\langle\Phi_L^{\mathrm{GS}}|\hat{U}_L^{(\alpha)}|\Phi_L^{\mathrm{GS}}\rangle = -1$$

corollaries of the theorem

$$\hat{H}_L^{\mathrm{Heis}} = \sum_{j=-L}^{L-1} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} - h(\hat{S}^{\mathrm{z}}_{-L} + \hat{S}^{\mathrm{z}}_{L})$$

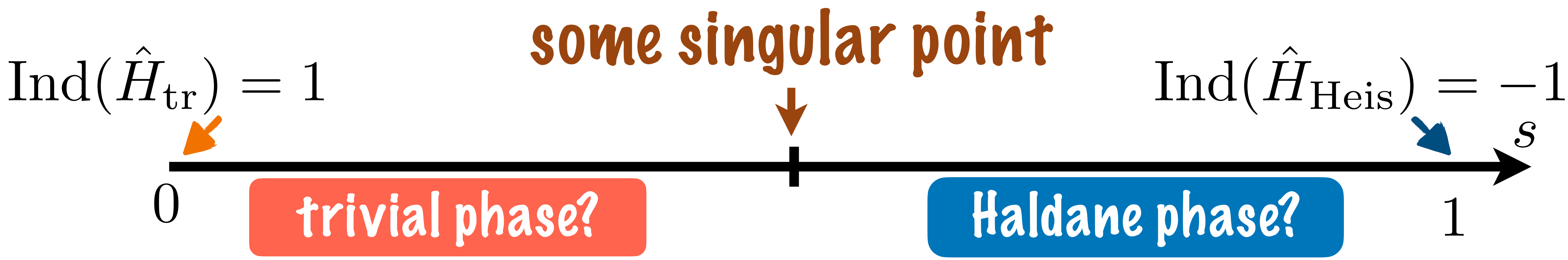
assumption: $\hat{H}_L^{\mathrm{Heis}}$ has a unique gapped ground state with a gap uniform in $L \geq L_0$

Theorem: $\mathrm{Ind}(\hat{H}_{\mathrm{Heis}})$ is well-defined and equals -1

☑ a gapless edge excitation in the half-infinite chain

☑ the existence of a g.s. phase transition in the interpolating model

$$\hat{H}^{(s)} = \sum_j \{s\,\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + (1-s)(\hat{S}^{\mathrm{z}}_j)^2\} \quad s \in [0,1]$$



index theorem: mathematically precise form

Theorem: Let $\hat{H}^{(s)} = \sum_{j\in\mathbb{Z}} \hat{h}_j^{(s)}$ with $s \in [0,1]$ where each $\hat{h}_j^{(s)}$ is short-ranged and $U(1)$ invariant

if $\mathrm{ind}(\hat{H}^{(0)}) = 1$ and $\mathrm{ind}(\hat{H}^{(1)}) = -1$, there exists $s_0 \in (0,1]$ at which the g.s. undergoes a phase transition in the sense that either (i) $\hat{H}^{(s_0)}$ does not have a locally unique gapped g.s., (ii) the energy gap approaches zero as $s \to s_0$, (iii) the g.s. of $\hat{H}^{(s_0)}$ has no site-inversion symmetry, or (iv) the g.s is discontinuous at $s = s_0$

Definition: a state $\omega : \mathfrak{A} \to \mathbb{C}$ is a g.s of $\hat{H}$ iff $\omega(\hat{V}^\dagger[\hat{H}, \hat{V}]) \geq 0$ for any $\hat{V} \in \mathfrak{A}_{\mathrm{loc}}$

a state ω is a locally unique gapped g.s. iff there is $\gamma > 0$ s.t. $\omega(\hat{V}^\dagger[\hat{H}, \hat{V}]) \geq \gamma\omega(\hat{V}^\dagger\hat{V})$ for any $\hat{V} \in \mathfrak{A}_{\mathrm{loc}}$ with $\omega(\hat{V}) = 0$

unconditional results

valid without any unproven assumptions

☑ **the $S=1$ AF Heisenberg chain may have**

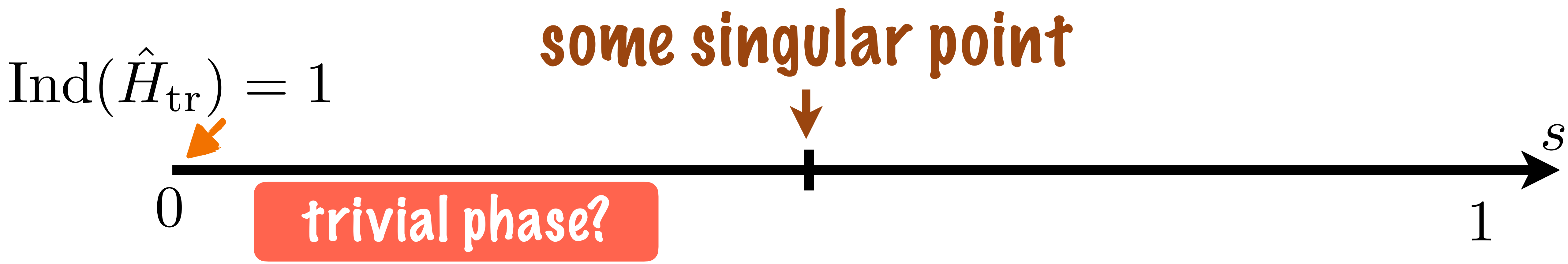
- ~~topologically trivial unique gapped ground state~~
- topologically nontrivial unique gapped ground state
- gapless or degenerate ground state(s)

☑ **a phase transition in the interpolating model**

in case the assumption does NOT hold, $\hat{H}_{\mathrm{Heis}}$ is singular

there exists a phase transition (at least) at $s=1$

$$\hat{H}^{(s)}=\sum_j\{s\,\hat{\boldsymbol{S}}_j\cdot\hat{\boldsymbol{S}}_{j+1}+(1-s)(\hat{S}^{\mathrm{z}}_j)^2\}\quad s\in[0,1]$$



some technical remarks

☑ the symmetry of the finite chain model

$$\hat{H}_L^{\text{Heis}} = \sum_{j=-L}^{L-1} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} - h(\hat{S}^{\text{z}}_{-L} + \hat{S}^{\text{z}}_L)$$

- ~~time-reversal symmetry~~
- ~~$\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry (π rotations about x, y, z axes)~~
- ~~bond-centered inversion symmetry~~
- $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry Fuji, Pollmann, Oshikawa 2015
  (π rotation about z axis + site-centered inversion)

other symmetries should be restored as $L \uparrow \infty$

☑ Ogata index

most general index, which works for any symmetry classes that can host SPT phases

defined in terms of projective representation of the symmetry group on $L \uparrow \infty$ ground sates

we still do not know how to determine $\text{Ind}_{\text{Ogata}}(\hat{H}_{\text{Heis}})$

summary of part 2: $S=1$ AF Heisenberg chain is topologically nontrivial if gapped

- ☑ we proved that the $S=1$ AF Heisenberg chain has a nontrivial topological index, under the assumption that the model has a unique gapped ground state
- ☑ we rigorously ruled out the possibility that the $S=1$ AF Heisenberg chain has a unique gapped ground state that is topologically trivial
- ☑ we established the existence of a phase transition in the model that interpolates $\hat{H}_{\mathrm{Heis}}$ and $\hat{H}_{\mathrm{tr}}$
- ☑ all the results extend to models with odd S
- ☑ the first nontrivial rigorous results on topological properties of the (realistic) AF Heisenberg chain

remaining issues

- ☑ clarify the relation of our index to projective representations and to the Ogata index
- ☑ develop a similar elementary index theory for general symmetries without $U(1)$ (related problem: constructive proof of the generalized LSM theorem)
- ☑ prove similar conditional results on "realistic" models that exhibit topological property
- ☑ justify the assumption = "Haldane conjecture" by developing a new strategy
computer-aided proof by a new finite-size criterion?

Haldane's discovery led to the valence-bond picture, matrix product states, tensor networks, symmetry protected topological phases, and much more

still, our understanding of the Heisenberg chain is incomplete, and there still remains much more to learn

there must be more surprises to come!