The Ground State of the S=1 Antiferromagnetic Heisenberg Chain is Topologically Nontrivial if Gapped

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webinar @ YouTube / July 2024

the $S=1$ antiferromagnetic Heisenberg chain

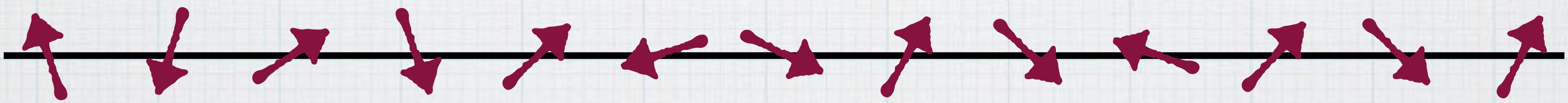
$$\hat{H}^{(1)} = \sum_{j\in\mathbb{Z}} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} \qquad \hat{\boldsymbol{S}}_j = (\hat{S}^{\mathrm{x}}_j, \hat{S}^{\mathrm{y}}_j, \hat{S}^{\mathrm{z}}_j) \qquad (\hat{\boldsymbol{S}}_j)^2 = 2$$

may have

- ☑ a unique gapped ground state that is topologically trivial

this is expected

- ☑ a unique gapped ground state that is topologically nontrivial
- ☑ gapless or degenerate ground states(s)



the $S=1$ antiferromagnetic Heisenberg chain

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may have

we rigorously rule out this possibility!

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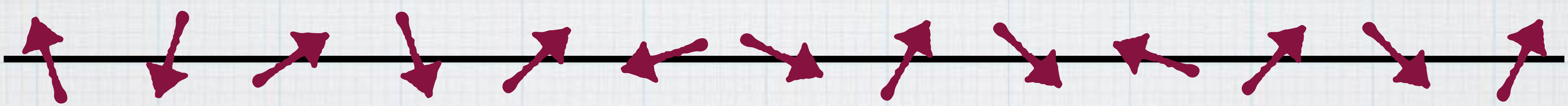
this is expected

- ☑ a unique gapped ground state that is topologically nontrivial

- ☑ gapless or degenerate ground states(s)



a rigorous and nontrivial result about the ground state of the $S=1$ antiferromagnetic Heisenberg chain

introduction/motivation

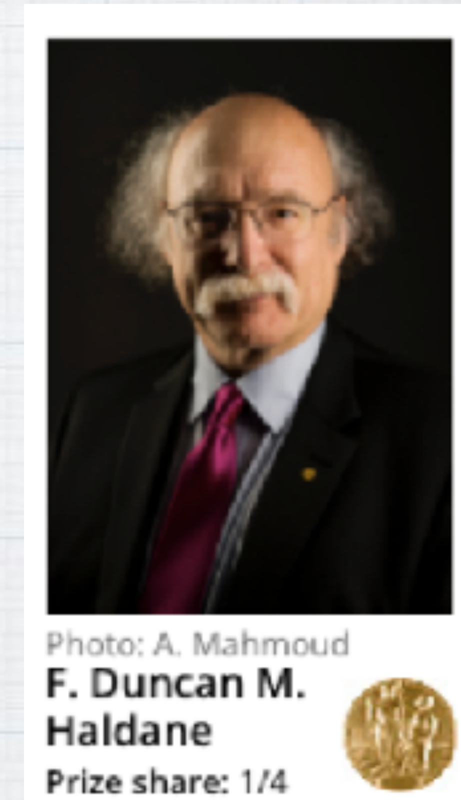
main results

idea of the proof

the ground state of the spin S antiferromagnetic Heisenberg chain

$$\hat{H}^{(1)} = \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} \quad \hat{\boldsymbol{S}}_j = (\hat{S}^{\mathrm{x}}_j, \hat{S}^{\mathrm{y}}_j, \hat{S}^{\mathrm{z}}_j) \quad (\hat{\boldsymbol{S}}_j)^2 = S(S+1)$$

$$S = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$$



Haldane's discovery

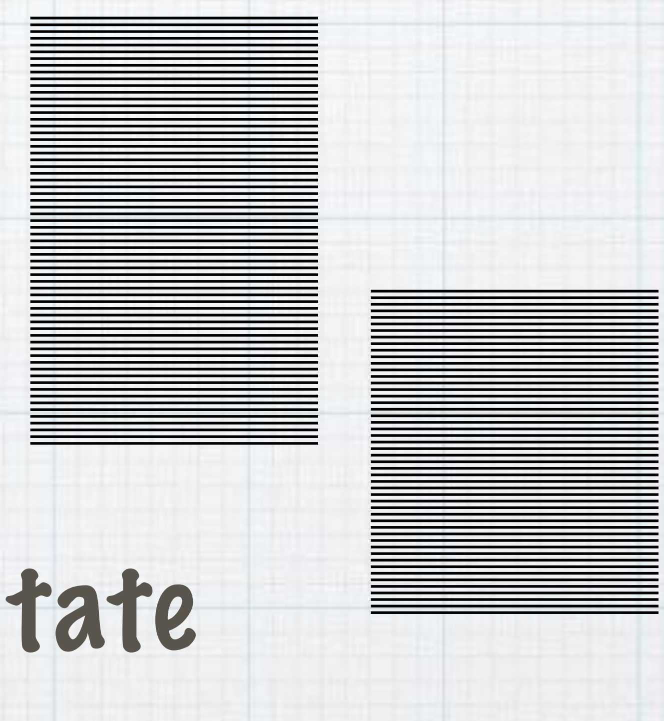
Haldane 1981, 1983, 1983

half-odd integer S

unique gapless ground state

integer S

unique **gapped** ground state



the picture of symmetry-protected topological (SPT) phases

Gu,Wen 2009, Pollmann, Turner, Berg, Oshikawa 2010, 2012

even S belongs to a trivial SPT phase

odd S belongs to a **nontrivial SPT phase**

nontrivial SPT phase of $S=1$ chain

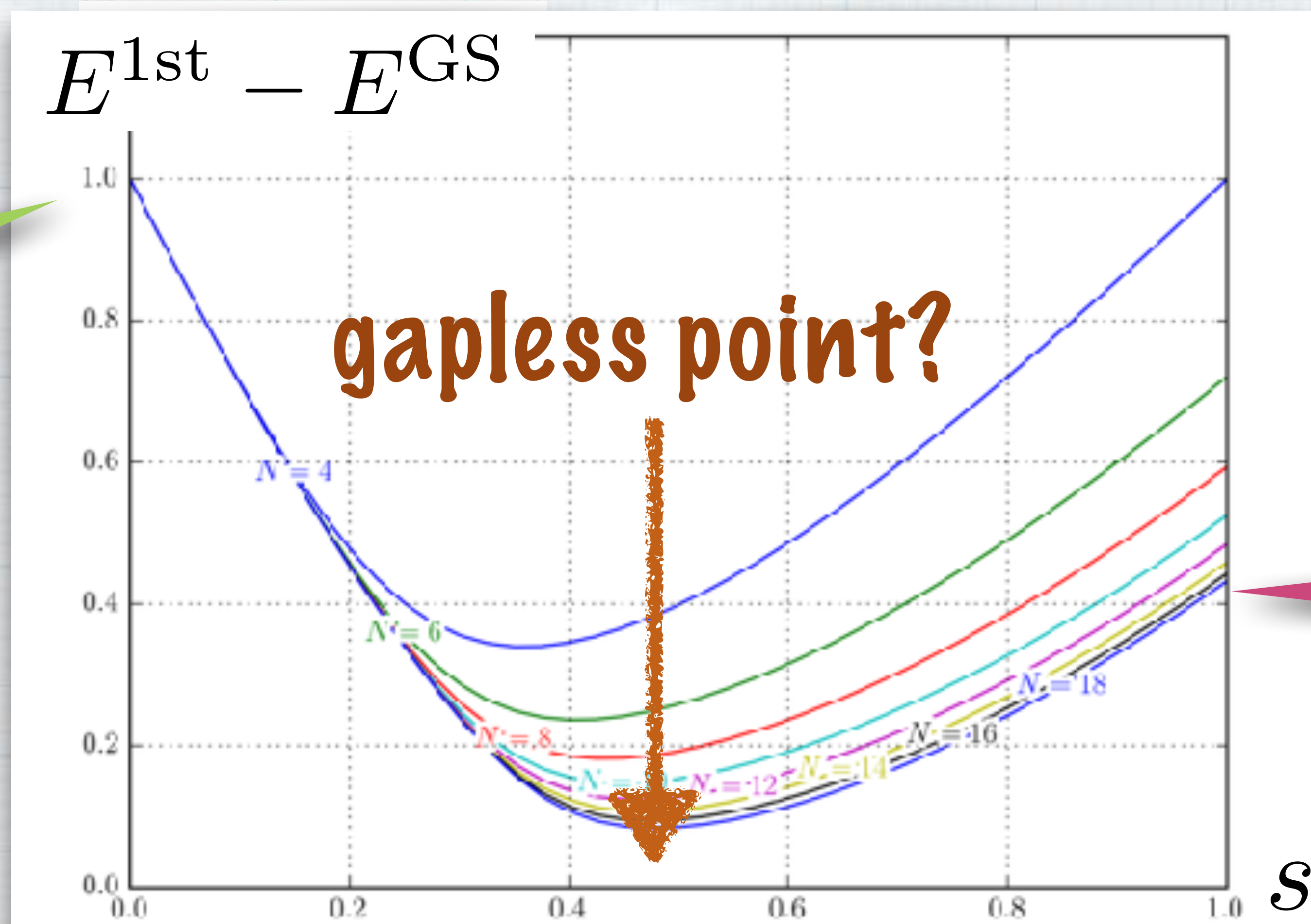
AF Heisenberg chain $\hat{H}^{(1)} = \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}$ unique gapped g.s.

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

interpolating model

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

energy gap



trivial gap

Haldane gap

plot by Emil Aagaard

there seems to be a phase transition

nontrivial SPT phase of $S = 1$ chain

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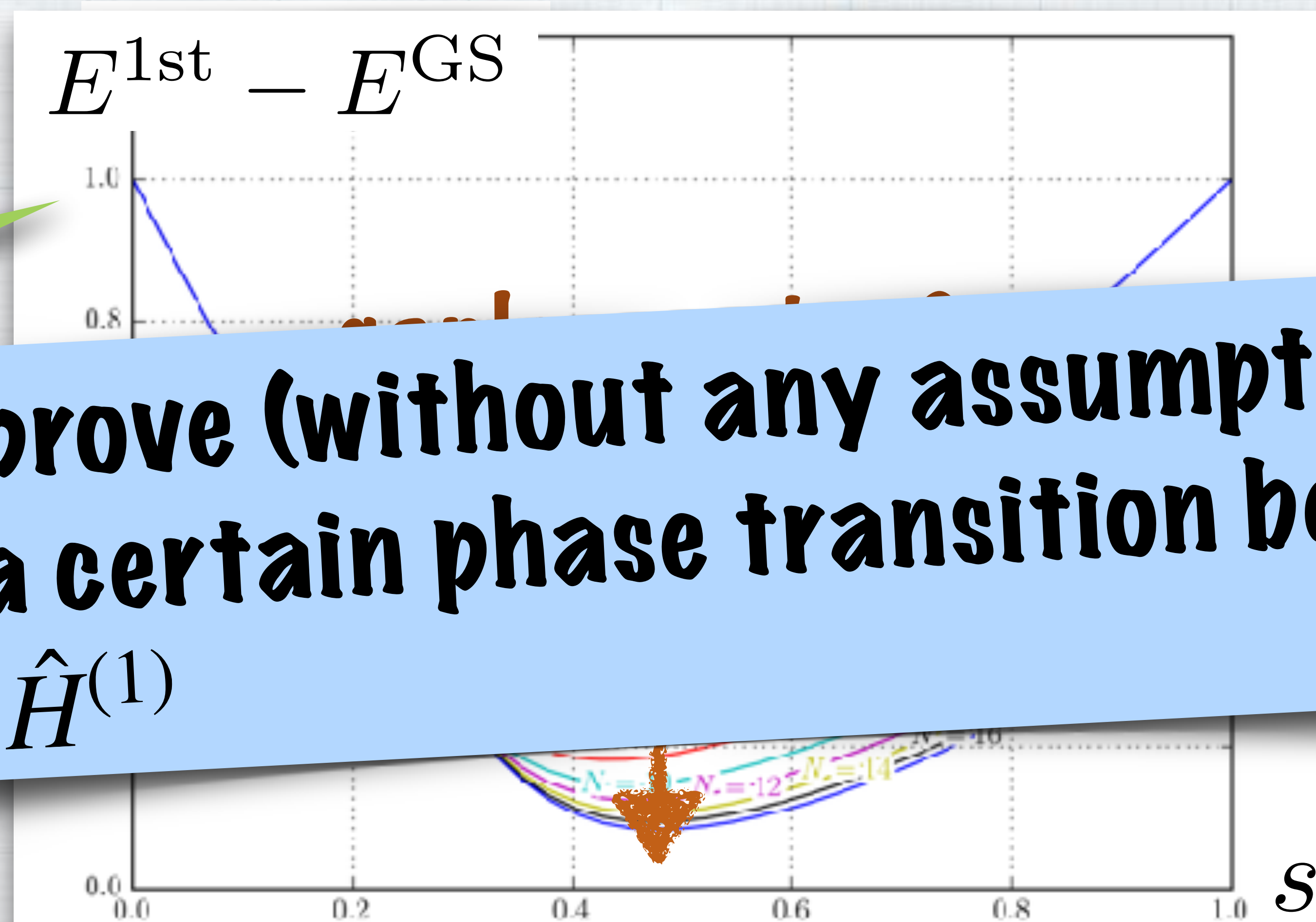
energy gap



trivial

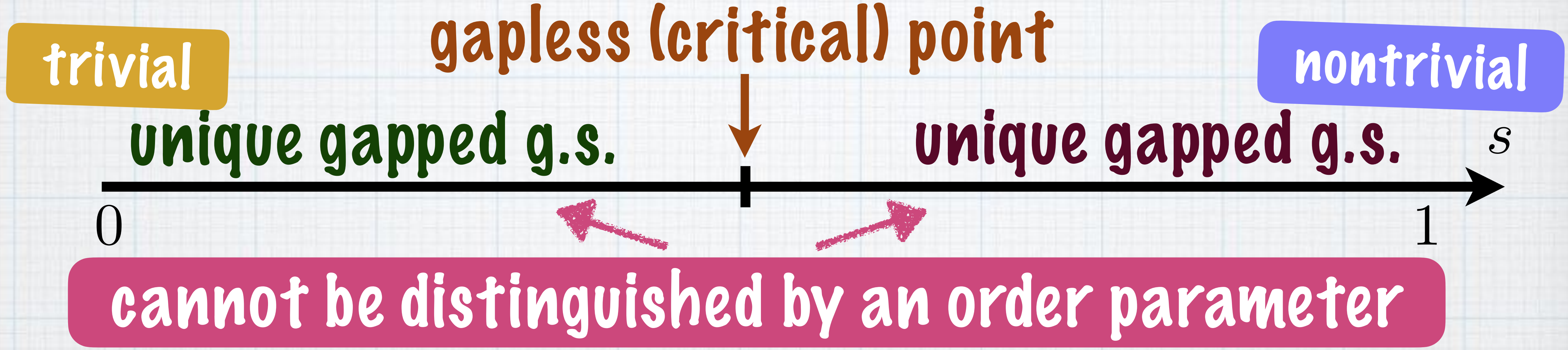
we here prove (without any assumptions) that there is a certain phase transition between $\hat{H}^{(0)}$ and $\hat{H}^{(1)}$

plot by Emil Aagaard

there seems to be a phase transition

nontrivial SPT phase of $S = 1$ chain

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



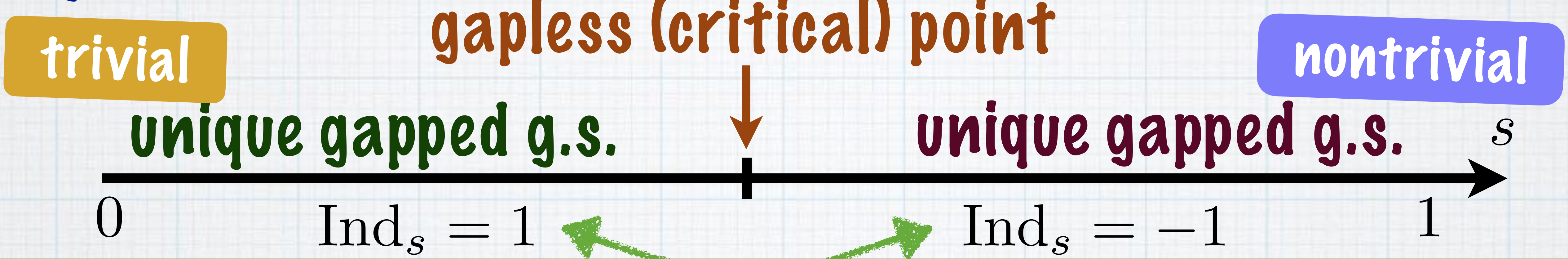
distinct symmetry-protected topological (SPT) phases

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
- $\mathrm{U}(1) \times \mathbb{Z}_2$ symmetry
  (any rotation about z axis + site-centered inversion)

Pollmann, Turner, Berg, Oshikawa 2010, 2012, Fuji, Pollmann, Oshikawa 2015

topological indices



the two phases are 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 locally-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

general unique gapped ground states Ogata 2018

$\mathrm{Ind} = 1$ and $\mathrm{Ind} = -1$ in the ground states of the trivial model and the Affleck-Kennedy-Lieb-Tasaki (AKLT) model

prototypical solvable model in the "Haldane phase"

Affleck, Kennedy, Lieb, Tasaki 1987

Haldane gap and SPT phases

general theory

- ☑ general picture of SPT phases by Gu and Wen and Pollmann, Turner, Berg, and Oshikawa
- ☑ well-defined indices and index theorem by Ogata

examples

- ☑ AKLT model provides a rigorous example of the Haldane gap and topologically nontrivial ground state

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

nothing rigorous has been proved about the antiferromagnetic Heisenberg chain with odd S!!

the goal of the present work

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

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

"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

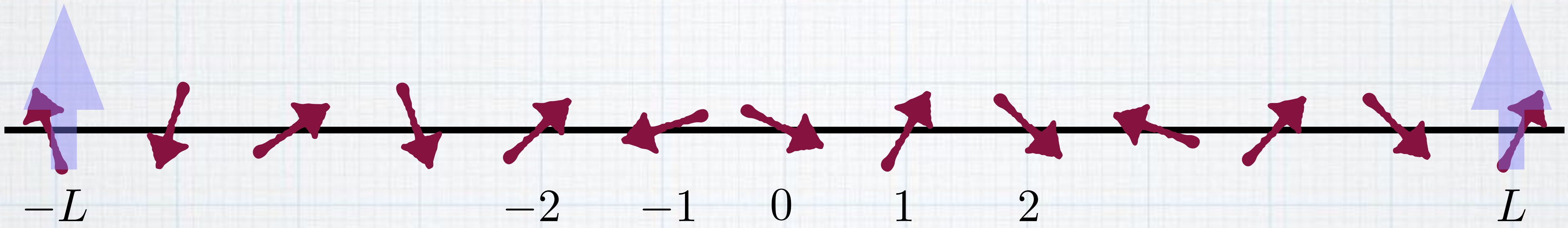
the model with general odd S can be treated similarly

introduction/motivation

main results

idea of the proof

$S=1$ model on finite chains



Hamiltonian on the finite open chain $\{-L,\cdots,L\}$

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

magnetic field at the edges

symmetry

- time-reversal symmetry
- $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry (π rotations about $\mathrm{x}, \mathrm{y}, \mathrm{z}$ axes)
- bond-centered inversion symmetry
- $\mathrm{U}(1) \times \mathbb{Z}_2$ symmetry Fuji, Pollmann, Oshikawa 2015
  (any rotation about z axis + inversion about 0)

lemma: $\hat{H}^{(1)}_L$ has a unique ground state $|\Phi^{\mathrm{GS}}_L\rangle$
it satisfies $\left(\sum_{j=-L}^{L}\hat{S}^{\mathrm{z}}_j\right)|\Phi^{\mathrm{GS}}_L\rangle = |\Phi^{\mathrm{GS}}_L\rangle$

assumption

Hamiltonian on the finite open chain $\{-L, \cdots, L\}$

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

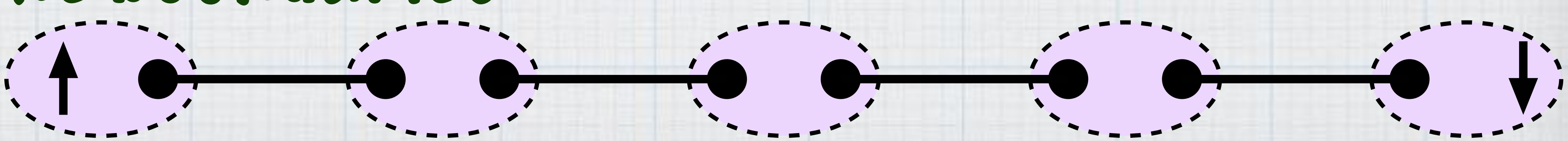
E_L^{GS}, E_L^{1st} the ground state and the 1st excited energies

highly nontrivial and unproven

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

expected hold with $\gamma \simeq 0.41$ and $h = 1$ (Haldane conjecture)

the boundary field $h \gtrsim 1$ is necessary to suppress gapless excitations at the boundaries



main result

$\omega^{(1)}(\hat{A}) = \lim_{L\uparrow\infty} \langle \Phi_L^{\mathrm{GS}} | \hat{A} | \Phi_L^{\mathrm{GS}} \rangle$ for any local operator $\hat{A}$

$\omega^{(1)}$ a locally-unique gapped g.s. of $\hat{H}^{(1)} = \sum_{j\in\mathbb{Z}} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}$

Index defined in Tasaki 2018

theorem: $\mathrm{Ind}[\omega^{(1)}] = -1$

interpolating model

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

$\omega^{(s)}$ the ground state of $\hat{H}^{(s)}$ $\qquad \mathrm{Ind}[\omega^{(0)}] = 1$

corollary: there is $s_0 \in (0,1)$ such that $\omega^{(s_0)}$ is not a unique gapped ground state or $\omega^{(s)}$ is discontinuous at s_0

remark: $\omega^{(1)}$ is critical if the assumption is not valid

the existence of a phase transition in the ground states of $\hat{H}^{(s)}$ has been proved without any assumptions!!

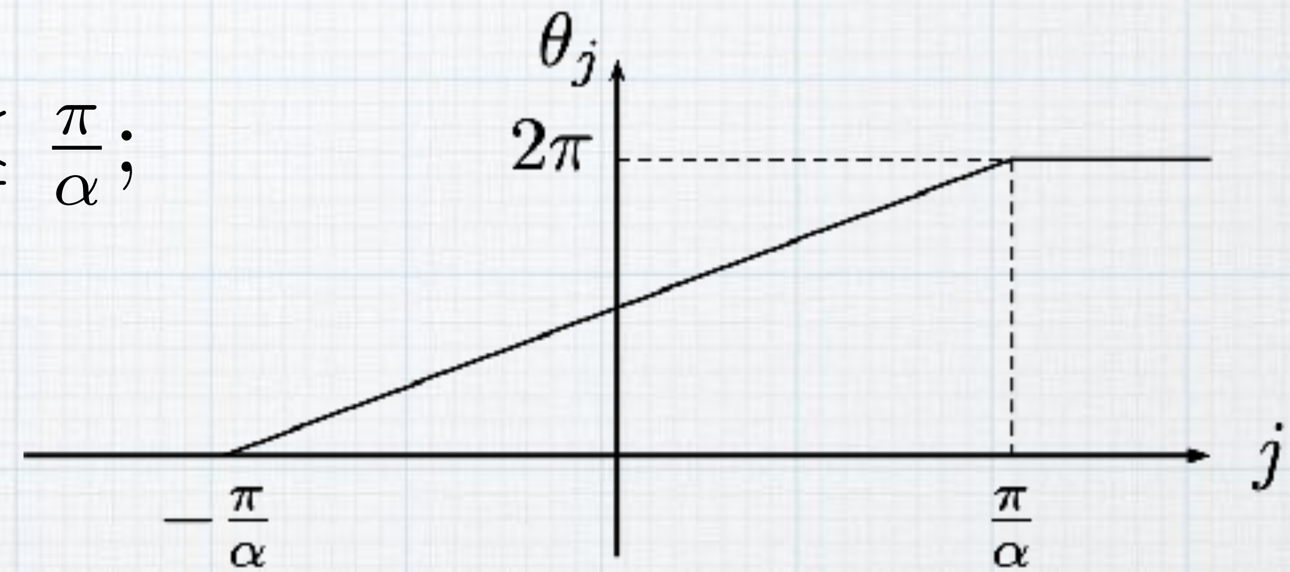
introduction/motivation
main results
idea of the proof

twist operator

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

twist angle with gradient $\alpha \in [0,4 - \pi]$

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



twist operator on finite chain

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

when $\alpha > 0$, we take the $L \uparrow \infty$ limit

$$e^{-i2\pi \hat{S}_j^{\mathrm{z}}} = \hat{1}$$

$$\hat{U}^{(\alpha)} = \exp\left[-i \sum_{j \in \mathbb{Z} \cap [-\frac{\pi}{\alpha}, \frac{\pi}{\alpha}]} \theta_j^{(\alpha)} \hat{S}_j^{\mathrm{z}}\right]$$

local operator on the infinite chain

$\hat{U}_L^{(\alpha)}$ and $\hat{U}^{(\alpha)}$ are continuous in α

topological index in terms of $\hat{U}^{(\alpha)}$

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

$\omega^{(s)}$ the ground state of $\hat{H}^{(s)}$

Tasaki 2018

theorem: if $\omega^{(s)}$ is a locally-unique gapped ground state and is invariant under inversion $j \to -j$, then the following index is well-defined. the index is invariant when s is varied, provided that $\omega^{(s)}$ satisfies the above conditions.

$$\mathrm{Ind}[\omega^{(s)}] = \lim_{\alpha\downarrow 0} \omega^{(s)}(\hat{U}^{(\alpha)}) \in \{1,-1\}$$

the (sign of) the ground state expectation value of $\hat{U}^{(\alpha)}$

Nakamura, Todo 2002

trivial model

$\hat{H}^{(0)} = \sum_j (\hat{S}^{\mathrm{z}}_j)^2 \qquad \omega^{(0)} \longleftrightarrow \bigotimes_j |0\rangle_j$

$\omega^{(0)}(\hat{U}^{(\alpha)}) = \omega^{(0)}(\exp[-i\sum_j \theta^{(\alpha)}_j \hat{S}^{\mathrm{z}}_j]) = 1 \qquad \mathrm{Ind}[\omega^{(0)}] = 1$

proof that $\mathrm{Ind}[\omega^{(1)}] = -1$

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

when $\alpha = 0$, we have $\theta_j^{(0)} = \pi$

$$\hat{U}_L^{(0)} = \exp\left[-i \sum_{j=-L}^{L} \theta_j^{(0)} \hat{S}_j^{\mathrm{z}}\right] = \exp\left[-i\pi \sum_{j=-L}^{L} \hat{S}_j^{\mathrm{z}}\right]$$

$$\left(\sum_{j=-L}^{L} \hat{S}_j^{\mathrm{z}}\right)|\Phi_L^{\mathrm{GS}}\rangle = |\Phi_L^{\mathrm{GS}}\rangle$$ from lemma

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

we have proved $\lim_{L\uparrow\infty} \lim_{\alpha\downarrow 0} \langle \Phi_L^{\mathrm{GS}} | \hat{U}_L^{(\alpha)} | \Phi_L^{\mathrm{GS}} \rangle = -1$

definition of the index $\mathrm{Ind}[\omega^{(1)}] = \lim_{\alpha\downarrow 0} \lim_{L\uparrow\infty} \langle \Phi_L^{\mathrm{GS}} | \hat{U}_L^{(\alpha)} | \Phi_L^{\mathrm{GS}} \rangle$

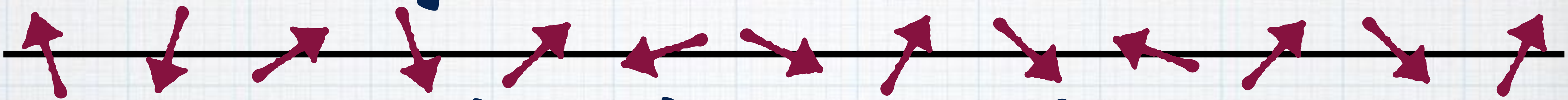
the assumption on the gap allows us to exchange the limits!

lemma: for $\alpha \in [0, \gamma/18]$ and sufficiently large L

$$\langle \Phi_L^{\mathrm{GS}} | \hat{U}_L^{(\alpha)} | \Phi_L^{\mathrm{GS}} \rangle \in [-1, -\tfrac{1}{3}] \cup [\tfrac{1}{3}, 1]$$

illustration by Chisato Naruse

summary



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

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

(1) it has a unique gapped ground state

(2) it belongs to a nontrivial SPT phase

- ☑ we proved (2), assuming (1)
- ☑ the proof makes use of the elementary index theory based on the twist operator
- ☑ it is desirable to prove also (1)
  it seems we need a new idea