Symmetry-protected topological (SPT) phases and topological indices in quantum spin chains

part 1: Haldane conjecture, topological phase transitions, SPT phases, and all that

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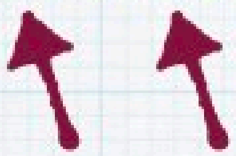
online lecture @ YouTube / August 2021

ground states of two-spin systems

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

ferromagnetic interaction

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



infinitely many g.s.

antiferromagnet interaction

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

infinitely many g.s.

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

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

ferromagnetic interaction

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

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

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

spin triplet

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

infinitely many g.s.

antiferromagnet 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

ground states of two-spin systems

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

ferromagnetic interaction

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

infinitely many g.s.

antiferromagnet interaction

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

infinitely many g.s.

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

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

ferromagn… …**interaction**

$\hat{H}=-$ …

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

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

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

spin triplet

infinitely many g.s.

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

spin singlet

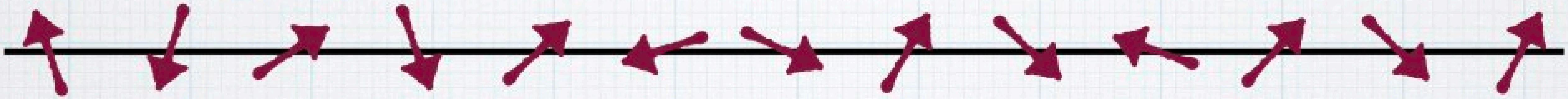
unique rotationally invariant ground state

we expect strong (and interesting) "quantum effects" in antiferromagnets!

Bethe ansatz
Haldane conjecture
and AKLT model

quantum antiferromagnetic Heisenberg chain

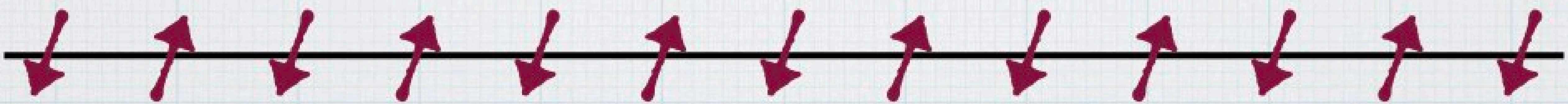
one of the most standard models of quantum many-body systems



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

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?



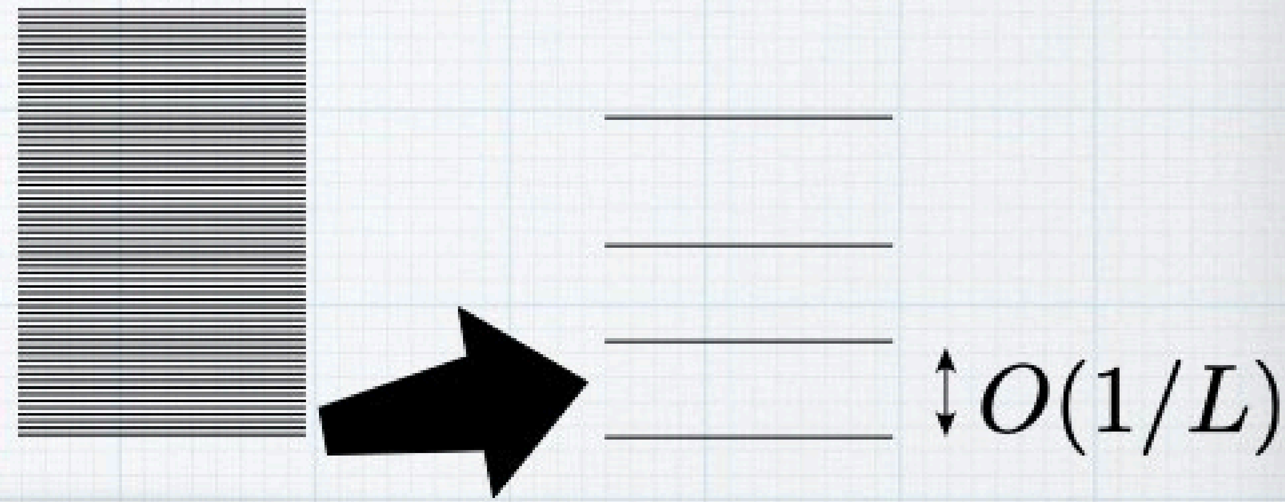
Néel state is NOT a ground state (quantum fluctuation!)

Results from the Bethe ansatz

Bethe 1931 and many others

$$\hat{H} = \sum_{j=1}^{L} \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1}$$

$$S = \frac{1}{2}$$



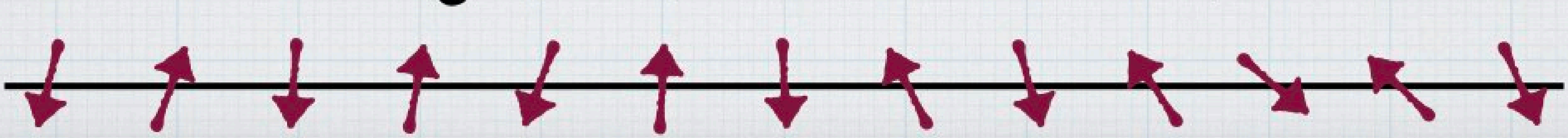
(i) ground state is unique (for finite or infinite L)

(ii) no energy gap above the ground state

(iii) g.s. correlation decays with power law

$$\langle \mathrm{GS} | \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_k | \mathrm{GS} \rangle \sim (-1)^{j-k} \frac{\sqrt{\log |j-k|}}{|j-k|}$$

the ground state is critical



Haldane's discovery

Haldane 1981, 1983, 1983

there is a qualitative difference in low energy properties of the AF Heisenberg chains with half-odd-integer spins $S = \frac{1}{2}, \frac{3}{2}, \cdots$ and integer spins $S = 1, 2, 3, \ldots$

half-odd-integer spins (the same as $S = 1/2$)

(i) ground state is unique (for finite or infinite L)

(ii) no energy gap above the ground state

(iii) g.s. correlation decays with power law

Haldane's discovery

integer spins

(i) ground state is unique (for finite or infinite L)

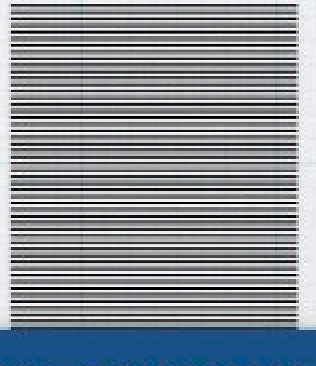
(ii) nonzero energy gap above the ground state

(iii) g.s. correlation decays exponentially

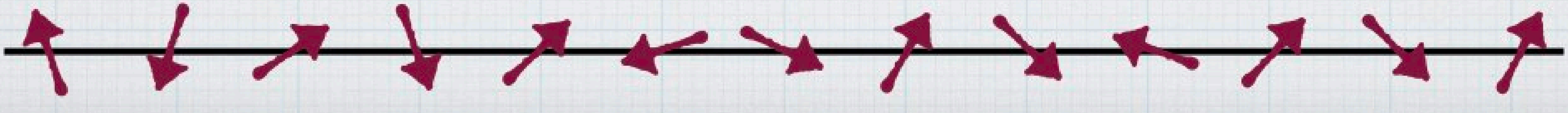
$$\langle \mathrm{GS}|\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_k|\mathrm{GS}\rangle \sim (-1)^{j-k} \frac{e^{-|j-k|/\xi}}{|j-k|^{1/2}}$$

the energy gap = Haldane gap

a **unique gapped ground state**
without any order



a unique ground sate accompanied by a nonzero energy gap $= O(1)$



Surprises (in early 80s) about Haldane's conclusions

- qualitative difference between models with half-odd-integer spins and integer spins
- it is "natural" that a system with continuous symmetry and unique g.s. is gapless (LSM theorem)
- the unique gapped g.s. of integer spin chains are predicted to be disordered like high-temperature states. can "quantum fluctuation" be that strong??

the referee report to Haldane's paper in 1981

"This is in manifest contradiction to fundamental principles of physics"

A rigorous example with $S = 1$

antiferromagnetic Hamiltonian with an extra term

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

Theorem (AKLT 1987)

(i) ground state is unique (for finite or infinite L)

(ii) nonzero energy gap above the ground state

(iii) g.s. correlation decays exponentially

$$\frac{\langle \mathrm{VBS} | \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_k | \mathrm{VBS} \rangle}{\langle \mathrm{VBS} | \mathrm{VBS} \rangle} = 4(-3)^{-|j-k|} \quad (j \neq k)$$

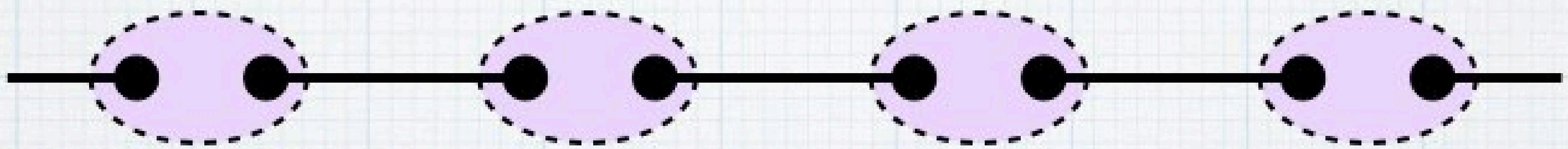
All the conclusions by Haldane for integer spin chains are verified (for an artificial model)

VBS (valence-bond solid) state

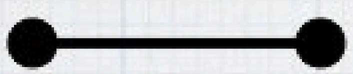
$$\hat{H}_{\mathrm{AKLT}} = \sum_{j=1}^{L} \left\{ \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1} + \frac{1}{3} (\hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+1})^2 \right\}$$

exact g.s. of AKLT model

starting point of the proof

$|\mathrm{VBS}\rangle =$ 

- a spin with $S = 1/2$

 $= \dfrac{1}{\sqrt{2}} \left\{ |\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle \right\}$ spin singlet

"quantum fluctuation"

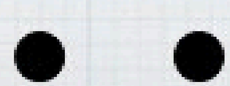
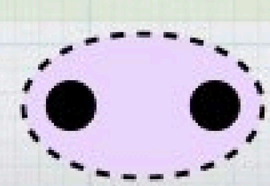
antiferromagnetic correlation

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

spin triplet

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

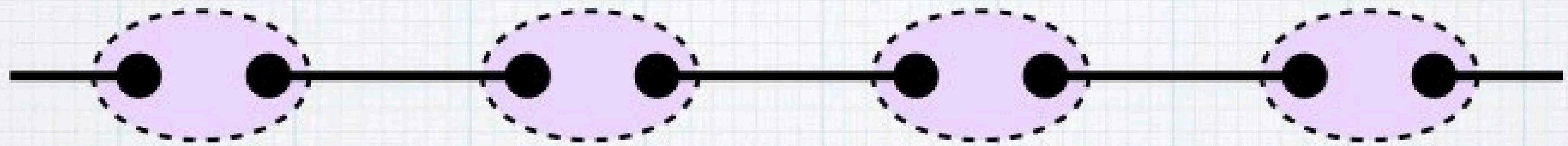
$\sigma, \sigma' = \uparrow, \downarrow$

Matrix product representation of the VBS state

Fannes, Nachtergaele, Werner 1989, 1992

exact g.s. of AKLT model

$|\mathrm{VBS}\rangle =$ 

$$= \sum_{\sigma_1,\ldots,\sigma_L=0,\pm 1} \mathrm{Tr}[\mathsf{M}^{\sigma_1}\ldots\mathsf{M}^{\sigma_L}]\,|\sigma_1,\ldots,\sigma_L\rangle \qquad \sigma_j = 0, \pm 1$$

coefficient

standard basis state

$$\mathsf{M}^{+} = \begin{pmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix} \quad \mathsf{M}^{0} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \quad \mathsf{M}^{-} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}$$

special case of a general class of states

matrix product states (MPS)

$$|\Phi\rangle = \sum_{\sigma_1,\ldots,\sigma_L=-S}^{S} \mathrm{Tr}[\mathsf{M}^{\sigma_1}\ldots\mathsf{M}^{\sigma_L}]\,|\sigma_1,\ldots,\sigma_L\rangle$$

any unique gapped ground state of a spin chain is approximated accurately by MPS

Exotic properties of the AKLT model

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

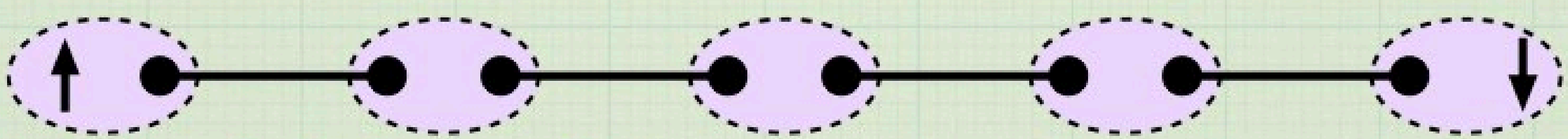
hidden antiferromagnetic order in the VBS state

$$\cdots +0-+0-+-0+0-+0-00+-+0-+0-\cdots$$

$$\cdots + \quad -+ \quad -+- \quad + \quad -+ \quad - \quad\quad +-+ \quad -+ \quad -\cdots$$

alternating sequence of + and −

effective $S = 1/2$ spins at the edge of an open chain



four-fold (near) degeneracy in an open chain

observed experimentally!

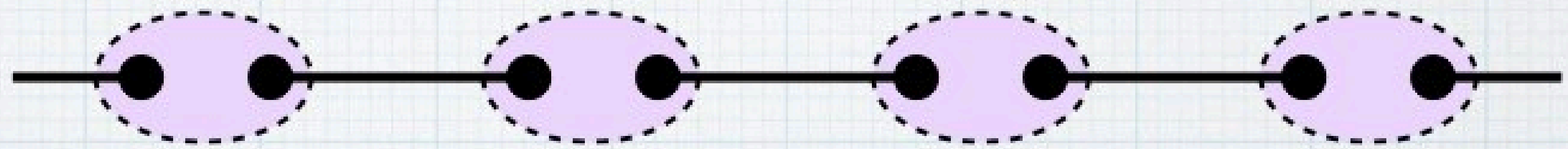
universal properties of the "Haldane phase"

topological phase transition
and
SPT phases

Two $S = 1$ chains with a unique gapped ground state

AKLT model

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

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

trivial model

$$\hat{H}_{\mathrm{trivial}} = \sum_j (\hat{S}^{\mathrm{z}}_j)^2 \qquad \hat{S}^{\mathrm{z}}_j|0\rangle_j = 0 \qquad \hat{S}^{\mathrm{z}}_j|\pm\rangle_j = \pm|\pm\rangle_j$$

$$|\mathrm{GS}_{\mathrm{trivial}}\rangle = |\cdots 00000000 \cdots\rangle$$

both models have a unique gapped ground state

are the two models "connected" smoothly?

property of a model which interpolates the two models

Interpolating model

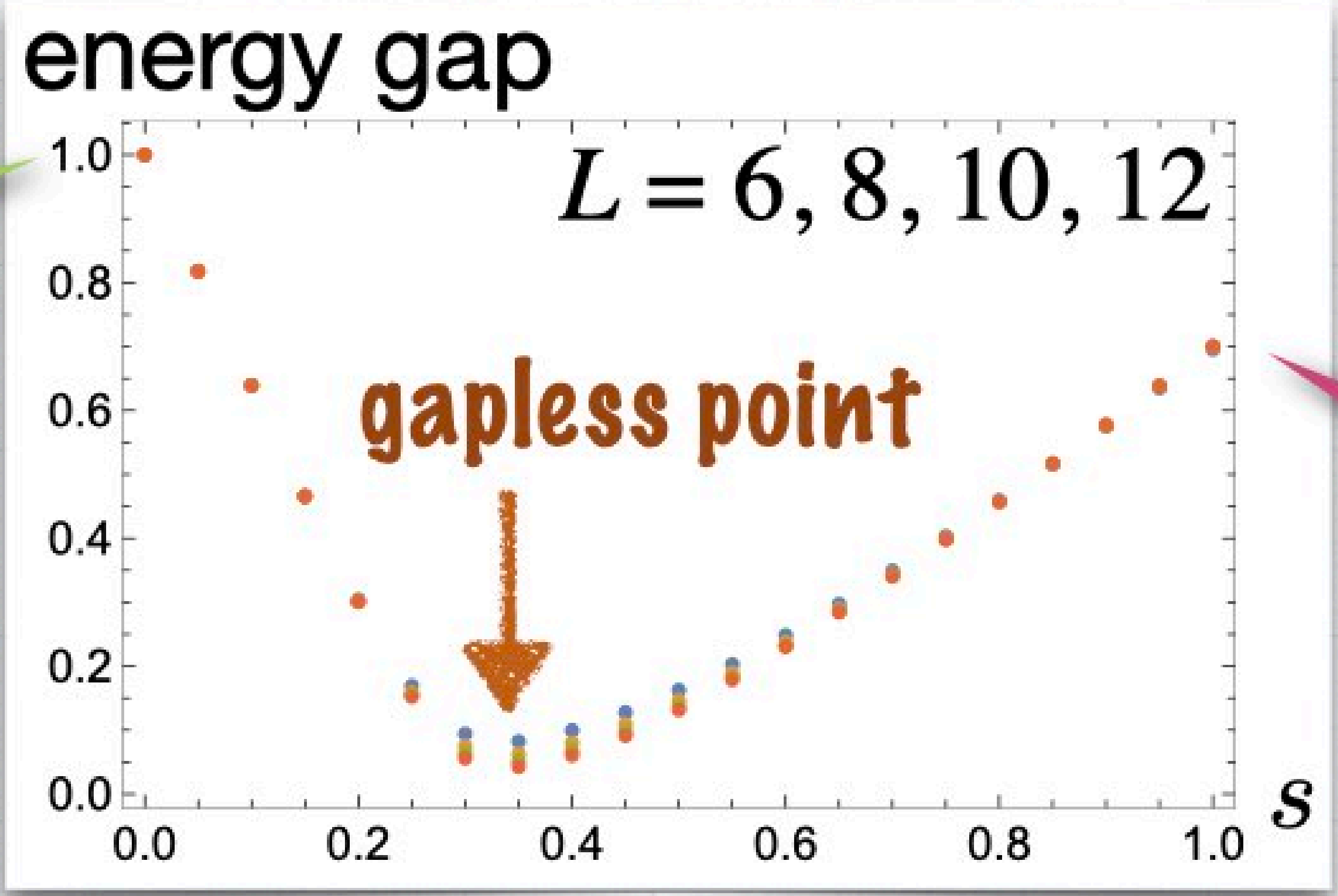
$$\hat{H}_s = s\hat{H}_{\mathrm{AKLT}} + (1-s)\hat{H}_{\mathrm{trivial}} \quad 0 \le s \le 1 \qquad S=1$$

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

$$\hat{H}_{\mathrm{trivial}} = \sum_j (\hat{S}^{\mathrm{z}}_j)^2$$

a unique gapped ground state at $s = 0, 1$

trivial gap



Haldane gap

numerical results by Hosho Katsura

there is a phase transition at intermediate s !!

Interpolating model

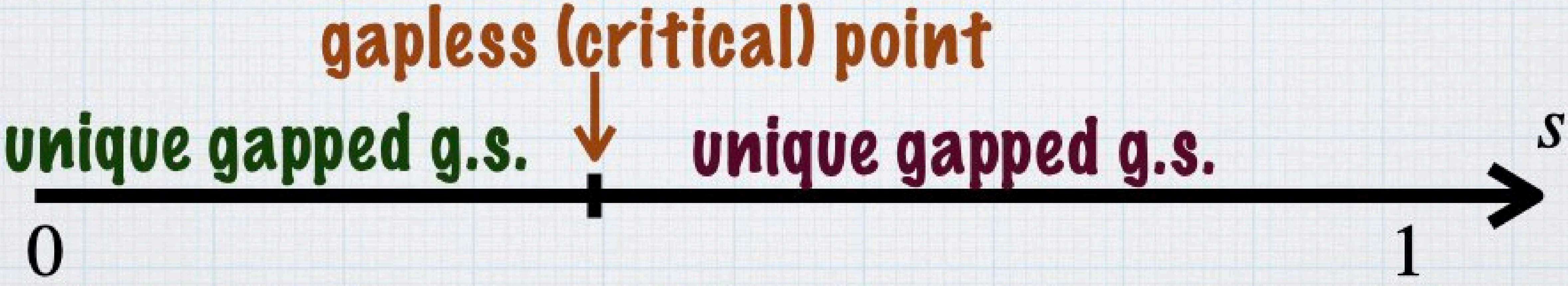
$$\hat{H}_s = s\hat{H}_{\mathrm{AKLT}} + (1-s)\hat{H}_{\mathrm{trivial}} \quad 0 \le s \le 1 \qquad S=1$$

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

$$\hat{H}_{\mathrm{trivial}} = \sum_j (\hat{S}^{\mathrm{z}}_j)^2$$

there is a phase transition at intermediate s !!

but, for $s = 0$ and 1, the ground state is unique, and breaks no symmetry



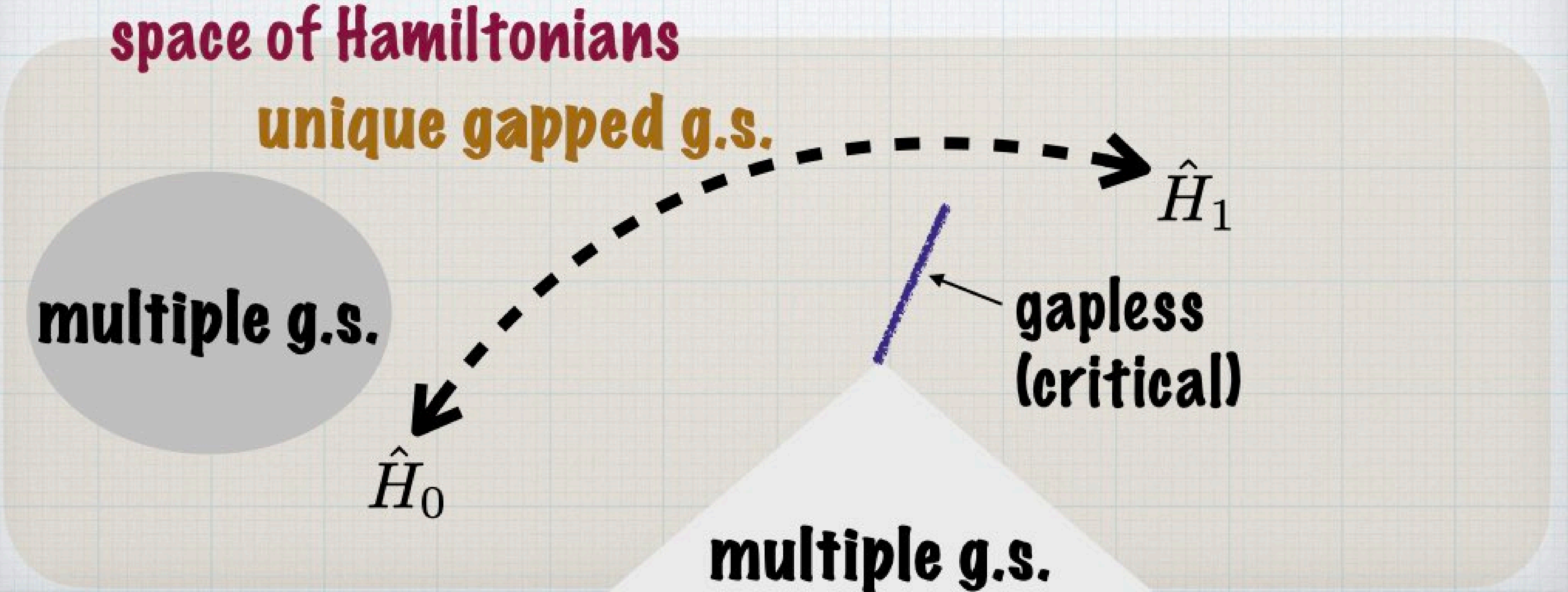
a "topological" phase transition (i.e., a phase transition which cannot be characterized by symmetry breaking)

proofs of the existence of a phase transition

Tasaki 2018 Ogata 2018

Smooth connection of two models

DEFINITION: $\hat{H}_0$ and $\hat{H}_1$ are said to be smoothly connected if there is a family $\hat{H}_s$ (with $0 \leq s \leq 1$), and, the Hamiltonian $\hat{H}_s$ has a unique gapped ground state for each s and the ground state depends smoothly on s



symmetry and phase transition

Gu, Wen 2009, Chen, Gu, Wen 2011

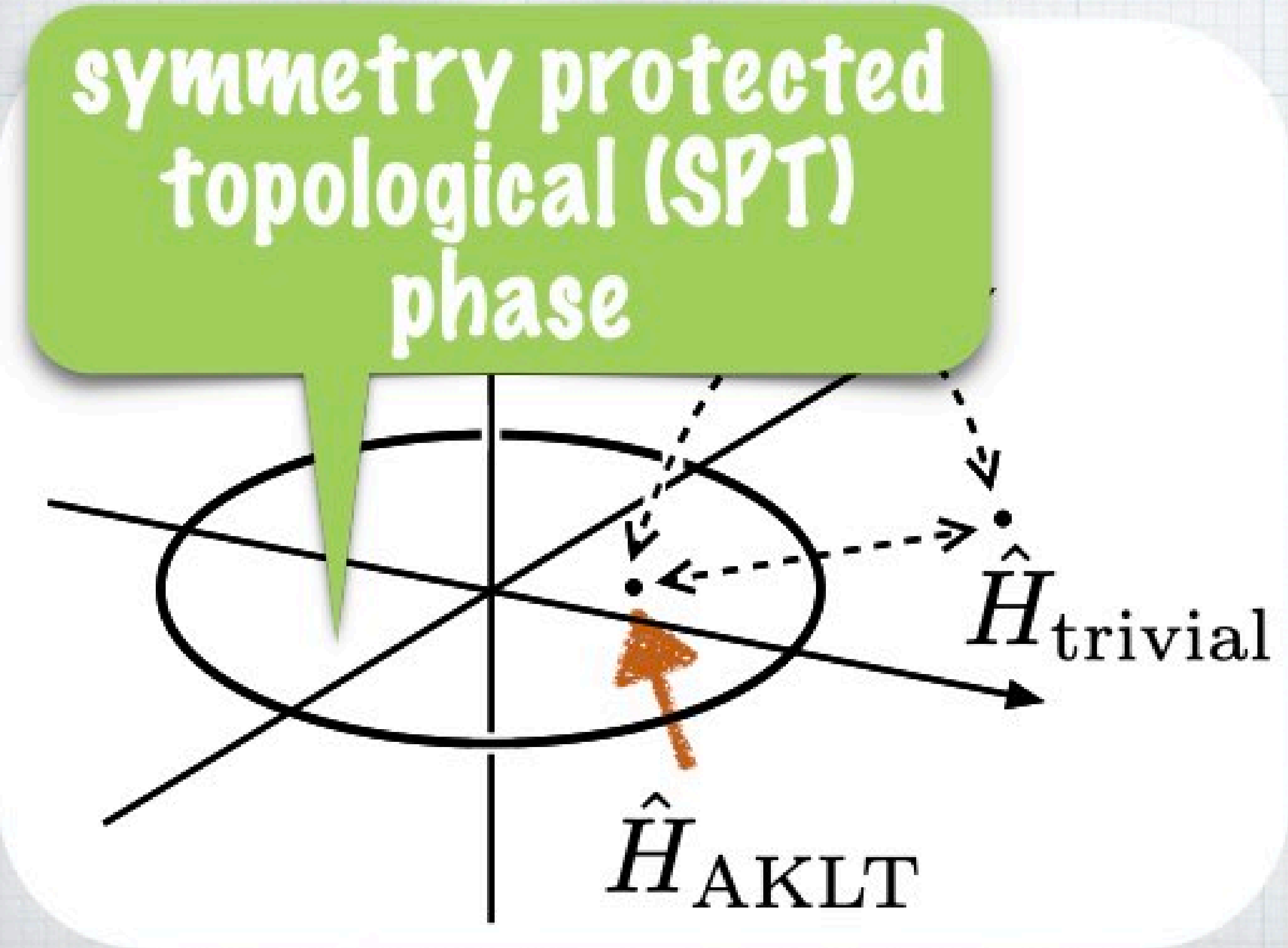
two Hamiltonians $\hat{H}_{\mathrm{AKLT}}$ and $\hat{H}_{\mathrm{trivial}}$

can be smoothly connected if any short ranged Hamiltonian is allowed

proof: Bachmann, Nachtergaele 2014, Ogata 2017

can never be smoothly connected if only Hamiltonians with certain symmetry are allowed

symmetry protected topological (SPT) phase



there must be a ground state phase transition!

Symmetry protected topological (SPT) phase

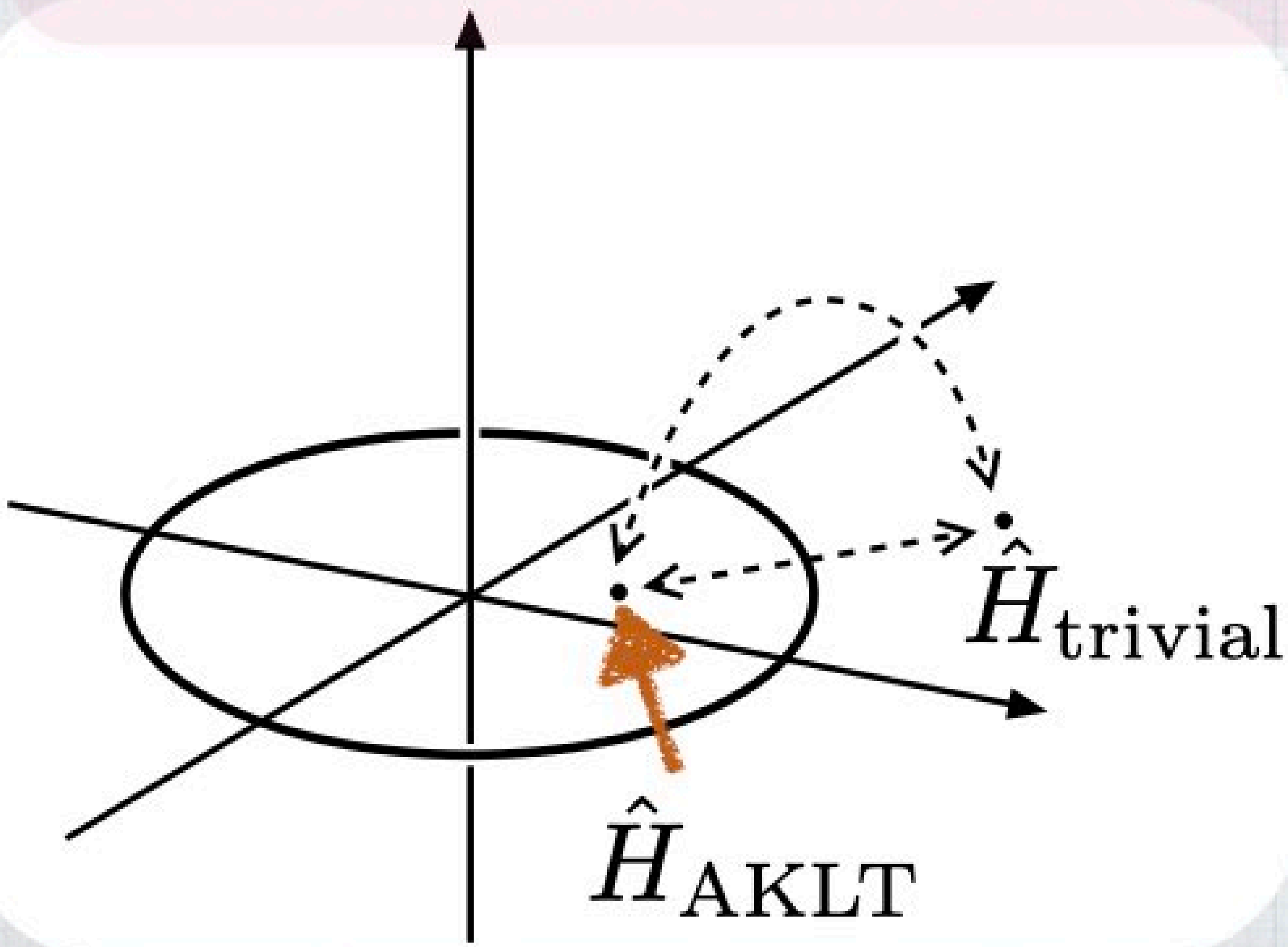
Gu,Wen 2009, Pollmann, Turner, Berg, Oshikawa 2010, 2012

Haldane phase (which includes AKLT model) of an $S=1$ chain is in a nontrivial SPT phase protected either by

S1 $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry (π-rotations about the three axes)

S2 time-reversal symmetry

S3 bond-centered reflection symmetry



SPT phases are characterized by "topological" indices, rather than order parameters