Matrix product state in symmetry protected topological phases

Hiroshi Ueda (Meiji Univ.)

HU and S. Onoda, Phys. Rev. B **90**, 214425 (2014).

T. Morimoto, HU, T. Momoi, and A. Furusaki, Phys. Rev. B **90**, 235111 (2014).

Outline

- Continuous phase transitions in Landau theory
- Continuous phase transitions outside Landau theory
  - Symmetry protected topological (SPT) phase transition
- How to classify SPT phases by use of matrix product states
- Our recent works

✓ SPT phase transition in a zigzag chain
✓ Z_3 SPT phase in SU(3) AKLT model

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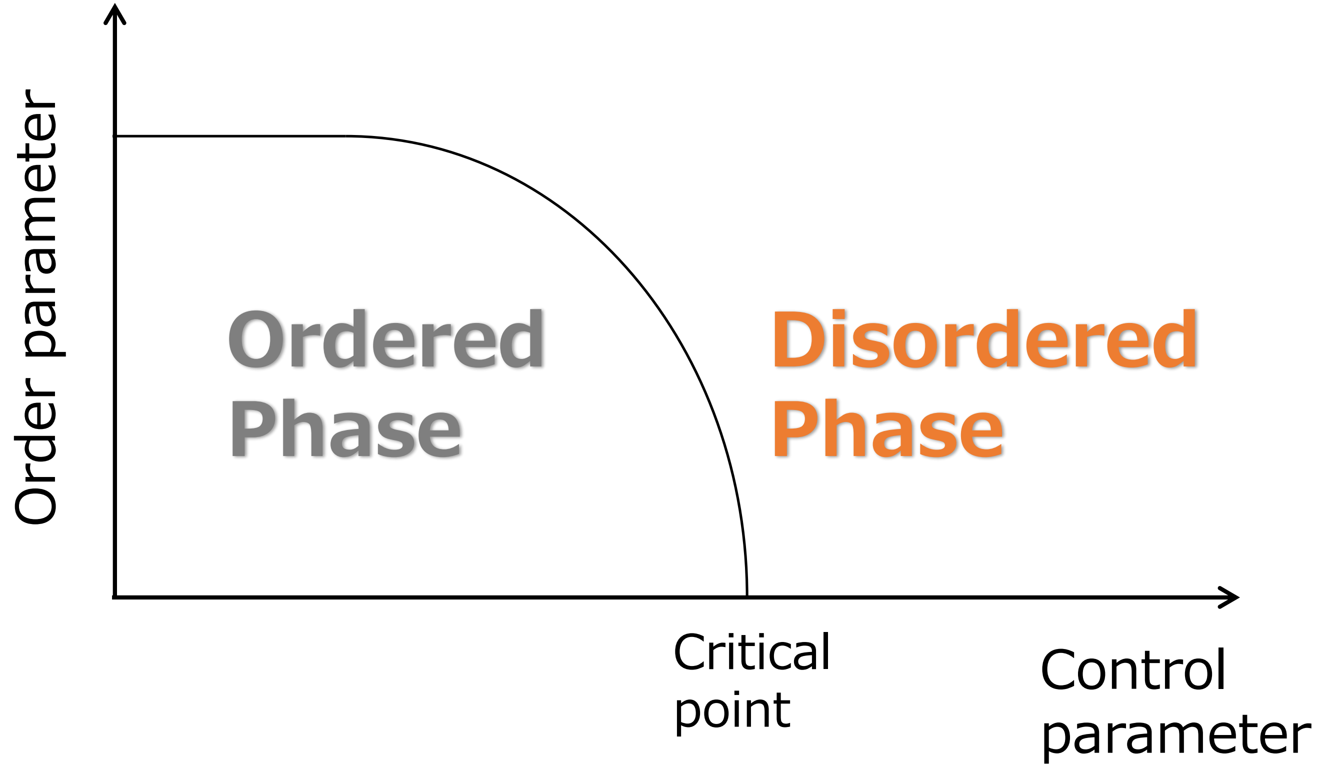
Continuous phase transitions in Landau theory



Classification of phases:

- Order parameter

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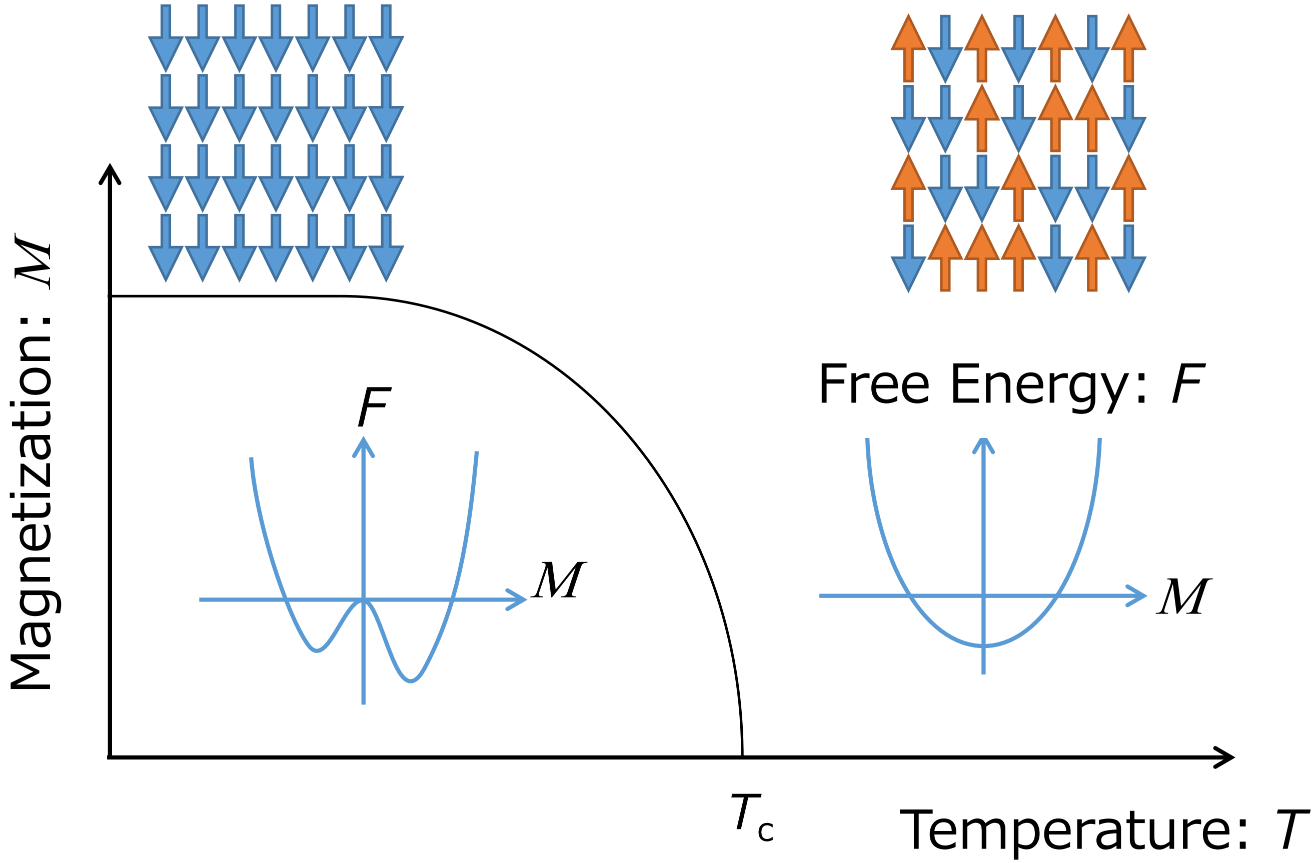
- Spontaneous symmetry breaking

Continuous phase transitions in Landau theory



Ex) Ising Model

$$H = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

$$Z = \mathrm{Tr}\left[\exp\left(-\frac{H}{k_\mathrm{B}T}\right)\right]$$

$$\begin{aligned} F &= -k_\mathrm{B} T \ln Z \\ &= a + rM^2 + sM^4 - hM + \cdots \end{aligned}$$

$$M = \sum_i \sigma_i$$

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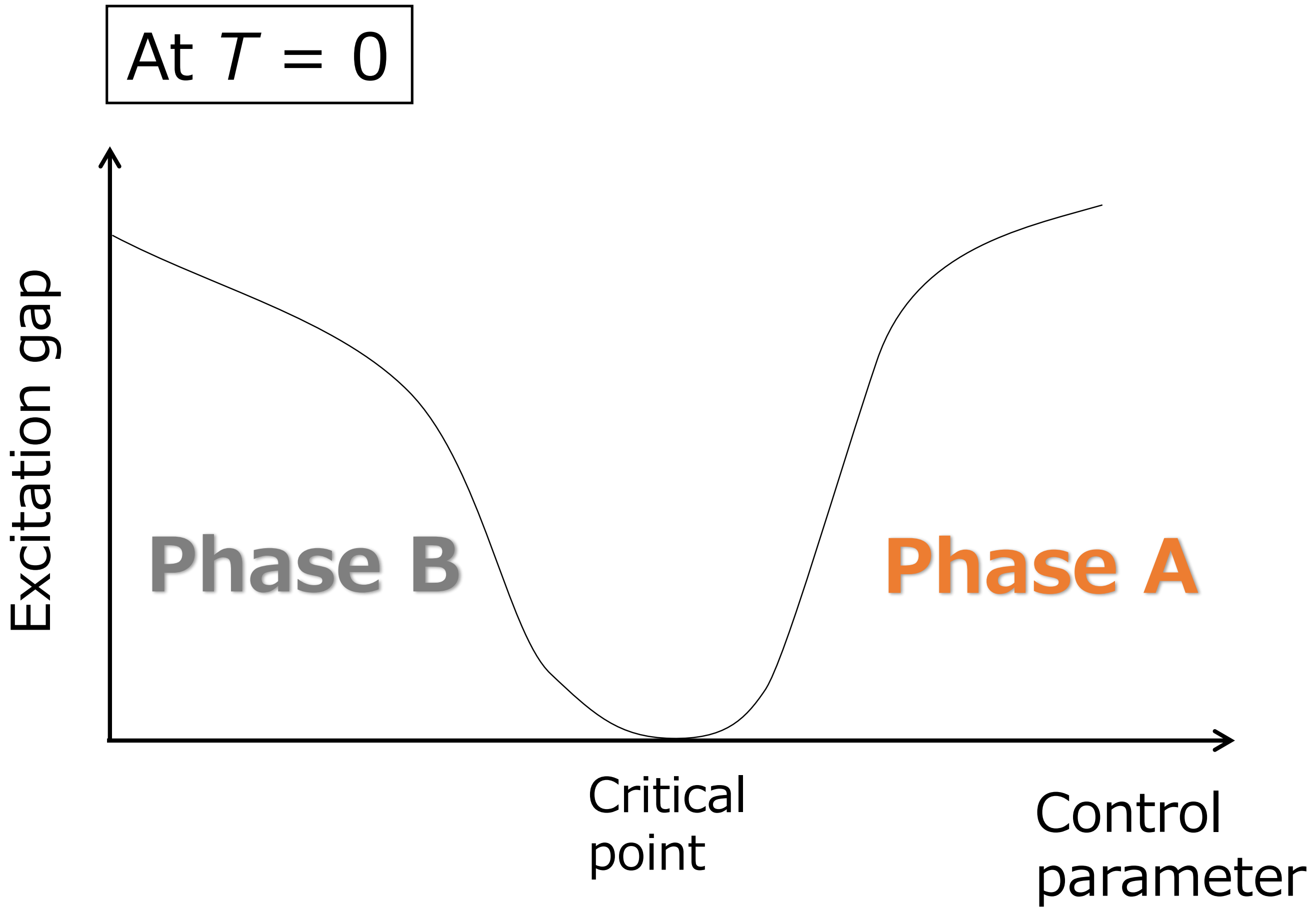
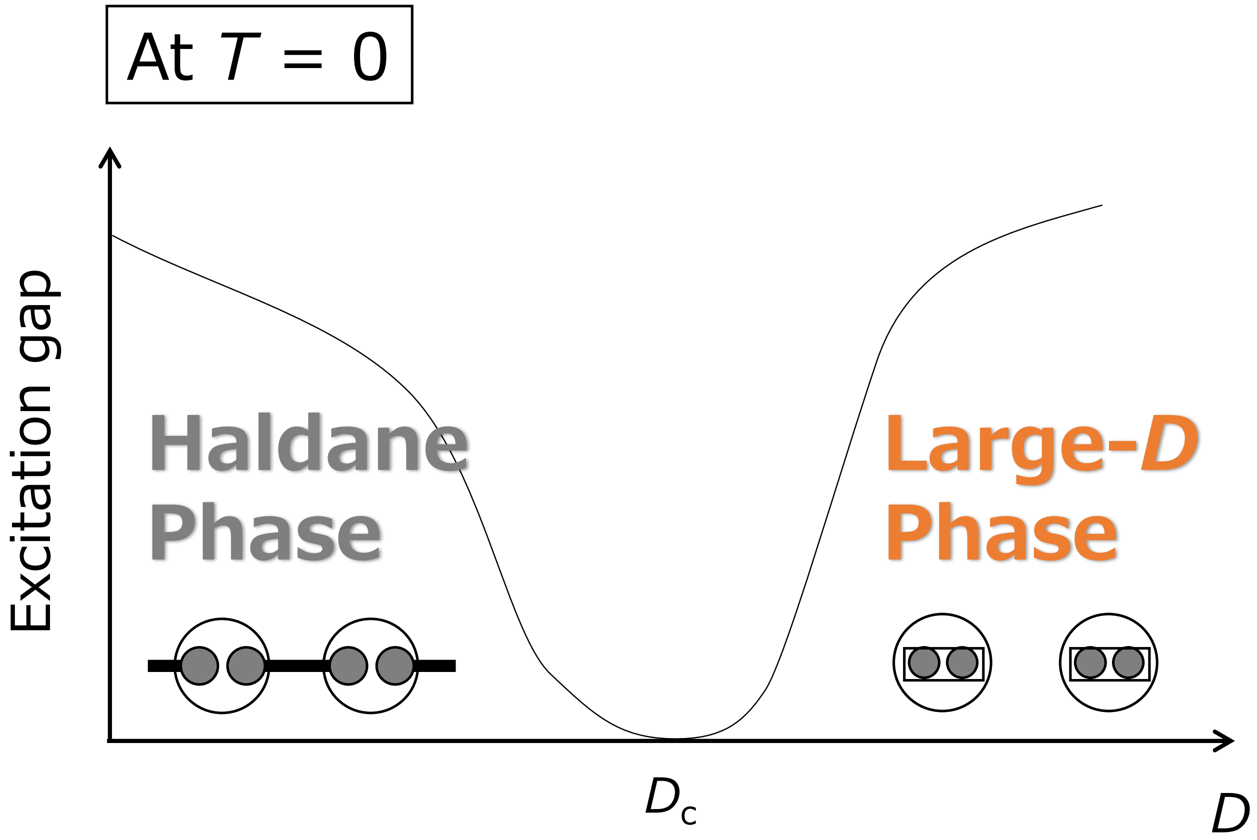
Continuous phase transitions outside Landau theory



Without any spontaneous symmetry breakings

- Translational symmetry
- Rotational symmetry
- Parity symmetry
- Time-reversal symmetry

Continuous phase transitions outside Landau theory



Ex) Spin-1 Heisenberg chain with a single-ion anisotropy

$$H = \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + D \sum_i (S_i^z)^2$$

Chen, Hida, Sanctuary, JPSJ (2000)

In both phases

$$\hat{T}|\Psi_{\rm gs}\rangle = |\Psi_{\rm gs}\rangle$$

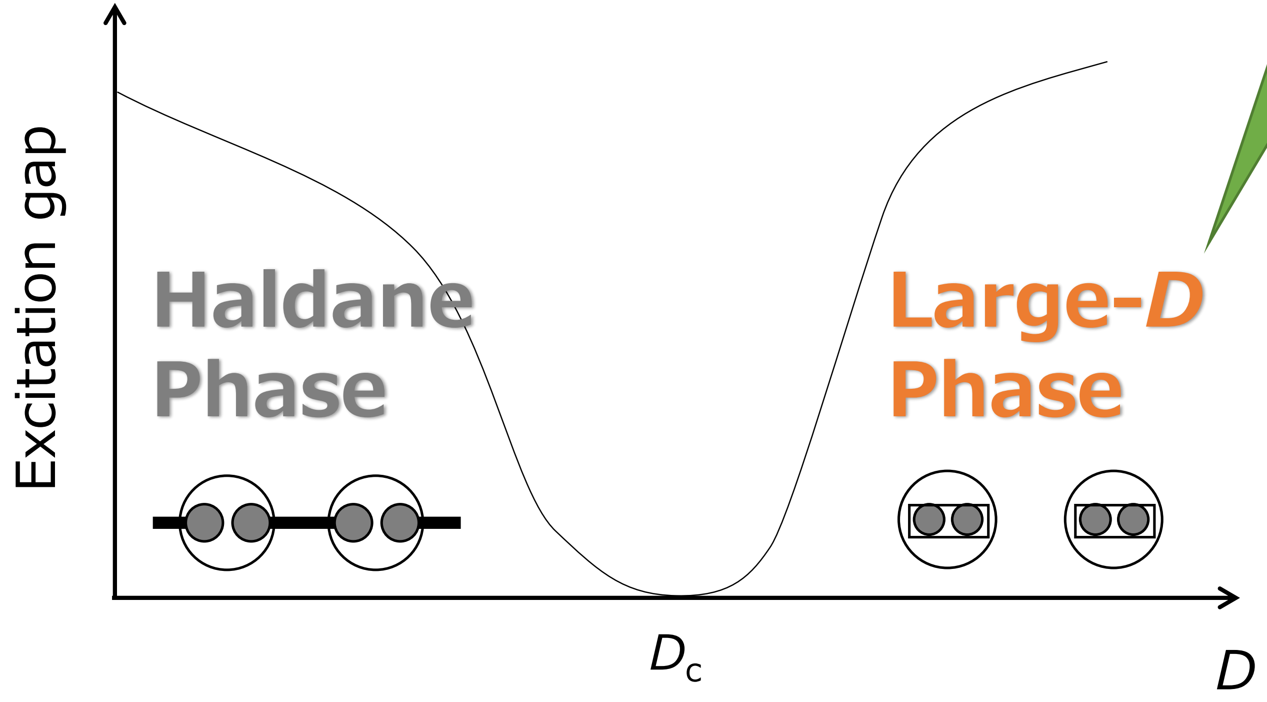
$$\langle\Psi_{\rm gs}|\boldsymbol{S}_i|\Psi_{\rm gs}\rangle = \boldsymbol{0}$$

$\hat{T}$: Translation operator

$|\Psi_{\rm gs}\rangle$: Ground state

$$H = D\sum_i (S_i^z)^2 \text{ when } D \to +\infty$$

$$|\Psi_{\rm gs}\rangle = \cdots \otimes |0\rangle \otimes |0\rangle \otimes |0\rangle \cdots$$



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$$\langle\Psi_{\rm gs}|\boldsymbol{S}_i|\Psi_{\rm gs}\rangle = \boldsymbol{0}$$

$\hat{T}$: Translation operator

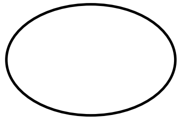
$|\Psi_{\rm gs}\rangle$: Ground state

$$H \xrightarrow{D \to 0} \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \longrightarrow \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \frac{1}{3}(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2$$

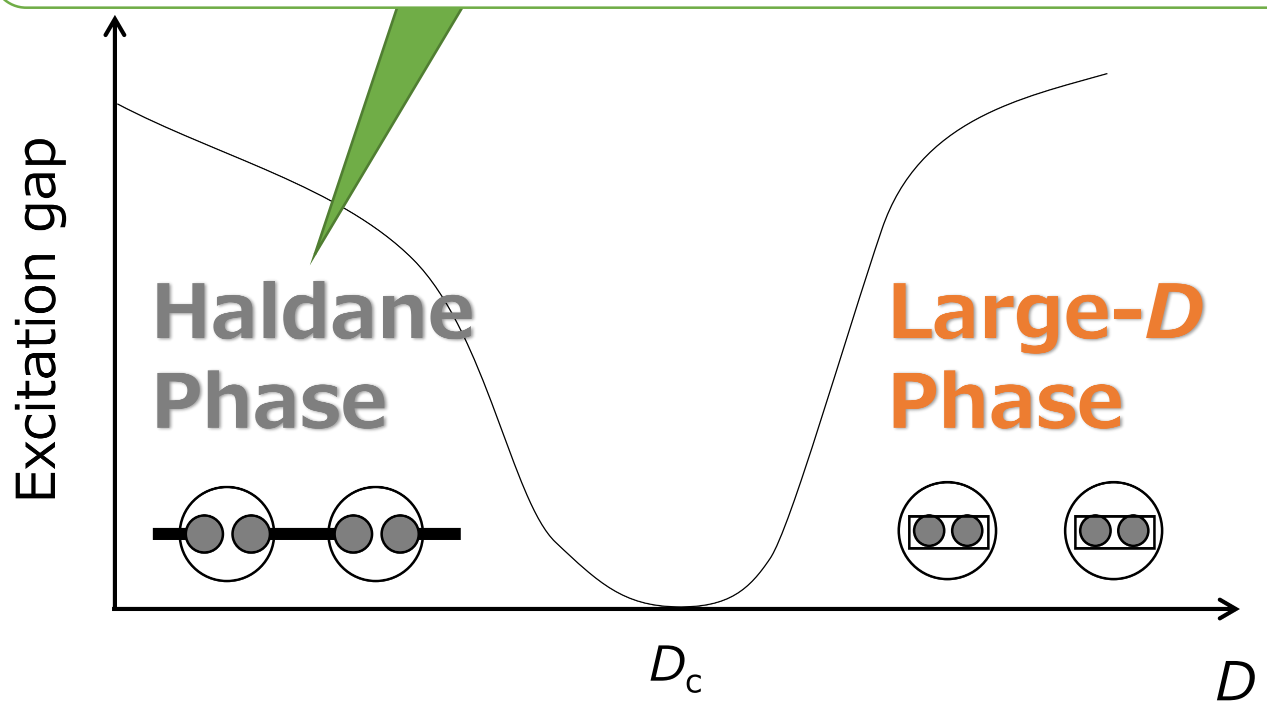
without a gap closing

AKLT model

$$= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\ ,$$



$$= |1\rangle\langle\uparrow\uparrow| + |0\rangle\left(\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}}\right) + |-1\rangle\langle\downarrow\downarrow|$$



$$H = \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + D\sum_i (S_i^z)^2$$

Chen, Hida, Sanctuary, JPSJ (2000)

In both phases

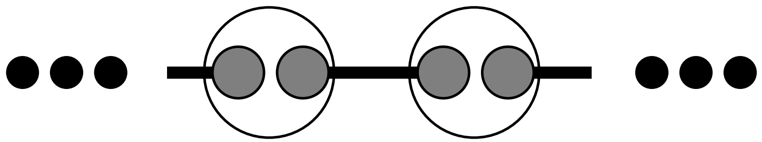
$$\hat{T}|\Psi_{\rm gs}\rangle = |\Psi_{\rm gs}\rangle$$

$$\langle\Psi_{\rm gs}|\boldsymbol{S}_i|\Psi_{\rm gs}\rangle = \boldsymbol{0}$$

$\hat{T}$: Translation operator

$|\Psi_{\rm gs}\rangle$: Ground state

Matrix product state (MPS) for the AKLT state



$$|\Psi_{\rm gs}\rangle = \sum_{\{m_i\}} \mathrm{Tr}\big[\cdots B\tilde{A}^{m_i} B\tilde{A}^{m_{i+1}} \cdots\big] |\cdots m_i m_{i+1} \cdots\rangle \quad (m_i = 1, 0, -1)$$

$$B = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},\ \tilde{A}^1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},\ \tilde{A}^0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \tilde{A}^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$= \sum_{\{m_i\}} \mathrm{Tr}\big[\cdots A^{m_i} A^{m_{i+1}} \cdots\big] |\cdots m_i m_{i+1} \cdots\rangle$$

$$A^m = \tilde{A}^m B,\ A^{\pm 1} = \frac{1}{2\sqrt{2}}(\pm\sigma_x + \mathbf{i}\sigma_y),\ A^0 = -\frac{1}{2}\sigma_z$$

MPS's for gapped ground states

$$|\Psi_{\rm gs}\rangle = \sum_{\{d_i\}} {\rm Tr}\left[\cdots A^{d_i} A^{d_{i+1}} \cdots\right] |\cdots d_i d_{i+1} \cdots\rangle \quad (d_i = 1, 2, \cdots, d)$$

Physical space

$$A^{d_i} = \left\{ A^{d_i}_{\alpha\beta} \right\}^{1 \leq \alpha \leq m}_{1 \leq \beta \leq m}$$

Auxiliary space

In MPS methods

m : input parameter to
control numerical accuracy

Bipartite entanglement entropy for MPS's

$$S \lesssim \log m$$

Entropic area law for 1D gapped system

$S \sim \log$ (Correlation length)

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Chen, Gu, Wen, PRB (2011)
Pollmann, Turner, Berg, Oshikawa, PRB (2010)

- Our recent works

Symmetry transformation of MPS

$$|\Psi_{\rm gs}\rangle = \sum_{\{m_i\}} \mathrm{Tr}\left[\cdots A^{m_i} A^{m_{i+1}} \cdots\right] |\cdots m_i m_{i+1} \cdots\rangle$$

$$\hat{g}|\Psi_{\rm gs}\rangle = \sum_{\{m_i\}} \mathrm{Tr}\left[\cdots A_g^{m_i} A_g^{m_{i+1}} \cdots\right] |\cdots m_i m_{i+1} \cdots\rangle$$

Ex) When *g* is a local operation: $A_g^{m_i} = \sum_{m_i'} g_{m_i m_i'} A^{m_i'}$

Invariant under a symmetry operation $\hat{g}$ ⇔ $\hat{g}|\Psi_{\rm gs}\rangle = a|\Psi_{\rm gs}\rangle$, a : Phase factor ⇔ $A_g^{m_i} = \alpha_g U_g^{-1} A^{m_i} U_g$

Phase factor α_g : 1D representation

U_g : representation matrix

Factor systems in projective representation

Unitary symmetry group: $G = \{g_1, g_2, g_3, \cdots\}$

$$g_1 g_2 = g_3 \Rightarrow U_{g_1} U_{g_2} = \alpha^{g_3}_{g_1 g_2} U_{g_3}$$

Factor systems

Ex) π-rotation around $a(= x, y, z)$ axis in the spin space

AKLT state: $U_a = \sigma_a \Rightarrow \alpha^{y}_{zx} = \mathbf{i}$

Large-D state: $U_a = 1 \Rightarrow \alpha^{y}_{zx} = 1$

Factor systems in projective representation

Unitary symmetry group: $G = \{g_1, g_2, g_3, \cdots\}$

g_1

Different factor systems

↕

Different SPT phases

Ex) … space

AKLT state: $U_a = \sigma_a$ ⇨ $\alpha^y_{zx} = \mathbf{i}$

Large-D state: $U_a = 1$ ⇨ $\alpha^y_{zx} = 1$

Practical estimation of factor systems

Unitary symmetry group: $G = \{g_1, g_2, g_3, \cdots\}$

$$g_1 g_2 = g_3 \Rightarrow U_{g_1} U_{g_2} = \alpha^{g_3}_{g_1 g_2} U_{g_3}$$

$\alpha^{g_3}_{g_1 g_2}$ is not unique.

U_{g_1}, U_{g_2}, U_{g_3} have arbitrary phase factors.

$$g_2 g_1 = g_3 \Rightarrow U_{g_2} U_{g_1} = \alpha^{g_3}_{g_2 g_1} U_{g_3}$$

$$U_{g_1} U_{g_2} = \omega_{g_1 g_2} U_{g_2} U_{g_1}, \quad \omega_{g_1 g_2} = \frac{\alpha^{g_3}_{g_1 g_2}}{\alpha^{g_3}_{g_2 g_1}}$$

$\omega_{g_1 g_2}$: unique

	ω_{zx}
AKLT state	-1
Large-*D* state	1

Parity symmetry

g=p: Bond center inversion

$$A_g^{m_i} = (A^{m_i})^T = \alpha_g U_g^{-1} A^{m_i} U_g$$

$$A_{gg}^{m_i} = (\alpha_g U_g^{-1} A^{m_i} U_g)^T = \alpha_g^2 U_g^T U_g^{-1} A^{m_i} U_g (U_g^{-1})^T = A^{m_i}$$

$$\Leftrightarrow \alpha_g = \pm 1,\ U_g^T = \beta_g U_g\ (\beta_g = \pm 1)$$

AKLT state: $\alpha_g = -1,\ U_g = \sigma_y,\ \beta_g = -1$

Large-D state: $\alpha_g = 1,\ U_g = 1,\ \beta_g = 1$

Parity symmetry

g=*p*: Bond center inversion

A_g^{m} ...

A_{g}^{m} ... $= A^{m_i}$

$(\beta_g = \pm 1)$

This phase transition is protected by the parity symmetry.

AKLT state: $\alpha_g = -1,\ U_g = \sigma_y,\ \beta_g = -1$

Large-*D* state: $\alpha_g = 1,\ U_g = 1,\ \beta_g = 1$

Time-reversal symmetry

g=Θ: π-rotation around *y* axis + complex conjugation

$$A_g^{m_i} = \sum_{m_i'} R_y(\pi)_{m_i m_i'} (A^{m_i'})^* = \alpha_g U_g^{-1} A^{m_i} U_g$$

$$A_{gg}^{m_i} = \sum_{m_i'} R_y(\pi)_{m_i m_i'} (\alpha_g U_g^{-1} A^{m_i'} U_g)^* = (U_g^{-1})^* U_g^{-1} A^{m_i} U_g U_g^* = A^{m_i}$$

⇔ $U_g^* = \beta_g U_g^{-1} \ (\beta_g = \pm 1)$

AKLT state: $U_g = \sigma_y, \ \beta_g = -1$

Large-*D* state: $U_g = 1, \ \beta_g = 1$

Time-reversal symmetry

g=Θ: π-rotation around *y* axis + complex conjugation

A_g^{m}

A_{gg}^{m} … $_g^{*} = A^{m_i}$

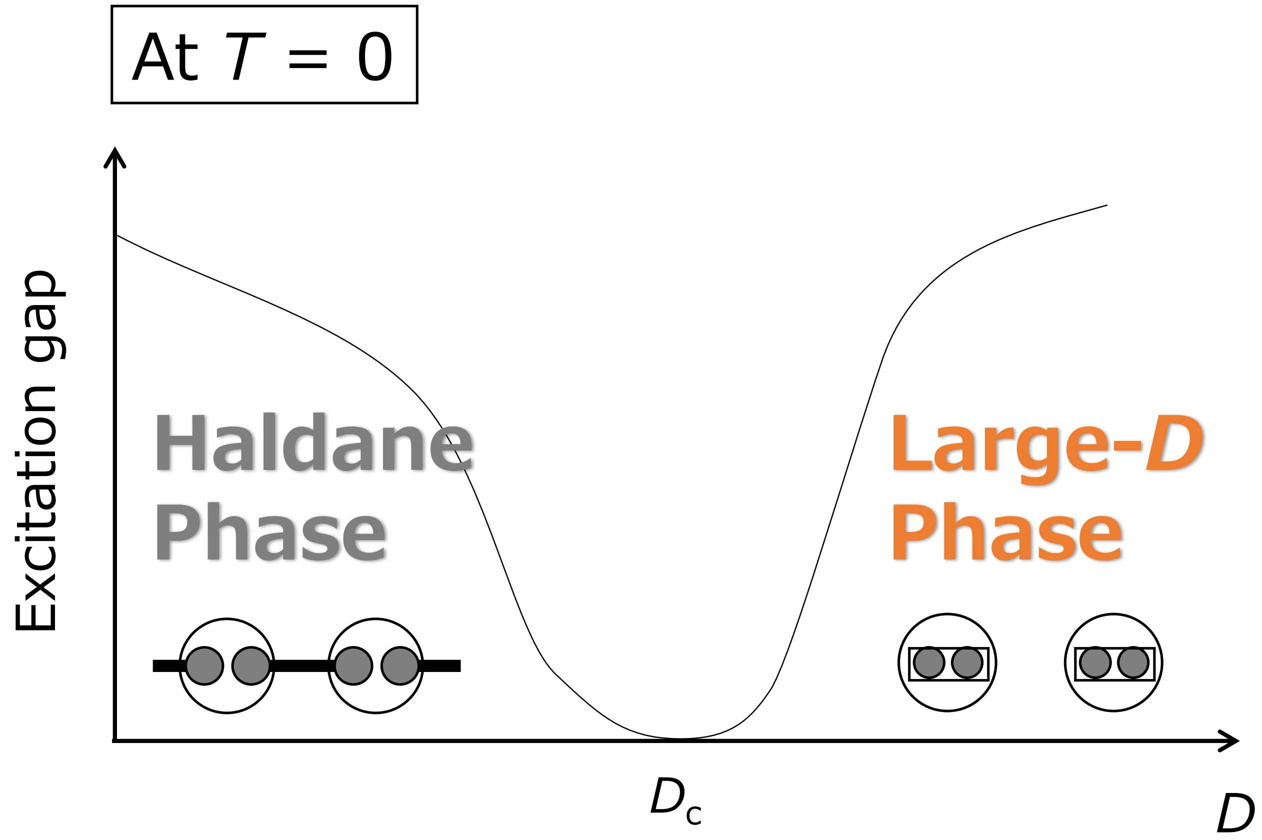
…1)

This phase transition is protected by the time-reversal symmetry.

AKLT state: $U_g = \sigma_y,\ \beta_g = -1$

Large-*D* state: $U_g = 1,\ \beta_g = 1$

SPT phase transition in S=1 Chain



Index	Haldane Phase	Large-D Phase
ω_{zx}	-1	1
α_p	-1	1
β_p	-1	1
β_Θ	-1	1
	Nontrivial	**trivial**

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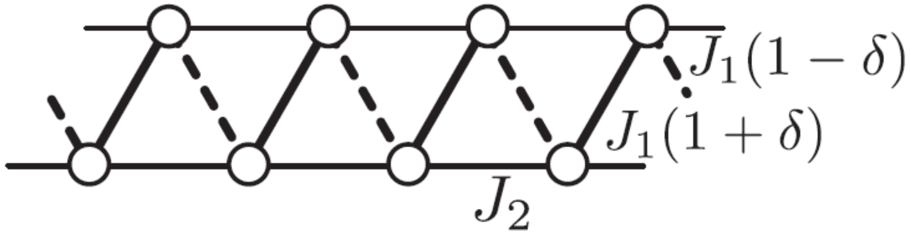
Spin-1/2 frustrated zigzag chain

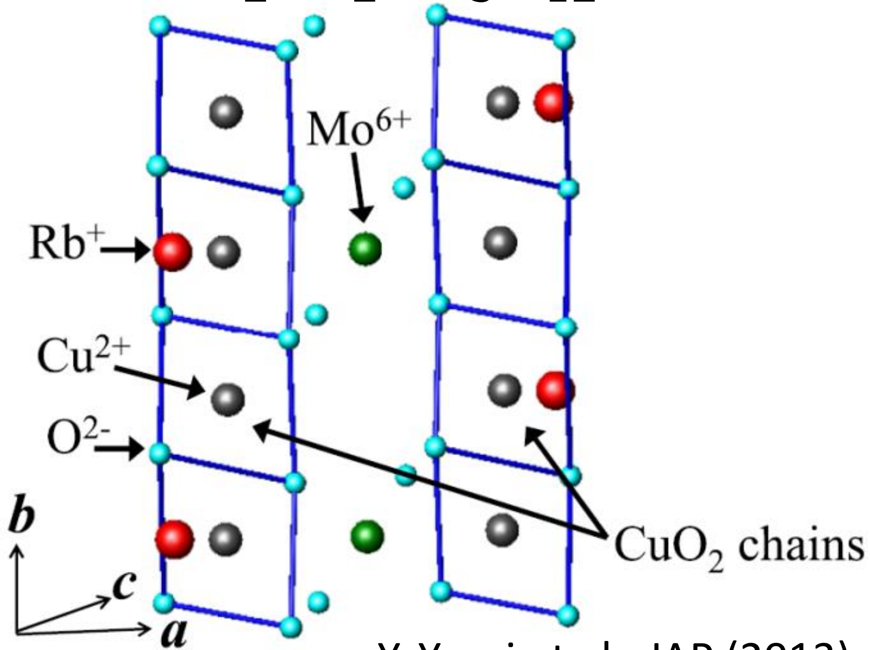
$$H = J_1 \sum_i (1-(-1)^i\delta)\left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right]$$
$$+ J_2 \sum_i \left[S_i^x S_{i+2}^x + S_i^y S_{i+2}^y + \Delta S_i^z S_{i+2}^z\right]$$



$$(J_1 < 0,\ J_2 > 0,\ |\delta| \ll 1)$$

✓ Relevant materials:
Quasi-1D spin-1/2 cuprate Mott insulators

$Rb_2Cu_2Mo_3O_{12}$



Y. Yasui et al., JAP (2013).

Phase diagram

Order parameters

$$\langle \hat{D}^a \rangle = \langle \Psi_{\rm gs} | S_1^a S_2^a - S_2^a S_3^a | \Psi_{\rm gs} \rangle$$

$$\langle \hat{\kappa}^z \rangle = \langle \Psi_{\rm gs} | S_1^x S_2^y - S_1^y S_2^x | \Psi_{\rm gs} \rangle$$

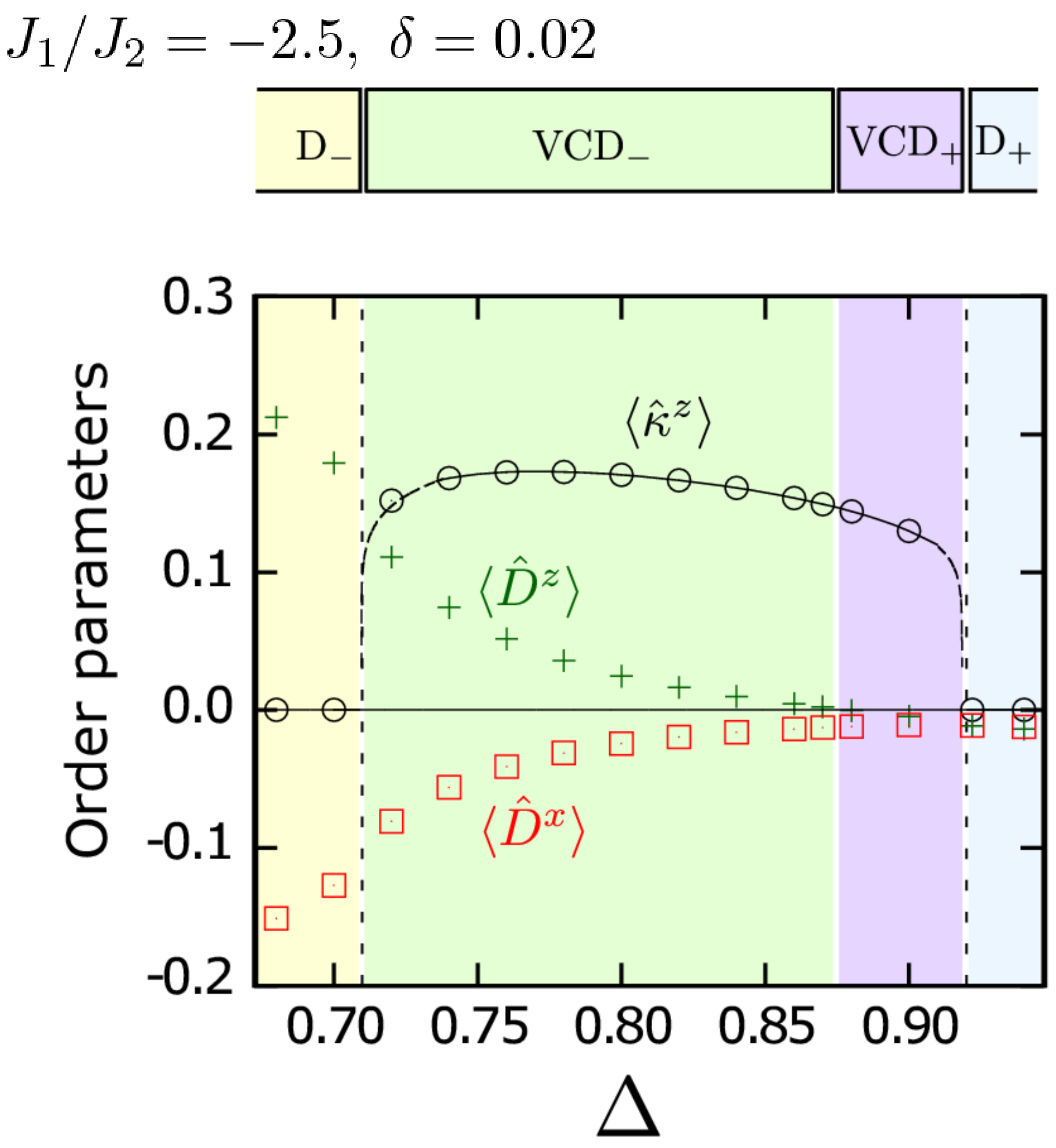
In VCD_+ and VCD_-

$$\hat{T}^2 | \Psi_{\rm gs} \rangle = | \Psi_{\rm gs} \rangle$$

$$\hat{\Theta} | \Psi_{\rm gs} \rangle = | \Psi_{\rm gs} \rangle$$

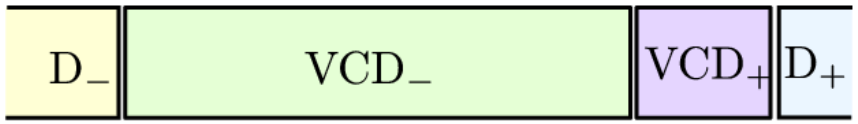
$$\hat{p} | \Psi_{\rm gs} \rangle \neq | \Psi_{\rm gs} \rangle$$

$$\langle \Psi_{\rm gs} | \boldsymbol{S}_i | \Psi_{\rm gs} \rangle = \boldsymbol{0}$$



Phase diagram

$J_1/J_2 = -2.5,\ \delta = 0.02$



Order parameters

$$\langle \hat{D}^a \rangle = \langle \Psi_{\rm gs} | S_1^a S_2^a - S_2^a S_3^a | \Psi_{\rm gs} \rangle$$

$$\langle \hat{\kappa}^z \rangle = \langle \Psi_{\rm gs} | S_1^x S_2^y - S_1^y S_2^x | \Psi_{\rm gs} \rangle$$

In VCD$_+$ and VCD$_-$

$$\hat{T}^2 | \Psi_{\rm gs} \rangle = | \Psi_{\rm gs} \rangle$$

$$\hat{\Theta} | \Psi_{\rm gs} \rangle = | \Psi_{\rm gs} \rangle$$

$$\hat{p} | \Psi_{\rm gs} \rangle \neq | \Psi_{\rm gs} \rangle$$

$$\langle \Psi_{\rm gs} | \boldsymbol{S}_i | \Psi_{\rm gs} \rangle = \boldsymbol{0}$$

Focus on the index β_Θ of MPSs with a two-site unit cell.

$$|\Psi\rangle = \sum_{\{m_i\}} \mathrm{Tr}[\cdots A^{m_1 m_2} A^{m_3 m_4} \cdots] \, |\cdots m_1 m_2 m_3 m_4 \cdots \rangle$$

$$= \sum_{\{m_i\}} \mathrm{Tr}[\cdots B^{m_2 m_3} B^{m_4 m_5} \cdots] \, |\cdots m_2 m_3 m_4 m_5 \cdots \rangle$$

Phase diagram

An SPT phase transition protected by the time-reversal symmetry

In VCD_+ and VCD_-

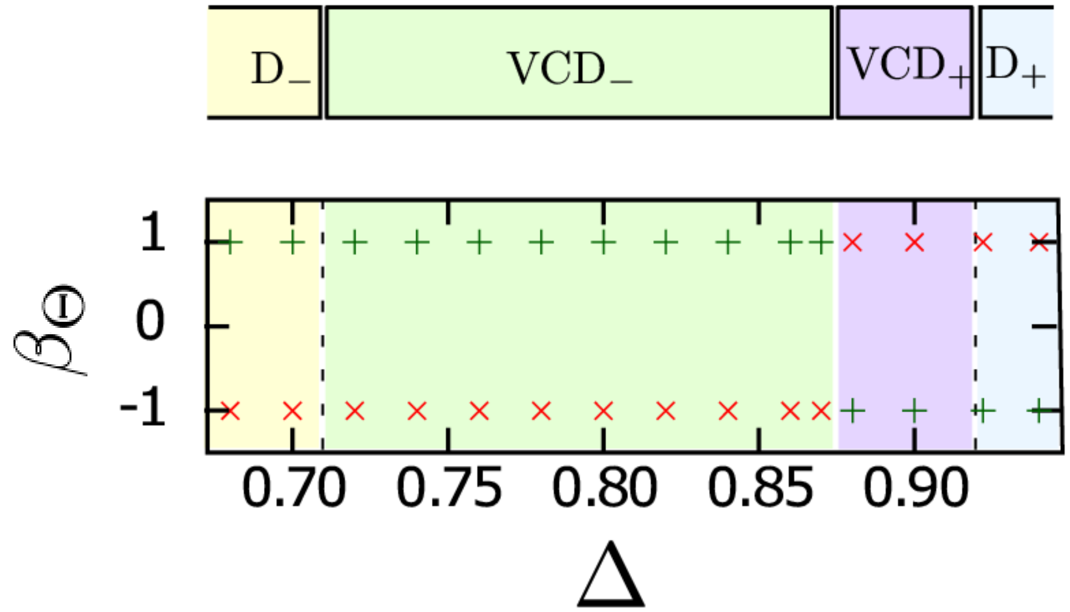
$$\hat{T}^2|\Psi_{\mathrm{gs}}\rangle = |\Psi_{\mathrm{gs}}\rangle$$

$$\hat{\Theta}|\Psi_{\mathrm{gs}}\rangle = |\Psi_{\mathrm{gs}}\rangle$$

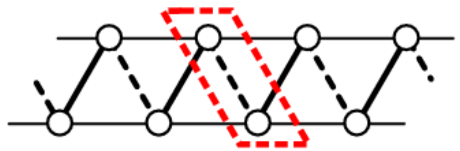
$$\hat{p}|\Psi_{\mathrm{gs}}\rangle \neq |\Psi_{\mathrm{gs}}\rangle$$

$$\langle\Psi_{\mathrm{gs}}|\boldsymbol{S}_i|\Psi_{\mathrm{gs}}\rangle = \boldsymbol{0}$$

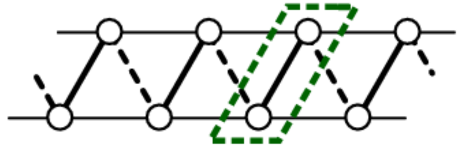
$J_1/J_2 = -2.5,\ \delta = 0.02$



$A^{m_1 m_2}$



$B^{m_2 m_3}$



Z_3 SPT phase

$$(d_i = 1, 2, \cdots, d)$$

$$|\Psi_{\rm gs}\rangle = \sum_{\{d_i\}} \mathrm{Tr}\big[\cdots A^{d_i} A^{d_{i+1}} \cdots\big] |\cdots d_i d_{i+1} \cdots\rangle$$

Symmetry operation: $\hat{g} = \hat{x}, \hat{y}$, $\hat{g}^3 = 1,\ \hat{x}\hat{y} = \hat{y}\hat{x}$

$$\hat{g}|\Psi_{\rm gs}\rangle = |\Psi_{\rm gs}\rangle \Leftarrow \sum_{d_i'} g_{d_i d_i'} A^{d_i'} = e^{\mathbf{i}\theta_g} U_g^{-1} A^{d_i} U_g$$

In nontrivial Z_3 SPT phases,

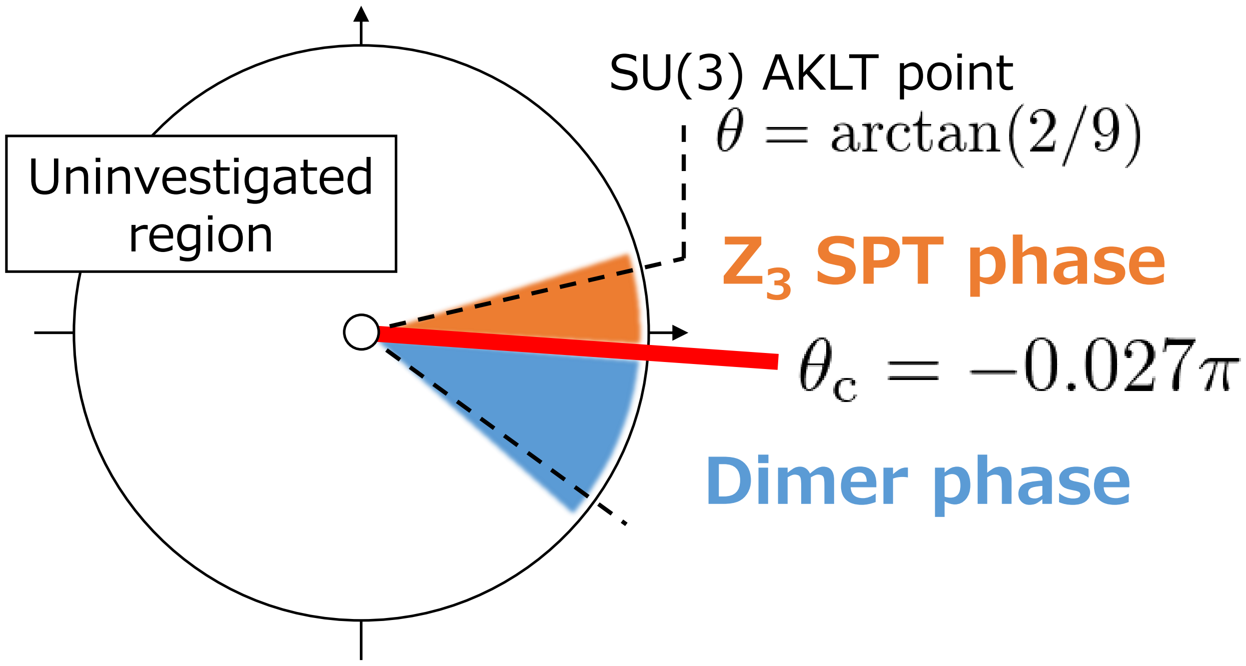
$$U_x U_y = e^{\pm i 2\pi/3} U_y U_x \ .$$

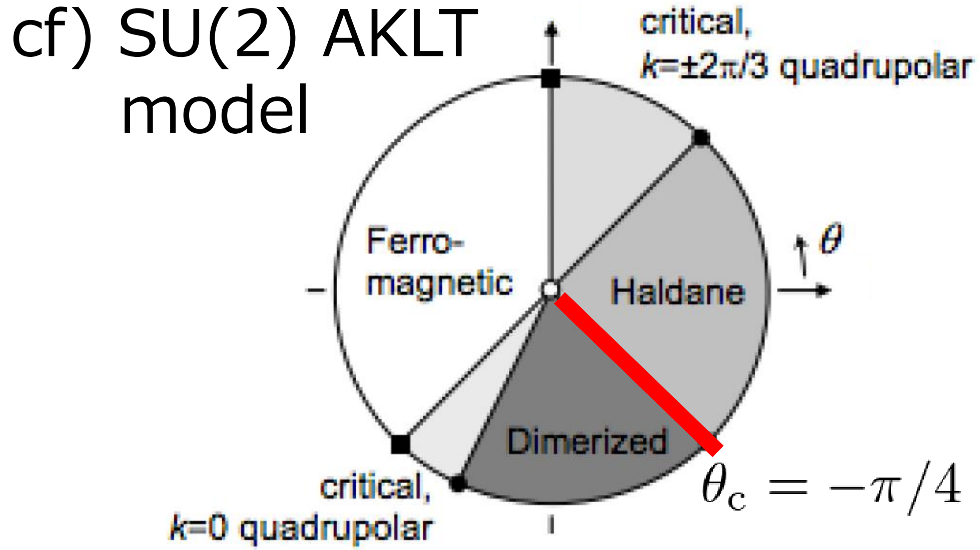
Z_3 SPT phase in SU(3) AKLT model

$$H = \sum_i \cos\theta \, \boldsymbol{T}_i \cdot \boldsymbol{T}_{i+1} + \sin\theta (\boldsymbol{T}_i \cdot \boldsymbol{T}_{i+1})^2$$

Gell-Mann matrix

$$\boldsymbol{T} = (T^1, \cdots, T^8) \, , \; (T^a)_{bc} = \frac{1}{4} \mathrm{Tr}[(\lambda_b)^\dagger (\lambda_a \lambda_c - \lambda_c \lambda_a)] \quad (a, b, c = 1, \cdots, 8)$$





Lauchli, Schmid, Trebst, PRB (2006).

Summary

- Symmetry-protected topological (SPT) phases and transitions in 1D systems

- Representation matrices on auxiliary space of MPS

- SPT phase transitions associated with the time-reversal symmetry in S=1/2 frustrated zigzag chain

- Z_3 SPT phases in SU(3) bilinear-biquadratic model