

# Duality, criticality, topology and integrability in quantum spin-1 chains

**Hosho Katsura (UTokyo)**

Collaborators:

Hong Yang, Linhao Li (UTokyo)

Koichi Okunishi (Niigata Univ.)

- Phys. Rev. B 107, 125158 (2023) [arXiv:2203.15791]

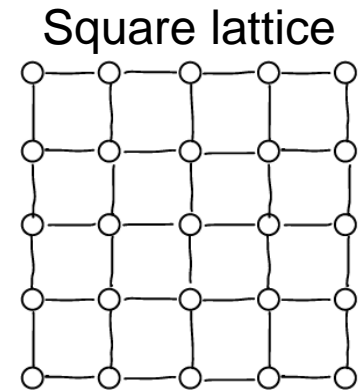
# 2D classical Ising model

## ■ Model

- Spin configuration  $\sigma = \{\sigma_1, \sigma_2, \dots, \sigma_N\}$ ,  $\sigma_i = \pm 1$
- Hamiltonian  $H(\sigma) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$  ( $J > 0$ )
- Partition function

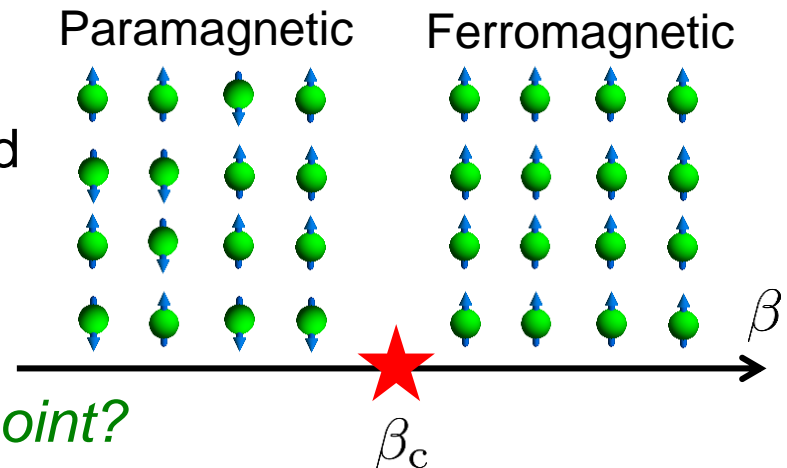
$$Z_N(\beta) = \sum_{\sigma} e^{-\beta H(\sigma)}$$

Solved by Onsager, Phys. Rev. **65**, 117 (1944)  
Majorana-fermion trick by Kauffmann (1949)



## ■ Phases

- Zero temperature ( $\beta = \infty$ )  
All-up and all-down states are realized
- Infinite temperature ( $\beta = 0$ )  
All states occur with equal probability



# Kramers-Wannier duality (1)

Phys. Rev. **60**, 252 (1941)

## ■ “High-temperature” expansion

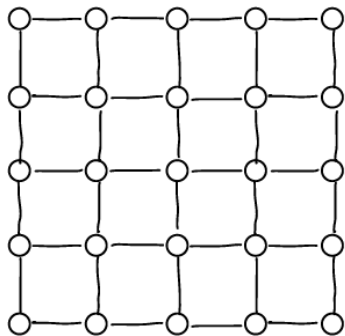
$$Z_N(\beta) = \sum_{\sigma} \exp \left( \underbrace{\beta J}_{\substack{\uparrow \\ K}} \sum_{\langle i,j \rangle} \sigma_i \sigma_j \right)$$

- Useful identity:  $e^{K\sigma_i\sigma_j} = \cosh K (1 + \sigma_i\sigma_j \tanh K)$

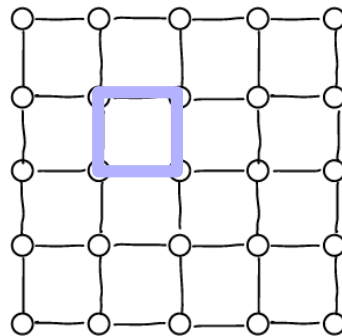
$$\begin{aligned} Z_N(K) &= (\cosh K)^{2N} \sum_{\sigma} \prod_{\langle i,j \rangle} (1 + \sigma_i\sigma_j \tanh K) \\ &= 2^N (\cosh K)^{2N} \sum_P (\tanh K)^{\ell(P)} \end{aligned}$$

$\downarrow \sum_{\sigma=\pm 1} \sigma^n = 1 + (-1)^n$

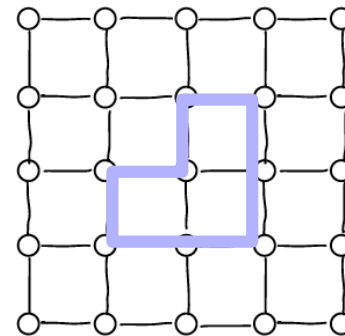
$\leftarrow$  Sum over loop configurations



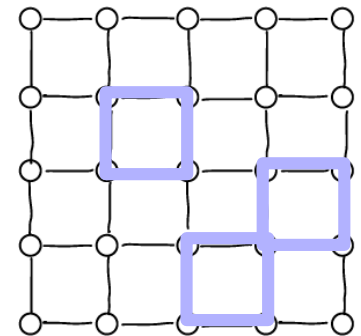
$$\ell(P) = 0$$



$$\ell(P) = 4$$



$$\ell(P) = 8$$



$$\ell(P) = 12$$

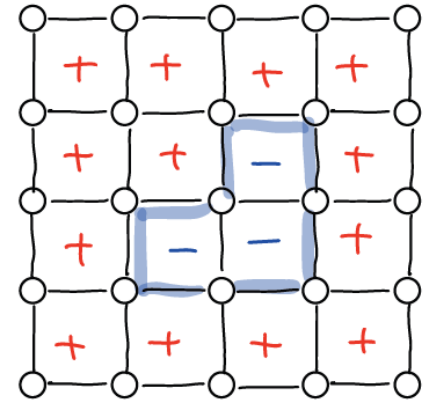
## Kramers-Wannier duality (2)

### ■ $Z$ in terms of dual variables

- Label dual lattice sites by  $a = 1, 2, \dots$
- Dual spin config.  $\mu = \{\mu_1, \mu_2, \dots\}$   
 $\mu = -1$  (+1) inside (outside) a loop

$$Z_N(K) = (\sinh K)^N \sum_{\mu} \prod_{\langle a,b \rangle} \exp(\tilde{K} \mu_a \mu_b)$$

- Dual coupling  $\tilde{K} = \frac{1}{2} \ln \coth K$



$$\ell(P) = \sum_{\langle a,b \rangle} \frac{1 - \mu_a \mu_b}{2}$$

### ■ Critical temperature

- Assumption: a **single** critical temperature
- Then  $K = \tilde{K} = \beta_c J$  must hold

Solving  $K = \frac{1}{2} \ln \coth K$  leads to  $\beta_c J = \frac{1}{2} \ln(1 + \sqrt{2}) \sim 0.44$

# Outline

## 1. Quantum Ising and Potts chains

- Duality and Majorana translation
- Kitaev chain: topology matters
- Duality and parafermion translation

## 2. Kennedy-Tasaki Duality in spin-1 chains

## 3. Criticalities in interpolating models

## 4. Summary

# Quantum Ising chain

## ■ Spin operators

- Pauli matrices

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Spin op. at site  $j$ :  $\sigma_j^\alpha = \overbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}^{j-1} \otimes \sigma^\alpha \otimes \overbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}^{N-j}$ ,

## ■ Hamiltonian ( $J, h > 0$ )

$$H_{\text{Ising}} = -J \sum_j \sigma_j^x \sigma_{j+1}^x - h \sum_j \sigma_j^z$$

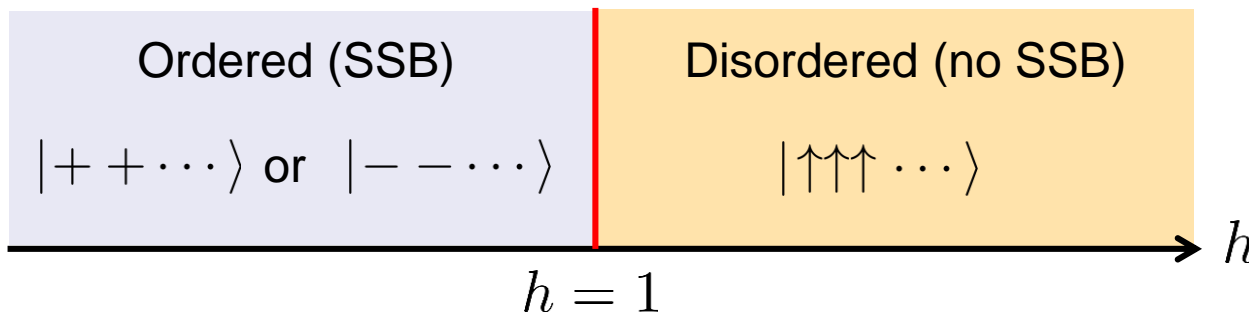
Local basis

$$\sigma^z |\uparrow\rangle = +|\uparrow\rangle$$

$$\sigma^z |\downarrow\rangle = -|\downarrow\rangle$$

$$\sigma^x |\pm\rangle = \pm|\pm\rangle$$

## ■ Phase diagram ( $J=1$ )



$h=1$  is a critical point described by Ising CFT ( $c=1/2$ )

# Kramers-Wannier Duality

## ■ Unitary transformation

Huang & Chen, *PRB* **91**, 195143 (2015)

$$U = \prod_j \frac{1 + i\sigma_j^z}{\sqrt{2}}, \quad V = \prod_j \frac{\sigma_j^x \sigma_{j+1}^x + \sigma_{j+1}^z}{\sqrt{2}}$$

$$(UV) \sigma_j^z (UV)^\dagger = \sigma_j^x \sigma_{j+1}^x$$

$$(UV) \sigma_j^x \sigma_{j+1}^x (UV)^\dagger = \sigma_{j+1}^z$$

## ■ Dual Hamiltonian

$$\tilde{H}_{\text{Ising}} = (UV) H_{\text{Ising}} (UV)^\dagger = -h \sum_j \sigma_j^x \sigma_{j+1}^x - J \sum_j \sigma_j^z$$

- The roles of  $J$  and  $h$  are interchanged
- Must have the same spectrum  
NOTE) Ignore the boundary terms
- If there exists a **single** gapless point, it should be at  $h = J$

*Anything to do with topology?*

# Quantum Ising chain = Kitaev chain

## ■ Jordan-Wigner tr.

- Majorana fermions

$$\gamma_{2j-1} = \left( \prod_{k < j} \sigma_k^z \right) \sigma_j^x, \quad \gamma_{2j} = \left( \prod_{k < j} \sigma_k^z \right) \sigma_j^y$$

$$\begin{aligned} (\gamma_m)^\dagger &= \gamma_m, \\ \{\gamma_m, \gamma_n\} &= 2\delta_{m,n} \end{aligned}$$

## ■ Fermionic Hamiltonian

A. Kitaev, *Phys. Usp.* (2001)

$$H_{\text{Ising}} = iJ \sum_j \gamma_{2j} \gamma_{2j+1} - ih \sum_j \gamma_{2j-1} \gamma_{2j}$$

Duality = Translation  
by 1 Majorana site

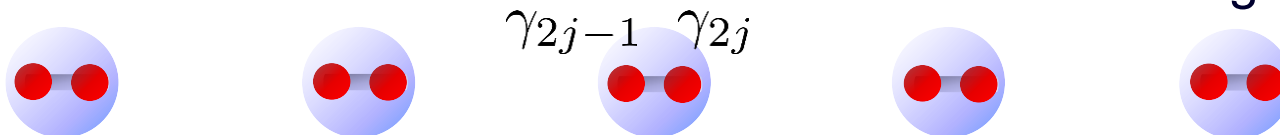
- Topological phase ( $J \gg h$ )

Edge zero modes!



- Trivial phase ( $J \ll h$ )

No edge modes...





# Self-duality = Translation symmetry

## ■ Topology matters

- “Bloch vector” of  $k$ -space Hamiltonian

$$H_{\text{Ising}} = \frac{1}{2} \sum_{0 \leq k \leq \pi} \Psi^\dagger(k) \mathcal{H}(k) \Psi(k), \quad \mathcal{H}(k) = \mathbf{d}(k) \cdot \boldsymbol{\sigma}$$

### Symmetry

$$d_{x,y}(k) = -d_{x,y}(-k), \quad d_z(k) = d_z(-k)$$

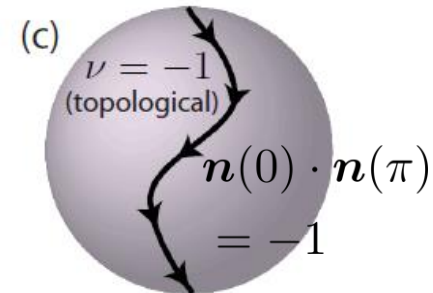
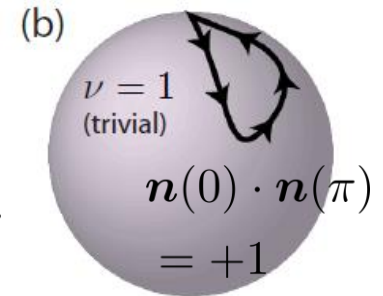
$$\text{n-vector } \mathbf{n}(k) := \frac{\mathbf{d}(k)}{|\mathbf{d}(k)|} \quad \text{Nonzero gap} \\ \Leftrightarrow |\mathbf{d}(k)| > 0$$

- There must be a critical point b/w (b) & (c)

## ■ At the critical point $J = h$

$$H_{\text{Ising}} = iJ \sum_m \gamma_m \gamma_{m+1}$$

- New symmetry: Translation by 1 Majorana site!



J. Alicea, *Rep. Prog. Phys.* **75** (2012)

# Quantum Potts chains

## ■ Shift & clock matrices

$$\sigma|i\rangle = |i-1\rangle, \quad \tau|i\rangle = \omega^i|i\rangle, \quad i = 1, \dots, N, \quad \omega = e^{2\pi i/N}$$

$$\sigma^N = \tau^N = 1, \quad \sigma^\dagger = \sigma^{N-1}, \quad \tau^\dagger = \tau^{N-1} \quad \sigma\tau = \omega\tau\sigma$$

## ■ Hamiltonian ( $J, h > 0$ )

$$H_{\text{Potts}} = -J \sum_j (\sigma_j^\dagger \sigma_{j+1} + \text{h.c.}) - h \sum_j (\tau_j + \tau_j^\dagger)$$

- **Duality:**  $\tau_j \rightarrow \sigma_j^\dagger \sigma_{j+1}, \quad \sigma_j^\dagger \sigma_{j+1} \rightarrow \tau_{j+1}$
- **Parafermions** Fradkin & Kadanoff, *NPB* **170** (1980)

$$\chi_{2j-1} = \sigma_j \prod_{k < j} \tau_k, \quad \chi_{2j} = -\omega^{1/2} \tau_j \sigma_j \prod_{k < j} \tau_k$$

$$H_{\text{Potts}} = J \sum_j (\omega^{1/2} \chi_{2j-1}^\dagger \chi_{2j} + \text{h.c.}) + h \sum_j (\omega^{1/2} \chi_{2j}^\dagger \chi_{2j+1} + \text{h.c.})$$

- Translation invariant at the self-dual point  $h = J$
- Gap closing (2nd order for  $N=2, 3, 4$ , 1st order for  $N > 4$ )

# Self-duality → Gap closing??

## ■ 3-state U(1)-invariant clock model

- Raising & lowering ops.  $S^+ = \frac{1}{3}(2 - \omega\tau - \omega^2\tau^\dagger)\sigma^\dagger, S^- = (S^+)^\dagger$

- Hamiltonian

$$H_0 = \sum_j \left[ 3((S_j^+)^2(S_{j+1}^-)^2 - S_j^+ S_{j+1}^- + \text{h.c.}) - \tau_j - \tau_j^\dagger \right]$$

Fateev & Zamolodchikov (1980), Vernier, O'Brien & Fendley,  
*J. Stat. Mech.* 043107 (2019); *PRB* **101**, 235108 (2020)

- ✓ U(1) symmetric, integrable, Onsager symmetries, ...
- ✓ Self-dual and gapless ( $c=1$  CFT)
- ✓ Criticality persists in the interpolating model

$$\alpha H_{\text{Potts}}(J = h) + (1 - \alpha)H_0$$

## ■ Today's subject

- Is this the end of the story?
- No! One can consider another duality transformation (KT tr.)

# Outline

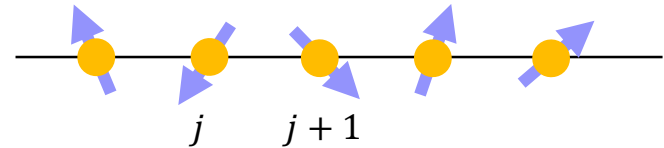
1. Quantum Ising and Potts chains
2. Kennedy-Tasaki Duality in spin-1 chains
  - Spin-1 bilinear-biquadratic chain
  - Haldane phase & AKLT model
  - SPT & Hidden symmetry breaking
3. Criticalities in interpolating models
4. Summary

# Haldane “conjecture” (early 80s)

## ■ Spin- $S$ Heisenberg antiferromagnetic chain

- Hamiltonian ( $J > 0$ )

$$H_{\text{Heis}} = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$



- $S=1/2, 3/2, 5/2, \dots$

Gapless, power-law decay of spin correlations

NOTE)  $S=1/2$  case is solvable (Bethe 1931)

- $S=1, 2, 3, \dots$ 
  - a. Unique ground state
  - b. Non-zero gap  $\Delta$  (Haldane gap)
  - c. Exponential decay of spin correlation

*Established in many different ways!*

AgVP<sub>2</sub>S<sub>6</sub>, NENP, ...; ED, QMC, ...

$$\Delta(S) = \begin{cases} 0.41048(6) & \text{for } S = 1 \\ 0.08917(4) & \text{for } S = 2 \\ 0.01002(3) & \text{for } S = 3 \end{cases}$$

Todo & Kato, *PRL* **87** (2001)

# Quantum spin-1 chain with SU(2)

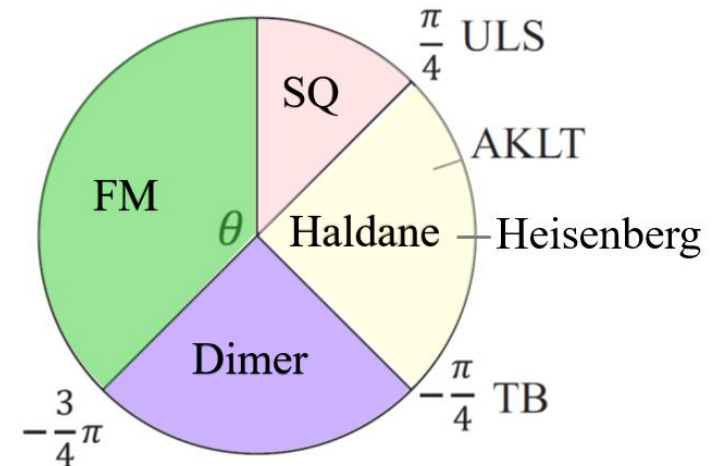
## ■ Bilinear-biquadratic (BLBQ) model

$$H_{\text{BLBQ}}(\theta) = \sum_{j=1}^L \left[ \cos \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1}) + \sin \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2 \right]$$

Spin-1 op. at site  $j$   
 $\mathbf{S}_j = (S_j^x, S_j^y, S_j^z)$

## ■ Phase diagram Lauchli, Schmid & Trebst, *PRB* **74**, 144426 (2006)

- Spin-quadrupolar (SQ): gapless, dominant nematic corr.
- Ferromagnetic (FM)
- Dimer: gapped, 2-fold degenerate g.s.
- Haldane phase
  - ✓ Gapped unique g.s.
  - ✓ Edge states
  - ✓ Hidden AFM order (string order)



Prototype of Symmetry-protected topological (SPT) phase!

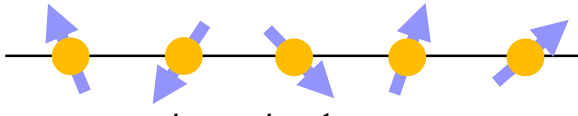
# AKLT model/state

## ■ S=1 AKLT model

Affleck, Kennedy, Lieb & Tasaki,  
*PRL* **59** (1987), *CMP* **115** (1987)

- Hamiltonian ( $\tan \theta = 1/3$ )

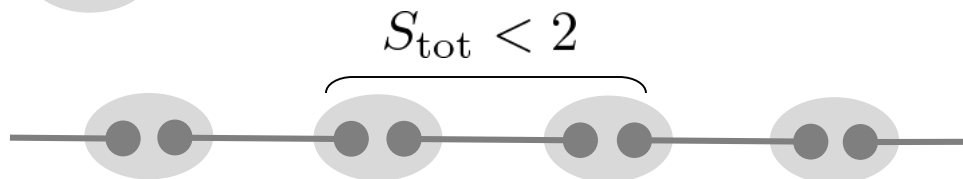
$$H_{\text{AKLT}} = \sum_j \left[ \underline{S_j \cdot S_{j+1} + \frac{1}{3} (S_j \cdot S_{j+1})^2} \right]$$

$$= 2P_{j,j+1}^{S=2} - \frac{2}{3}$$


- Exact ground state

● — ● : Spin singlet  $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$

○ : Projection to spin-1 space



**Frustration-free!** The g.s. minimizes each local Hamiltonian

(i) Non-zero gap above the g.s, (ii) exponential decay of correlations, supporting Haldane conjecture

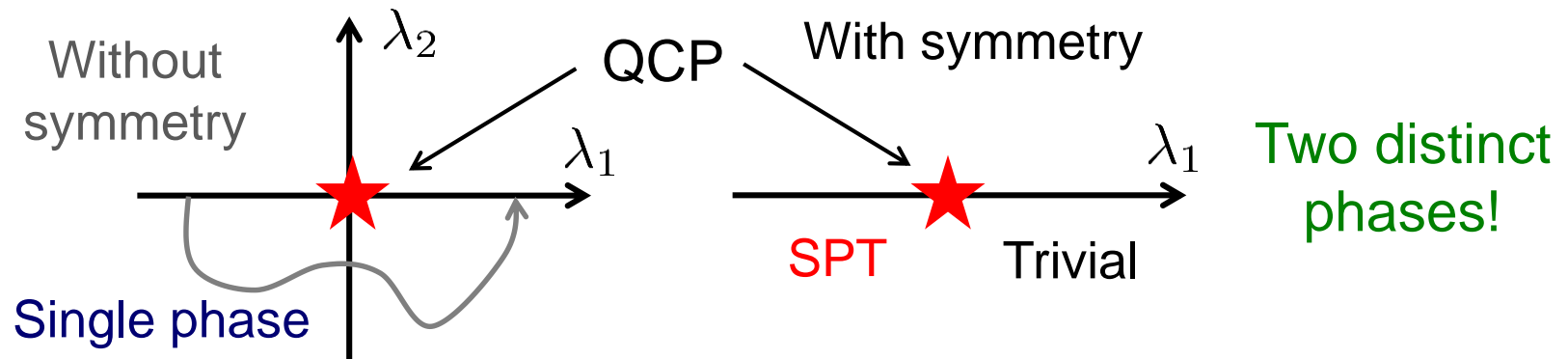


Edge states = nearly free  
edge spin-1/2s in open chain

# Haldane phase as SPT phase

## ■ What is SPT?

Gu & Wen, *PRB* **80** (2009). Pollmann, Berg, Turner & Oshikawa, *PRB* **81** (2010); **85** (2012)



## ■ Symmetry protection

S=1 Haldane phase is protected by ANY one of three symmetries:

(i)  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , (ii) time-reversal, (iii) bond centered inversion

$$Z_\pi = X_\pi Y_\pi = \exp(-i\pi \sum_j S_j^z)$$

$$Y_\pi = \exp(-i\pi \sum_j S_j^y)$$

$$X_\pi = \exp(-i\pi \sum_j S_j^x)$$

$$\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, X_\pi, Y_\pi, Z_\pi\}$$

BLBQ has symmetries (i), (ii) & (iii)



# Symmetry-breaking interpretation? (1)

## ■ Kennedy-Tasaki transformation

- Non-local unitary

Kennedy & Tasaki, *PRB* **45** (1992), Oshikawa, *JPC* **4** (1992)

$$U_{\text{KT}} = \prod_{j < k} \exp(i\pi S_j^z S_k^x), \quad U_{\text{KT}}^\dagger = U_{\text{KT}}, \quad (U_{\text{KT}})^2 = 1$$

- Transformation rules

Any local operator with  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry is transformed into a local operator in the new basis

$$\begin{array}{ccc}
 S_j^x S_{j+1}^x & & U_{\text{KT}} S_j^x S_{j+1}^x U_{\text{KT}} = -S_j^x S_{j+1}^x \\
 S_j^y S_{j+1}^y & \longleftrightarrow U_{\text{KT}} & S_j^y e^{i\pi(S_j^z + S_{j+1}^z)} S_{j+1}^y \\
 S_j^z S_{j+1}^z & & -S_j^z S_{j+1}^z
 \end{array}$$

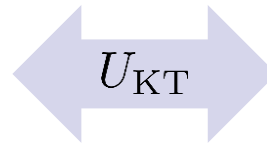
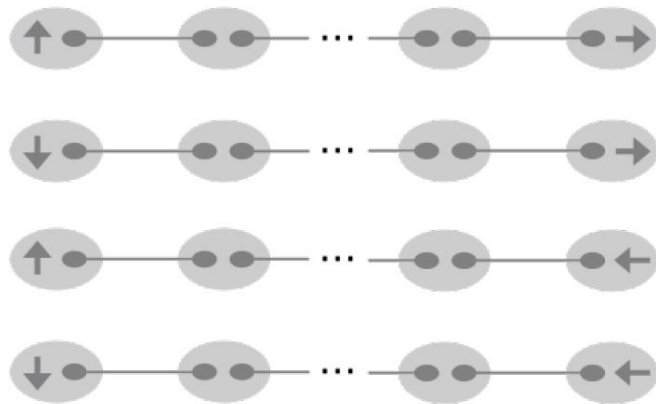
- “Hidden order”  $\Leftrightarrow$  Ferromagnetic order ( $\alpha = x, z$ )

$$- \lim_{r \rightarrow \infty} \langle S_j^\alpha \exp[i\pi \sum_{k=j+1}^{j+r-1} S_k^\alpha] S_{j+r}^\alpha \rangle \longleftrightarrow U_{\text{KT}} \lim_{r \rightarrow \infty} \langle S_j^\alpha S_{j+r}^\alpha \rangle$$

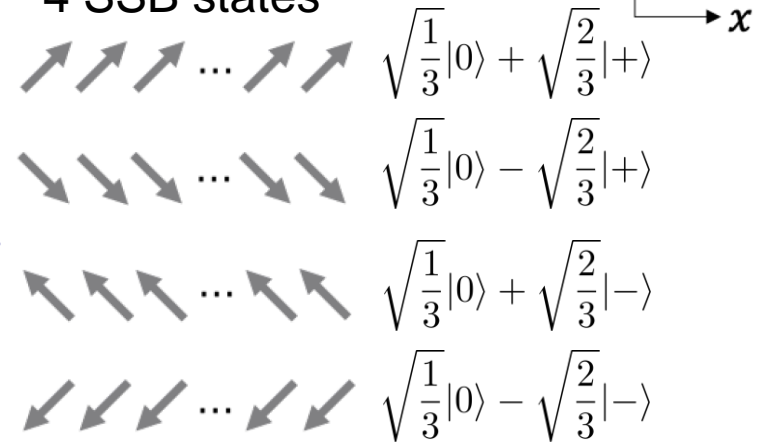
# Symmetry-breaking interpretation? (2)

## ■ What AKLT states look like after KT tr.?

4 ground states on open chain



4 SSB states



Break  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry!

## ■ Trivial state remains trivial

- Trivial model

$$H_{\text{triv}} = \sum_j (S_j^z)^2$$

has  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry. Invariant under KT transformation.

Ground state  $|0, 0, \dots, 0\rangle$  is also invariant under KT.

No FM order. It does not break  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry.

# Outline

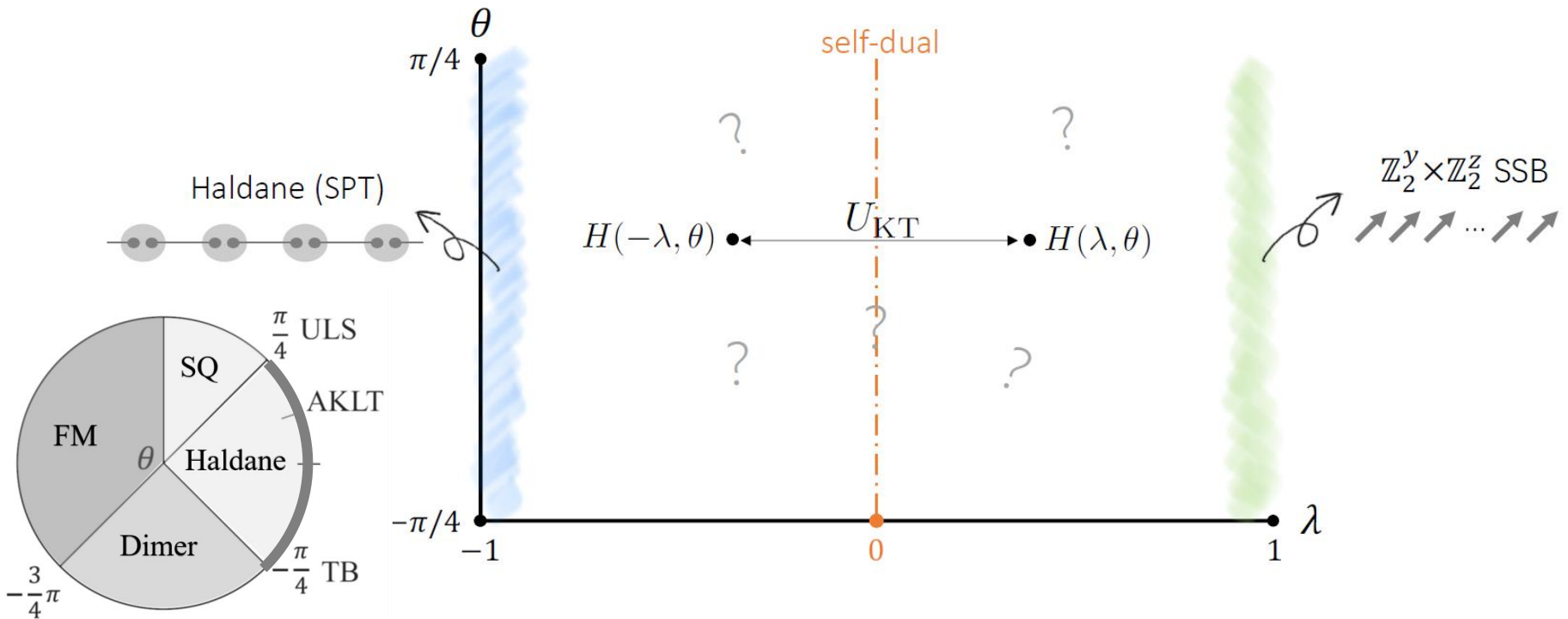
1. Quantum Ising and Potts chains
2. Kennedy-Tasaki Duality in spin-1 chains
- 3. Criticalities in interpolating models**
  - Model & phase diagram
  - Self-duality and Gaussian criticality
  - SPT & trivial Ising criticalities
4. Summary

# Model

## ■ Hamiltonian

$$\begin{aligned}
 H(\lambda, \theta) &= (1 - \lambda) H_{\text{BLBQ}}(\theta) + (1 + \lambda) \tilde{H}_{\text{BLBQ}}(\theta) \quad (-1 \leq \theta \leq 1) \\
 &= \sum_j [\cos \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1}) + \sin \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2] \\
 &= U_{\text{KT}} H_{\text{BLBQ}}(\theta) U_{\text{KT}}
 \end{aligned}$$

## ■ Phase diagram?



# Self-duality and criticality (1)

## ■ Self-dual model

- Hamiltonian  $H(0, \theta) = H_{\text{BLBQ}}(\theta) + \tilde{H}_{\text{BLBQ}}(\theta)$
- Commutes with  $U_{\text{KT}}$   $[H(0, \theta), U_{\text{KT}}] = 0$
- Change of basis

$S^z$  basis :  $\{|+\rangle, |0\rangle, |-\rangle\}$

$$\rightarrow \left\{ \begin{array}{l} |\uparrow\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle) \\ |\downarrow\rangle = |0\rangle \\ |h\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) \end{array} \right\}$$

Effective spin-1/2 subspace

$$\left\{ \begin{array}{l} \sigma^x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow| \\ \sigma^y = -i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow| \\ \sigma^z = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow| \\ n = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| \\ h = |h\rangle\langle h| \end{array} \right.$$

## ■ Connection to integrable XXZ

$$H(0, \theta) = H_{\text{XXZ}} + \sin \theta \sum_j (2h_j h_{j+1} + n_j n_{j+1} + 2)$$

$$H_{\text{XXZ}} = (\cos \theta - \sin \theta) \sum_j (-\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \sin \theta \sum_j \sigma_j^z \sigma_{j+1}^z$$

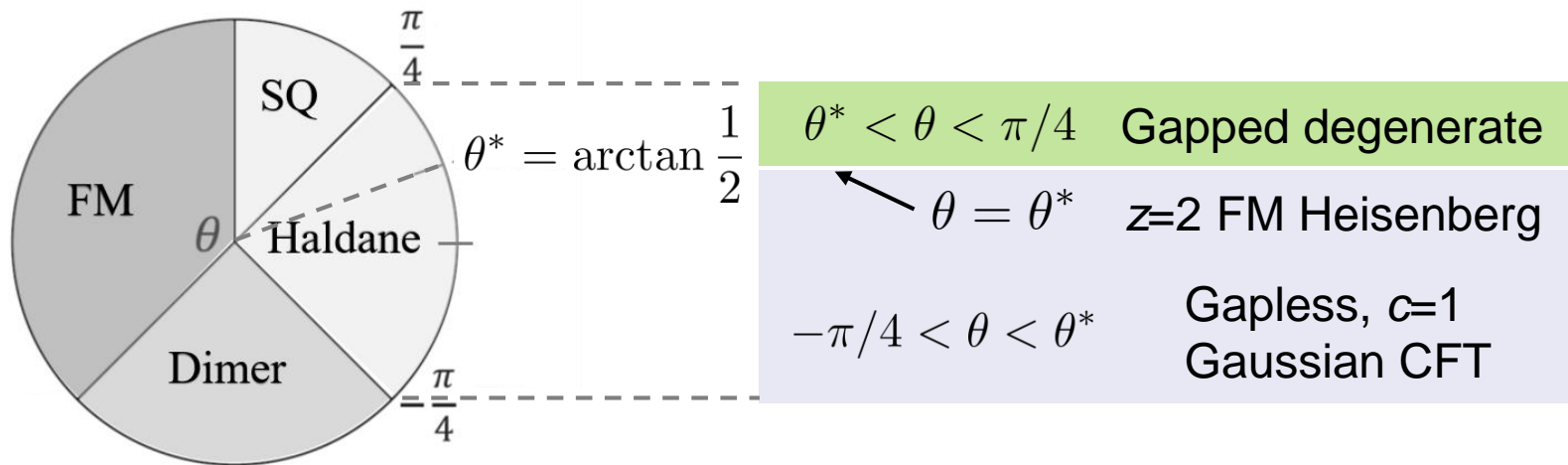
- ✓ Holes are not dynamical (fragmented model)
- ✓ Heisenberg point ( $\theta=0$ )  $\rightarrow$  XY (free-fermion) model!

# Self-duality and criticality (2)

## ■ Phase diagram at $\lambda=0$

- Anisotropy

$$\Delta(\theta) = \frac{\sin \theta}{|\cos \theta - \sin \theta|} \quad \left\{ \begin{array}{ll} -1 \leq \Delta(\theta) < 1 & c = 1 \text{ Gaussian CFT} \\ \Delta(\theta) = 1 & z = 2 \text{ FM Heisenberg} \\ |\Delta(\theta)| > 1 & \text{gapped degenerate} \end{array} \right.$$



- Presence or absence of holes in g.s.

$\theta^* \leq \theta < \pi/4$  Holes are present

$-\pi/4 < \theta < \theta^*$  Holes are absent

Can be proved using *classic* Bethe ansatz results

Yang-Yang, *PR* (1966), Hamer, Quispel & Batchelor, *JPA* (1987)

# Around self-dual line

## ■ Perturbation theory around $\lambda = 0$

Hole motion

$$H(\lambda, \theta) \sim H_{\text{XYZ}} + \sin \theta \sum_j (n_j n_{j+1} + 2) + 2\lambda \cos \theta \sum_{j, \sigma} (|h\sigma\rangle_{j, j+1} \langle \sigma h| + \text{h.c.})$$

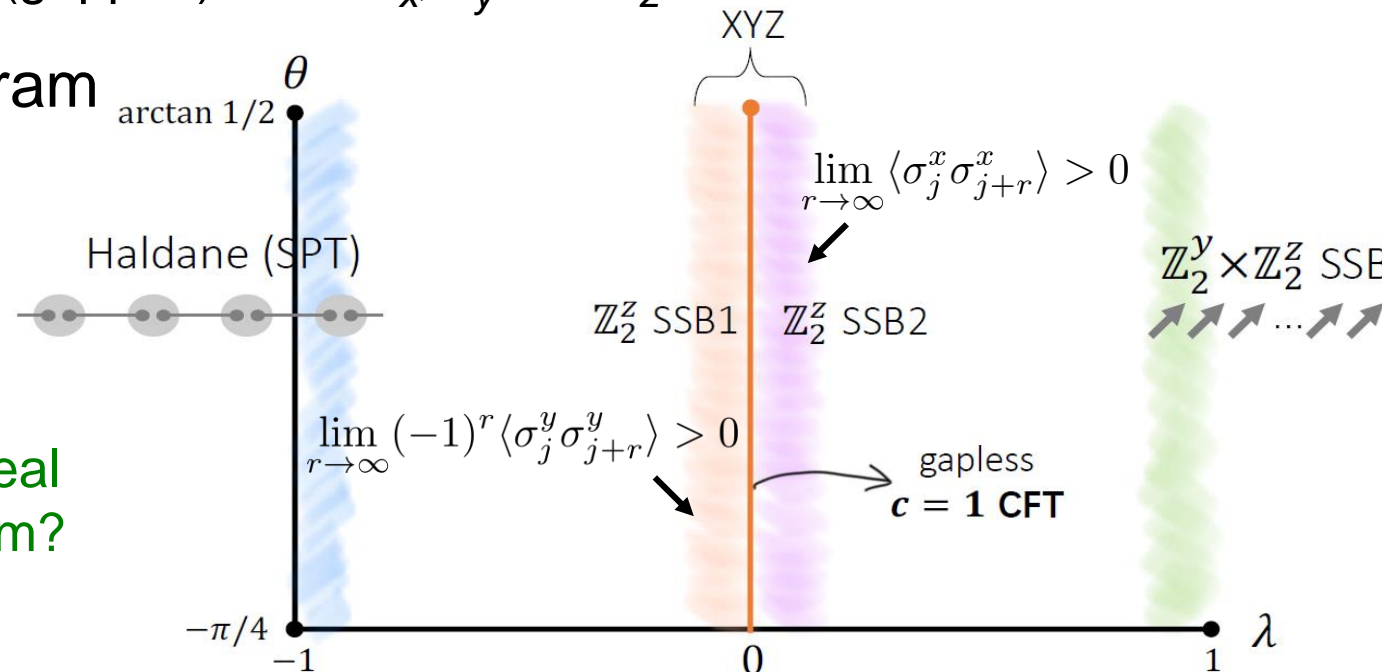
$$H_{\text{XYZ}} = \sum_j [-J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z]$$

$$J_x = [(1 + \lambda) \cos \theta - \sin \theta], \quad J_y = [(1 - \lambda) \cos \theta - \sin \theta], \quad J_z = \sin \theta$$

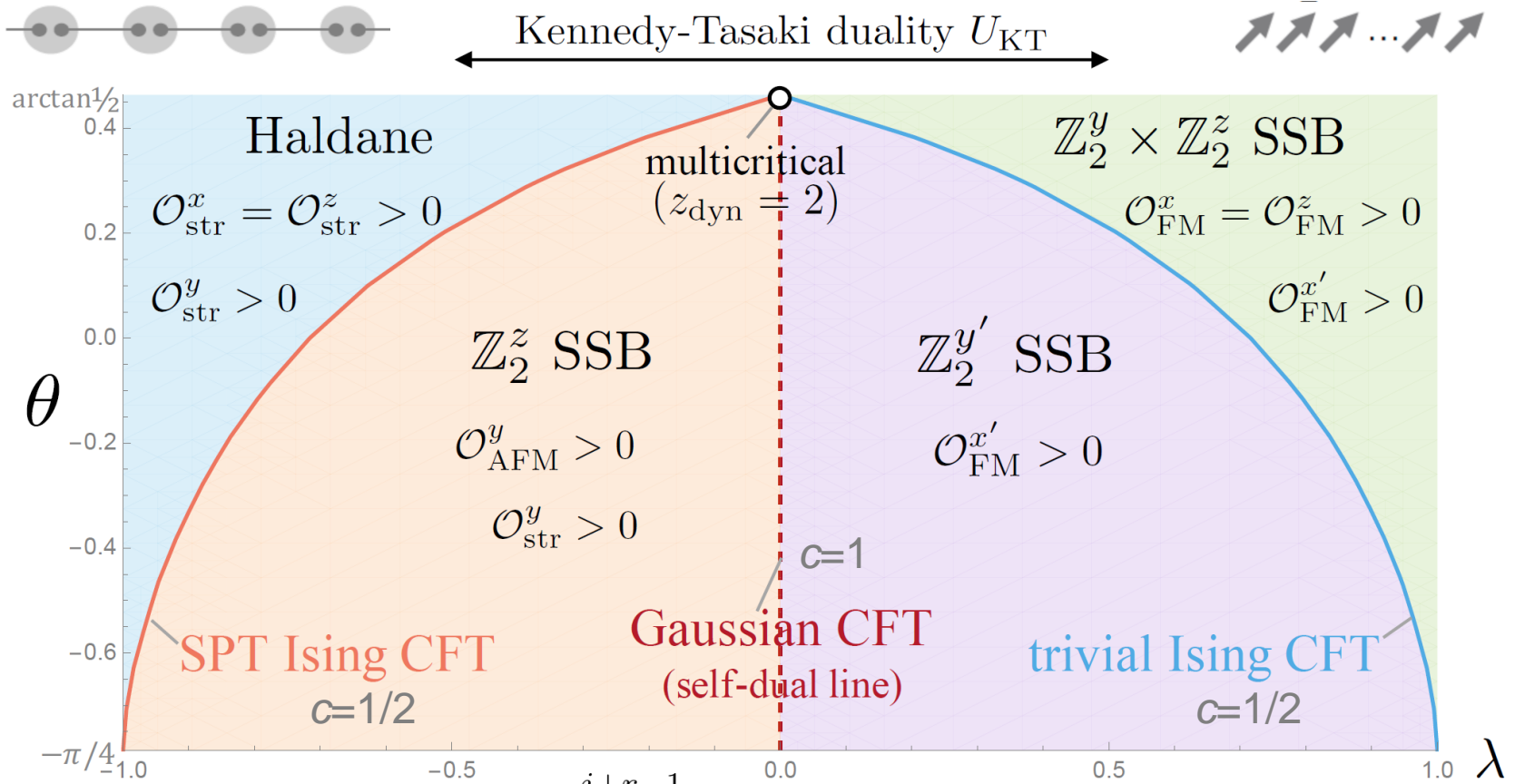
- S=1/2 XYZ chain is integrable
- Massive (gapped) when  $J_x$ ,  $J_y$  and  $J_z$  are distinct

## ■ Phase diagram (updated)

What is the real phase diagram?



# DMRG results



$$\mathcal{O}_{\text{str}}^\alpha = - \lim_{r \rightarrow \infty} \langle S_j^\alpha \exp[i\pi \sum_{k=j+1}^{j+r-1} S_k^\alpha] S_{j+r}^\alpha \rangle$$

$$\mathcal{O}_{\text{AFM}}^y = \lim_{r \rightarrow \infty} (-1)^r \langle S_j^y S_{j+r}^y \rangle$$

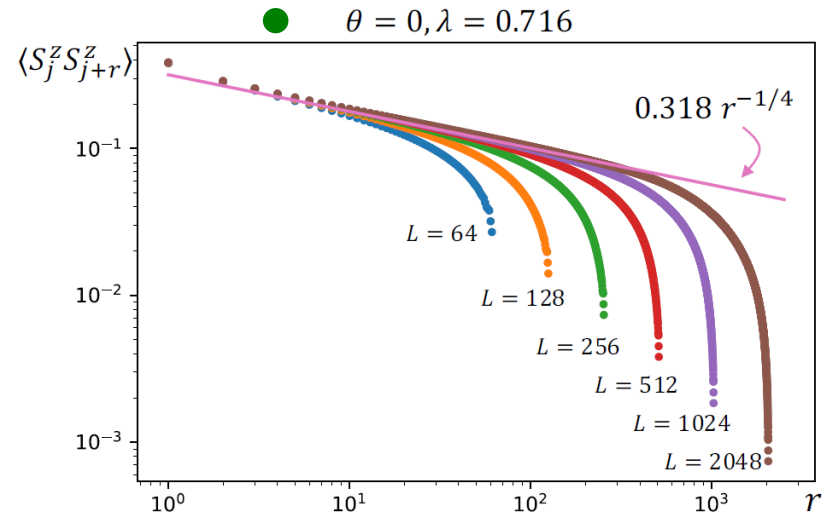
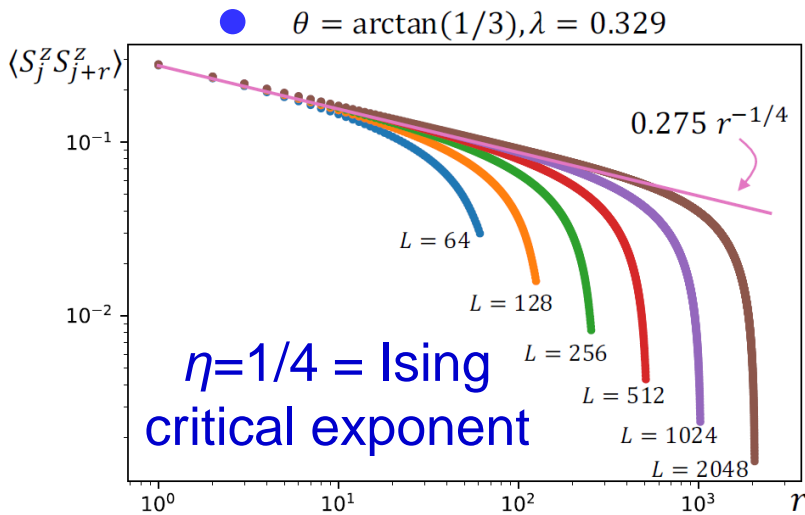
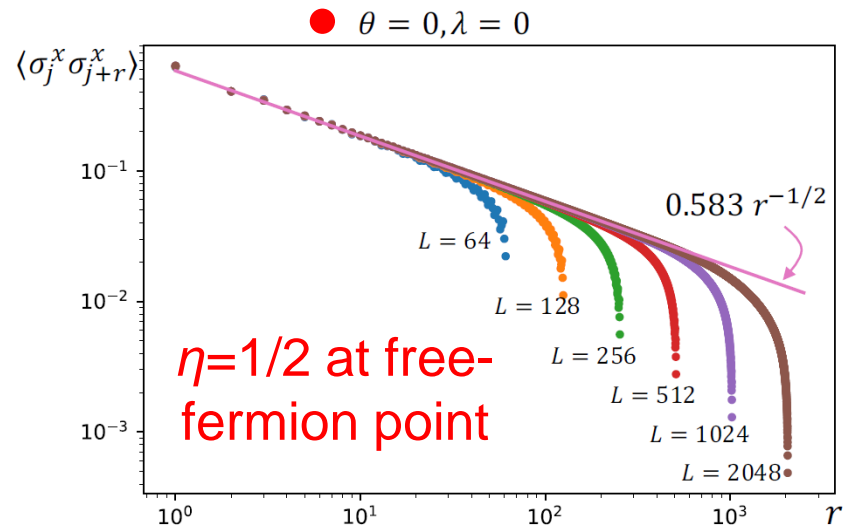
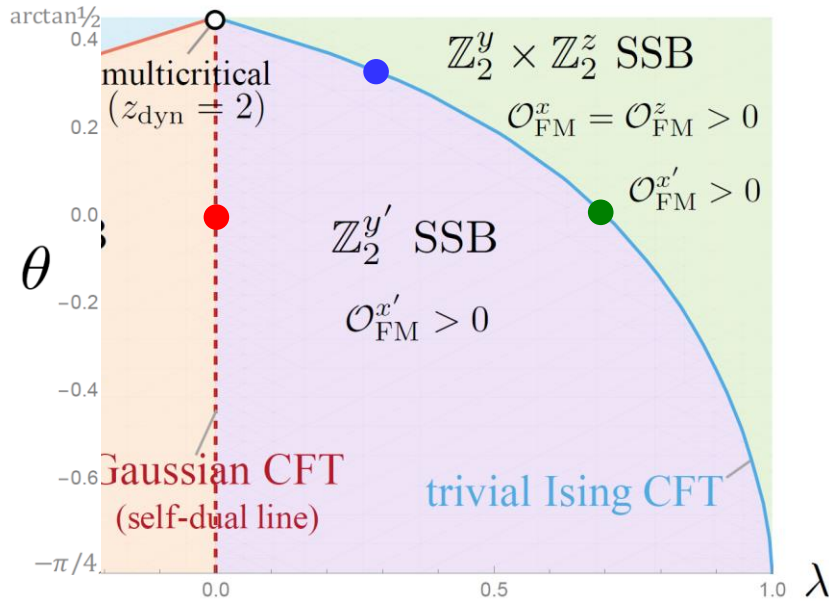
$$\mathcal{O}_{\text{FM}}^{x'} = \lim_{r \rightarrow \infty} \langle \sigma_j^x \sigma_{j+r}^x \rangle$$

$$\mathcal{O}_{\text{FM}}^\alpha = \lim_{r \rightarrow \infty} \langle S_j^\alpha S_{j+r}^\alpha \rangle$$

- $\mathcal{O}_{\text{str}}^y > 0$  on the SPT Ising, while  $\mathcal{O}_{\text{FM}}^{x'} > 0$  on the trivial Ising

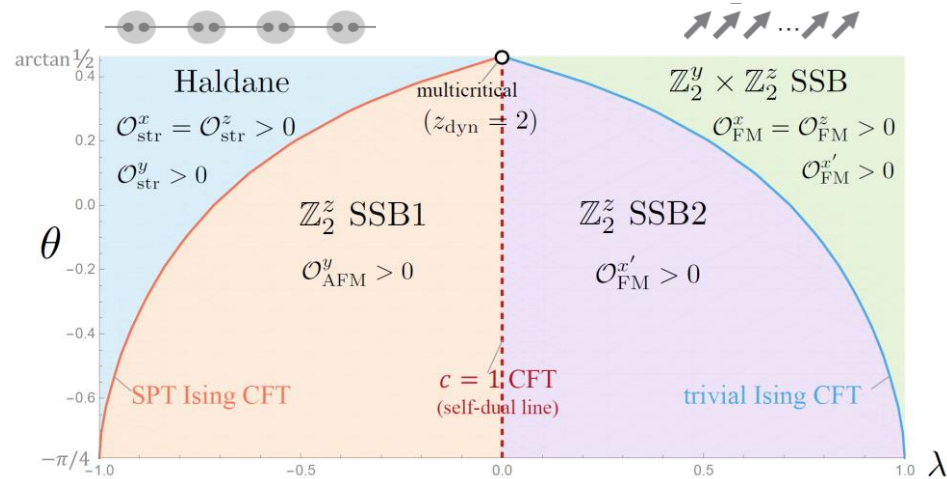


# Critical properties



# Summary

- Studied interpolating models between BLBQ chain in SPT and its Kennedy-Tasaki dual
- Rich phase diagram
- Gaussian, SPT Ising & trivial Ising criticalities



## Future directions

- What about higher integer spins?  $H_{\text{SD}}^{(S)} = H_{\text{Heis}}^{(S)} + U_{\text{KT}} H_{\text{Heis}}^{(S)} U_{\text{KT}}$   
 Conjecture:  $S = 1, 3, 5, \dots \rightarrow$  Critical  
 $S = 2, 4, 6, \dots \rightarrow$  Gapped & trivial
- $\text{SO}(2n+1)$  generalizations?  
 KT tr.: H. Tu, G-M. Zhang & T. Xiang, *PRB* **78** (2008)
- More general duality transformations?  
 Lootens, Delcamp, Ortiz & Verstraete, arXiv:2112.09091