S=1スピン鎖における対称性に守られたトポロジカル秩序と非局所ユニタリ変換

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Part 1

Physics of the Kennedy-Tasaki Transformation for the SPT entanglement and the negative sign problem

“Topological disentangler for the valence-bond-solid chain”
K Okunishi
Phys. Rev. B **83**, 104411 (2011)

“Symmetry-protected topological order and negative-sign problem for bilinear-biquadratic chains”
K Okunishi, K Harada, Phys. Rev. B **89**, 134422 (2014)

Motivation : beginning of this research

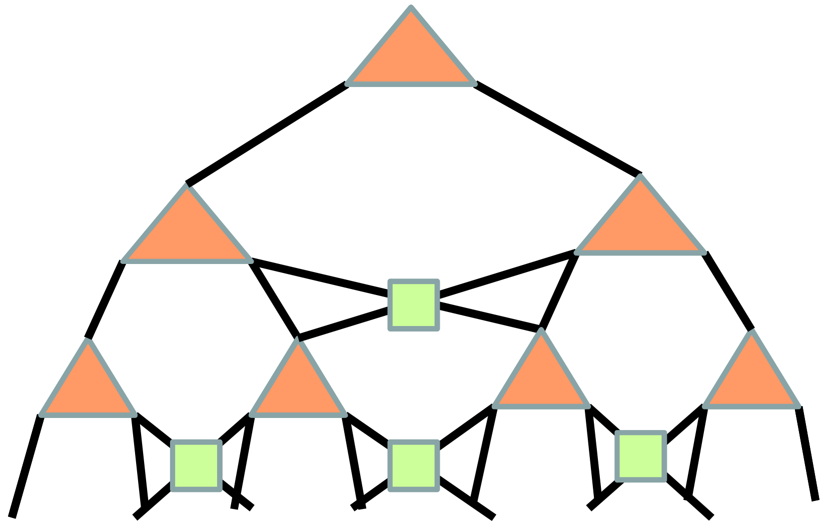
MERA : G. Vildal: active controlling of the entanglement.
real space RG + disentangler

- The disentangler is a local unitary in the MERA network.
- The disentangler is obtained as a result of the highly
  nontrivial numerical optimization

- Global entanglement is reduced by the disentanglers
  in the MERA type network.

Exact example of the disentangler
for through understanding of the disentangler

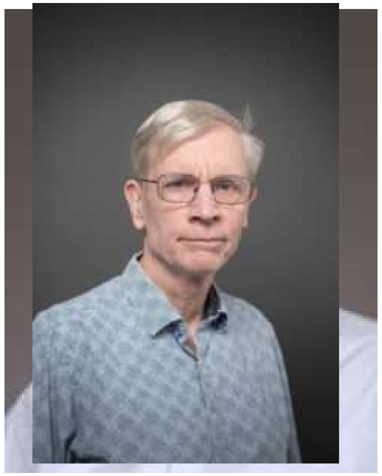
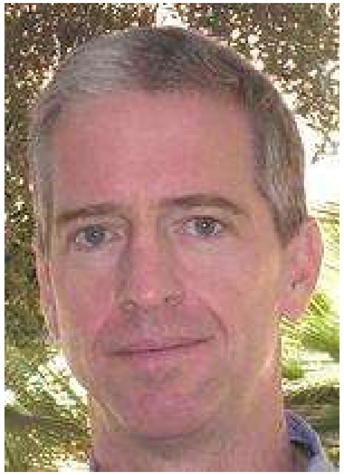
Tree network = block spin tranformation



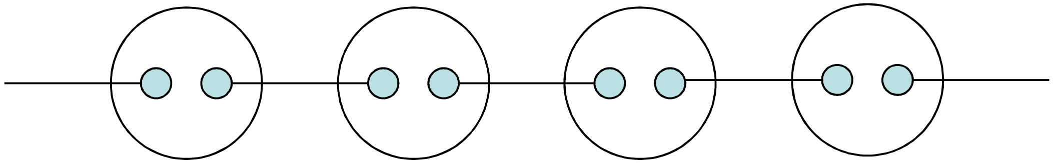
Entanglement between two blocks is maintained by only single bond!

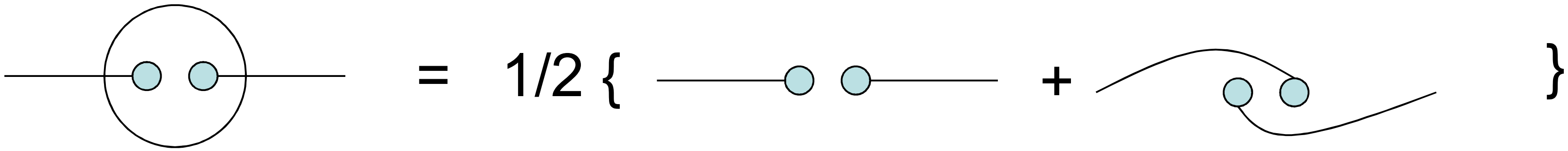
AKLT model and VBS state: Exact MPS (1986)

$$H = \sum S_i \cdot S_{i+1} + \frac{1}{3}(S_i \cdot S_{i+1})^2 = \sum P_{i,i+1}^{S=2}$$

VBS state





symmetrization = projection to
the triplet sector

Z2 x Z2 symmetry and string order

Hidden antiferromagneitc order (SPT order)

$-0+-00+00-+0-$

If "0" spins are skipped, Neel type order can be recognized.

⇨ $(+-)$ of the edge spins generates the Z2 x Z2 symmetry.

In order to detect the hidden Neel order, nonlocal string order parameter was constructed by den Nijis and Rommers.

$$\left\langle S_i^z \exp\left(i\pi \sum_{k=i+1}^{n-1} S_k^z \right) S_j^z \right\rangle$$

phase factor $e^{i\pi S_k^z}$ skips "0" spin and picks up string of the Neel type array of spins.

Analogy with the 2D interface system: disordered flat phase.

Kennedy-Tasaki transformation

minus sign is assigned for a state vector, if the number of 0 spin at the odd sites in the entire chain is odd

"+" or "−" spin is flipped, if there is odd number of + or – spins in the left side of a site j.

$$(0+-00+00-+0-) \Rightarrow -(0++00+00++0+)$$

$$|\Psi_j\rangle = \cdots |\phi_j\rangle \otimes |\phi_j\rangle \otimes |\phi_j\rangle \otimes \cdots$$ manifest Z2 x Z2 symmetry

$$|\phi_1\rangle = \sqrt{\frac{2}{3}}|+\rangle + \sqrt{\frac{1}{3}}|0\rangle \qquad |\phi_3\rangle = \sqrt{\frac{2}{3}}|-\rangle + \sqrt{\frac{1}{3}}|0\rangle$$

$$|\phi_2\rangle = -\sqrt{\frac{2}{3}}|+\rangle + \sqrt{\frac{1}{3}}|0\rangle \qquad |\phi_4\rangle = -\sqrt{\frac{2}{3}}|-\rangle + \sqrt{\frac{1}{3}}|0\rangle$$

$$|\Psi\rangle = \cdots |\phi_j\rangle \otimes |\phi_j\rangle \otimes |\phi_j\rangle \otimes \cdots$$

Classical state

There is no quantum entanglement!

Problem

Highly nonlocal transformation.

It is difficult to handle by hand

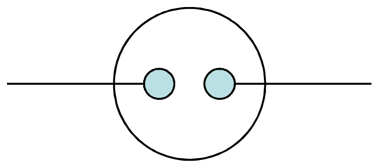
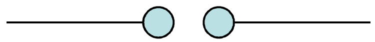
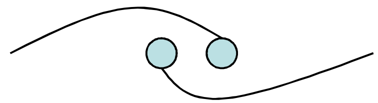
The classical state itself was obtained by diagonalization of the KT-transformed Hamiltonian.

generalization is not straightforward…

⇒ How does the KT transformation disentangle the quantum entanglement in the VBS state?

matrix product representation

$$|\Psi\rangle = A_1 A_2 A_3 \cdots A_N \Omega \qquad A_j = \begin{pmatrix} -\sqrt{\frac{1}{3}}|0\rangle & \sqrt{\frac{2}{3}}|+\rangle \\ -\sqrt{\frac{2}{3}}|-\rangle & \sqrt{\frac{1}{3}}|0\rangle \end{pmatrix}$$

 = 1/2 {   }

symmetrization = projection to the triplet sector

$$\Omega = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

boundary matrix yields linear combinations of 4 degenerating groundstates

$$e^{i\pi/2 S_j^y} A_j = \Omega^{-1} A_j \Omega$$

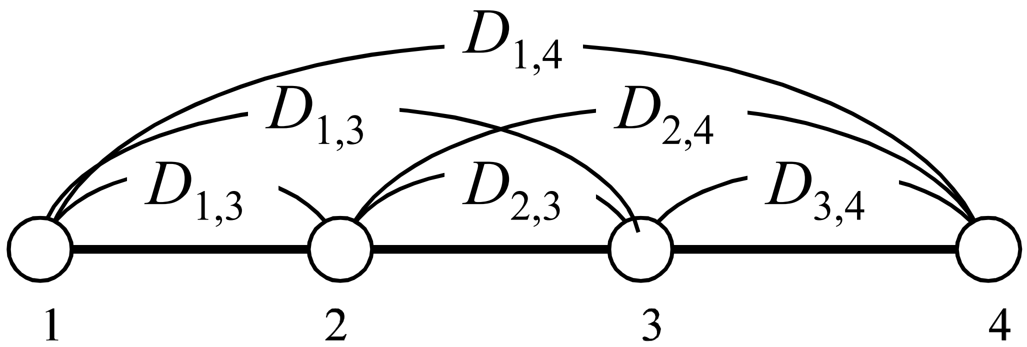
problem

The disentangled wavefunction is represented as a 4 x 4 matrix with the diagonal elements. However, matrix operation of any 2 x 2 matrix **can never** convert 2 x 2 into 4 x 4 !

1st step

Kennedy-Tasaki transformation can be represented as an assembly of the pair disentanglers

$$D_{KT} := \prod_{allpairs} D_{i,j}$$



$$D_{i,j} = e^{i\pi S_i^z S_j^x} \qquad \left[D_{i,j}, D_{k,l}\right] = 0$$

M. Oshikawa, (1992)

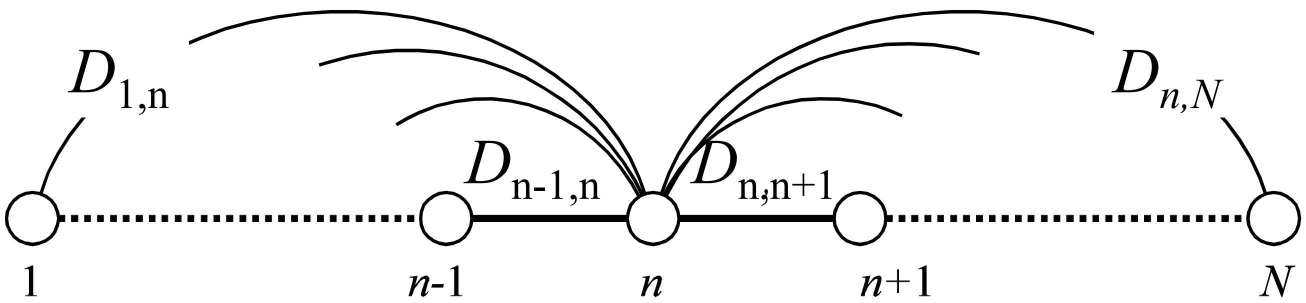
equivalently

$$D_{i,j} = P_i^0 \otimes \mathbf{1} + P_i^{\pm} \otimes e^{i\pi S_j^x} = \mathbf{1} \otimes Q_j^0 + e^{i\pi S_j^z} \otimes Q_j^{\pm}$$

$$P_j^0 = \frac{1}{2}(\mathbf{1} + e^{i\pi S_j^z}), P_j^{\pm} = \frac{1}{2}(\mathbf{1} - e^{i\pi S_j^z})$$

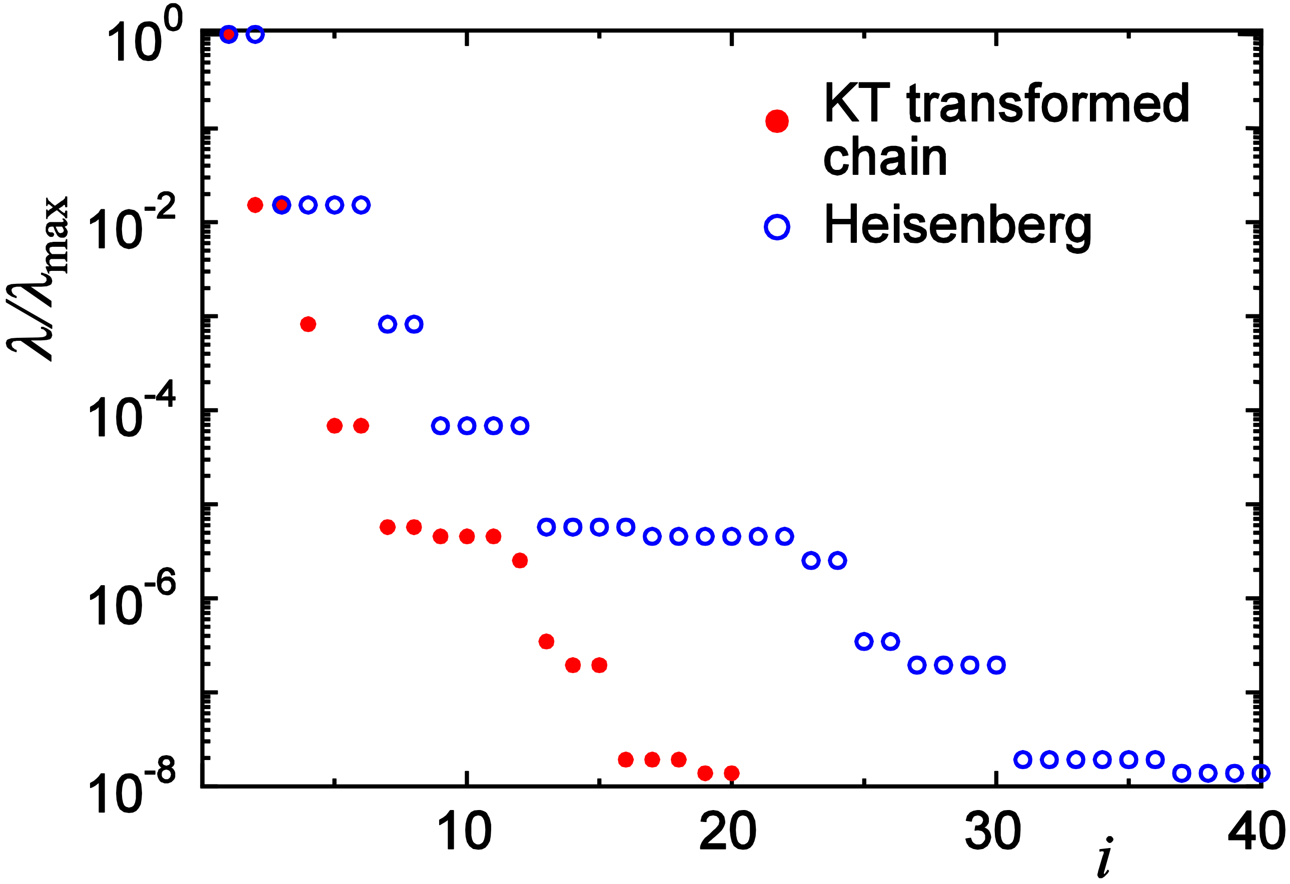
Disentangling single site

$$D := \prod_{i=1}^{n-1} D_{i,n} \prod_{j=1}^{N} D_{n,j}$$



n-th site is equally entangled with the other spins.

Heisenberg chain



Two fold degeneracy is removed in the KT transformed chain

$S-\widetilde{S}=\ln 2$ topological entanglement entropy

S=1 Heisenberg chain $H = \sum S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z$

<u>KT transform</u>

$$\widetilde{H} = \sum - S_i^x S_{i+1}^x - S_i^y S_{i+1}^y + S_i^z e^{i\pi (S_i^z + S_{i+1}^x)} S_{i+1}^z$$

The SU(2) symmetry becomes hidden by the KT transformation.

Haldane state: Pollman, Berg, Turner, Oshikawa, (2010)

Z2 ~ time reversal symmetry at the MPS level.

two fold degeneracy in the entanglement spectrum

DMRG for the AKLT model

m=4, parity is imposed(equivalent right and left blocks)

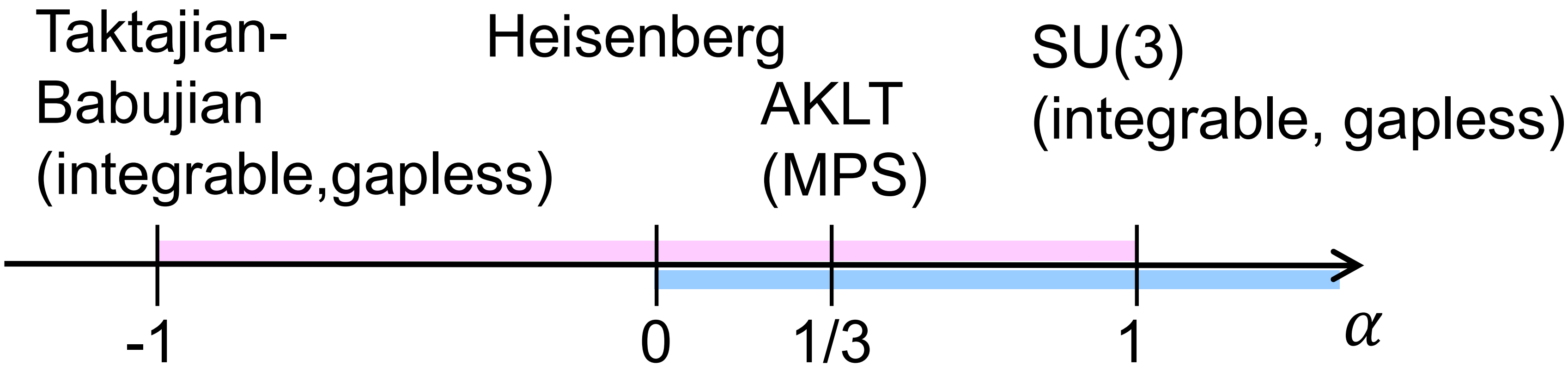
m=2, “canonical” MPS dimension

m=1, the KT transformed AKLT.

そこでふと考えた！

S=1 bilinear-biquadratic chain

$$h_{i,i+1} = \vec{S}_i \cdot \vec{S}_{i+1} + \alpha[(\vec{S}_i \cdot \vec{S}_{i+1})^2 - 1]$$



The ground state is also well-understand by DMRG

QMC : The region of α>0 is the dark side;

negative sign problem!

Hamiltonian : matrix elements

$$h_{i,i+1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha-1 & 0 & \alpha-1 & 0 & \alpha & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha-1 & 0 & \alpha & 0 & \alpha-1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & \alpha & 0 & \alpha-1 & 0 & \alpha-1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$\alpha>0$; negative sign problem

Kennedy-Tasaki Transformation U
+
Local unitary transformation V (dimer-R)

KT transformation : classical ground state(disentangled)

$$|\Psi_j\rangle = \cdots |\phi_j\rangle \otimes |\phi_j\rangle \otimes |\phi_j\rangle \otimes \cdots$$

manifest Z2 x Z2 symmetry

$$|\phi_1\rangle = \sqrt{\frac{2}{3}}|+\rangle + \sqrt{\frac{1}{3}}|0\rangle \qquad |\phi_3\rangle = \sqrt{\frac{2}{3}}|-\rangle + \sqrt{\frac{1}{3}}|0\rangle$$

$$|\phi_2\rangle = -\sqrt{\frac{2}{3}}|+\rangle + \sqrt{\frac{1}{3}}|0\rangle \qquad |\phi_4\rangle = -\sqrt{\frac{2}{3}}|-\rangle + \sqrt{\frac{1}{3}}|0\rangle$$

However, a naive use of the KT transformation does not yet remove the negative sign.

local unitary transformation : V (p-wave basis)

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

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

$$|3\rangle = |0\rangle$$

$$V = \begin{pmatrix} 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \end{pmatrix}$$

$$V^2 = I$$

$$|\phi_1\rangle = \sqrt{\frac{1}{3}}(|1\rangle + |2\rangle + |3\rangle)$$

$$|\phi_3\rangle = \sqrt{\frac{1}{3}}(|1\rangle + |2\rangle - |3\rangle)$$

$$|\phi_2\rangle = \sqrt{\frac{1}{3}}(-|1\rangle + |2\rangle - |3\rangle)$$

$$|\phi_4\rangle = \sqrt{\frac{1}{3}}(-|1\rangle + |2\rangle + |3\rangle)$$

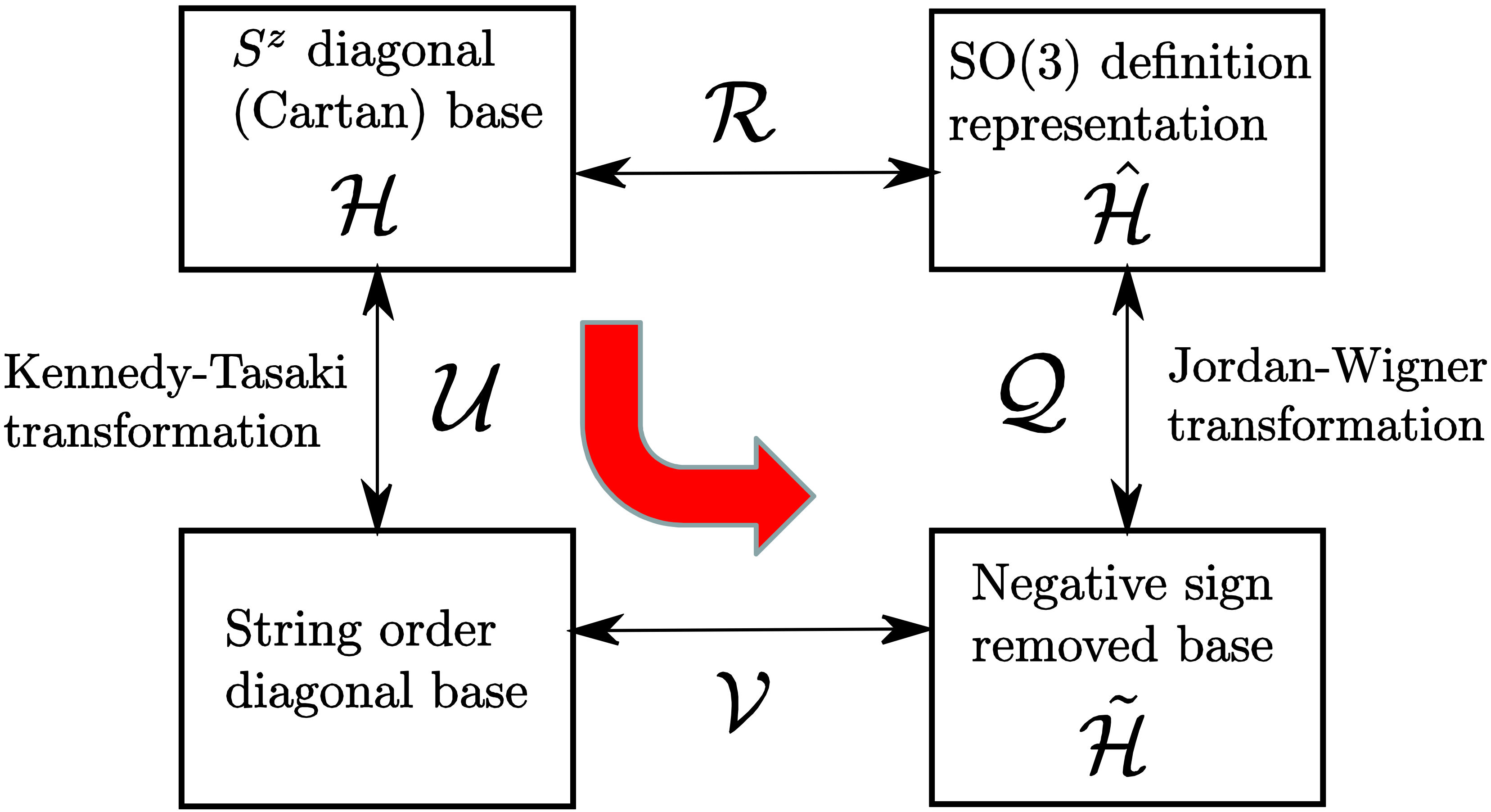
T. Kennedy, J. Phys. condens matt. 6, 8015 (1994)
: Perron-frobenius theorem

KT transformation + V transformation

$$VUh_{i,i+1}U^{-1}V^{-1} = \left(\begin{array}{ccc|ccc|ccc} \alpha & 0 & 0 & 0 & \alpha-1 & 0 & 0 & 0 & \alpha-1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ \hline 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \alpha-1 & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & \alpha-1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ \hline 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ \alpha-1 & 0 & 0 & 0 & \alpha-1 & 0 & 0 & 0 & \alpha \end{array}\right)$$

This Hamiltonian has NO negative sign for 1>= α .

KT + V transformations



Physical meaning of the matrix elements

$$\langle n'_1 \, n'_2 | \widetilde{h}_{1,2} | n_1 n_2 \rangle = -\Gamma_c - (1-\alpha)\Gamma_h + \alpha\Gamma_r$$

n=1,2,3 -> 3 colors of world line

Γ_c exchange of particles

Γ_h pair creation & anihiration of particles

Γ_r repulsion between particles of the same color (diagonal elements)

SU(3) matrices /Schwinger boson

$$\Gamma^c = \sum_{\mu\neq\nu} S^{\mu\nu} S^{\nu\mu} \qquad \Gamma^h = \sum_{\mu\neq\nu} S^{\mu\nu} S^{\mu\nu} \qquad \Gamma^r = \sum_{\mu} S^{\mu\mu} S^{\mu\mu}$$

$\approx$ [1,0] representation $\approx$ [1,1] representation

SU(3) algebra $\left[S^{\mu\nu}, S^{\mu'\nu'}\right] = \delta_{\nu\mu'} S^{\mu\nu'} - \delta_{\mu\nu'} S^{\mu'\nu}$

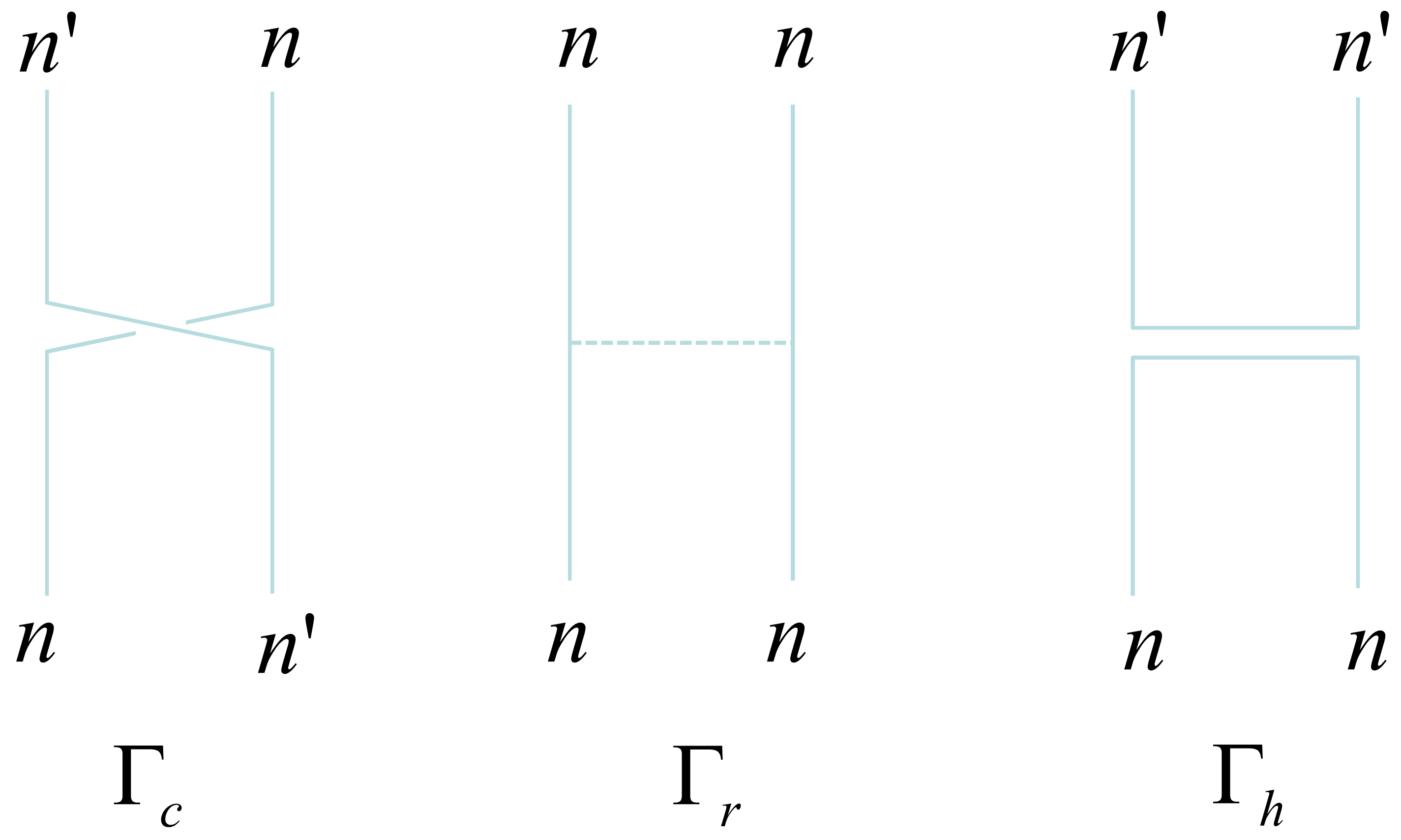
Scwinger boson

$$S^{\mu\nu} = b_\mu^+ b_\nu$$

constraint $\sum_\mu b_\mu^+ b_\mu = N$

Γ ⇨ scattering of bosonic particles

diagrammatic representation



diagonal

Continuous time worm type algorithm is possible

generalized Jordan-Wigner transformation

$$Q_{i,j} = diag(1 \quad -1 \quad -1 \quad 1 \quad 1 \quad -1 \quad 1 \quad 1 \quad 1)$$

Assign minus sign if particles of different colors are exchanged

generalized Jordan-Wigner

$$Q = \prod_{<i,j>} Q_{i,j}$$

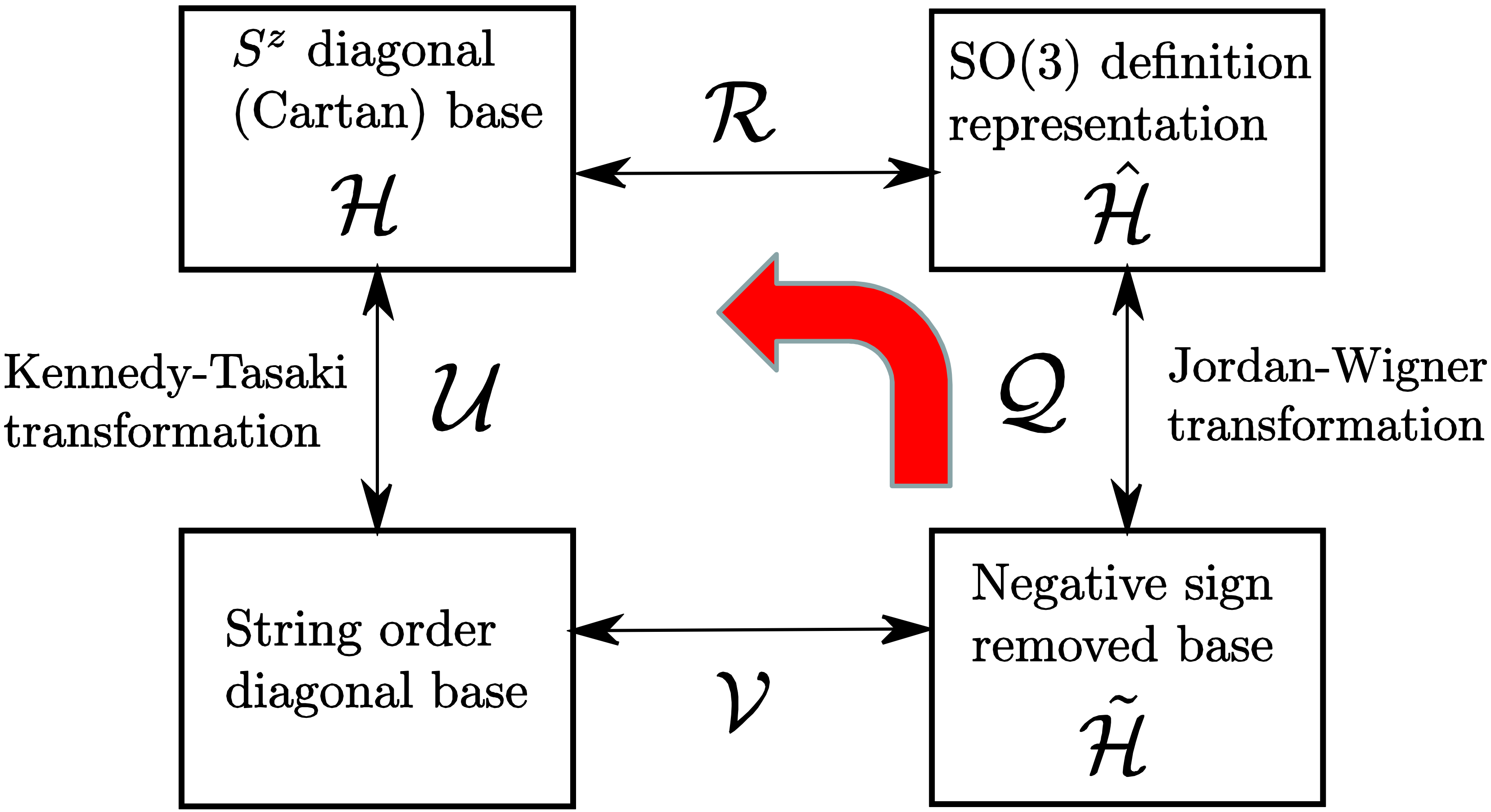
Product is taken for all spin pairs

L. Messio and F. Mila, Phys. Rev. Lett. **109,** 205306 (2012).

$$\Rightarrow \quad Q\Gamma_c Q = -\Gamma_c \qquad Q\Gamma_h Q = \Gamma_h \qquad Q\Gamma_r Q = \Gamma_r$$

What is this Hamiltonian?

gJW transformation and definition rep.



H and $\hat{H}$

$$R = \begin{pmatrix} -i/\sqrt{2} & 0 & i/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \end{pmatrix}$$

$$R\vec{S}R^{+} = \vec{L}$$

$$L^{x} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad L^{y} = -\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad L^{z} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Rightarrow \quad \hat{h}_{i,i+1} = \vec{L}_{i} \cdot \vec{L}_{i+1} + \alpha[(\vec{L}_{i} \cdot \vec{L}_{i+1})^{2} - 1]$$

bilinear-biquadratic chain in the definition representation

Correlation functions

$$\begin{aligned}\langle S_i^a S_j^a \rangle_{\mathcal{H}} &= \langle L_i^a L_j^a \rangle_{\hat{\mathcal{H}}} \\ &= -\langle T_i^a e^{i\pi \sum_{i<k<j} L_k^a} T_j^a \rangle_{\tilde{\mathcal{H}}} \\ &= -\langle T_i^a e^{i\pi \sum_{i<k<j} T_k^a} T_j^a \rangle_{\tilde{\mathcal{H}}}\end{aligned}$$

$$\begin{aligned}\langle S_i^a e^{i\pi \sum_{i<k<j} S_k^a} S_j^a \rangle_{\mathcal{H}} &= \langle L_i^a e^{i\pi \sum_{i<k<j} L_k^a} L_j^a \rangle_{\hat{\mathcal{H}}} \\ &= -\langle T_i^a T_j^a \rangle_{\tilde{\mathcal{H}}},\end{aligned}$$

Both of the KT and JW transformations yield the same correlation functions

SO(N) generalization

$$\hat{h}_{i,i+1} = \sum_{b>a} L_i^{ab} L_{i+1}^{ab} + \frac{\alpha}{N-2}[(\sum_{b>a} L_i^{ab} L_{i+1}^{ab})^2 - 1]$$

SO(N) generator: a-b plane $(L^{ab})_{x,y} = -i(\delta_{a,x}\delta_{b,y} - \delta_{b,x}\delta_{a,y})$

Diagrammatic representation

$$\hat{h}_{i,i+1} = \Gamma^{\mathrm{c}}_{i,i+1} + \alpha\Gamma^{\mathrm{r}}_{i,i+1} - (1-\alpha)\Gamma^{\mathrm{h}}_{i,i+1}$$

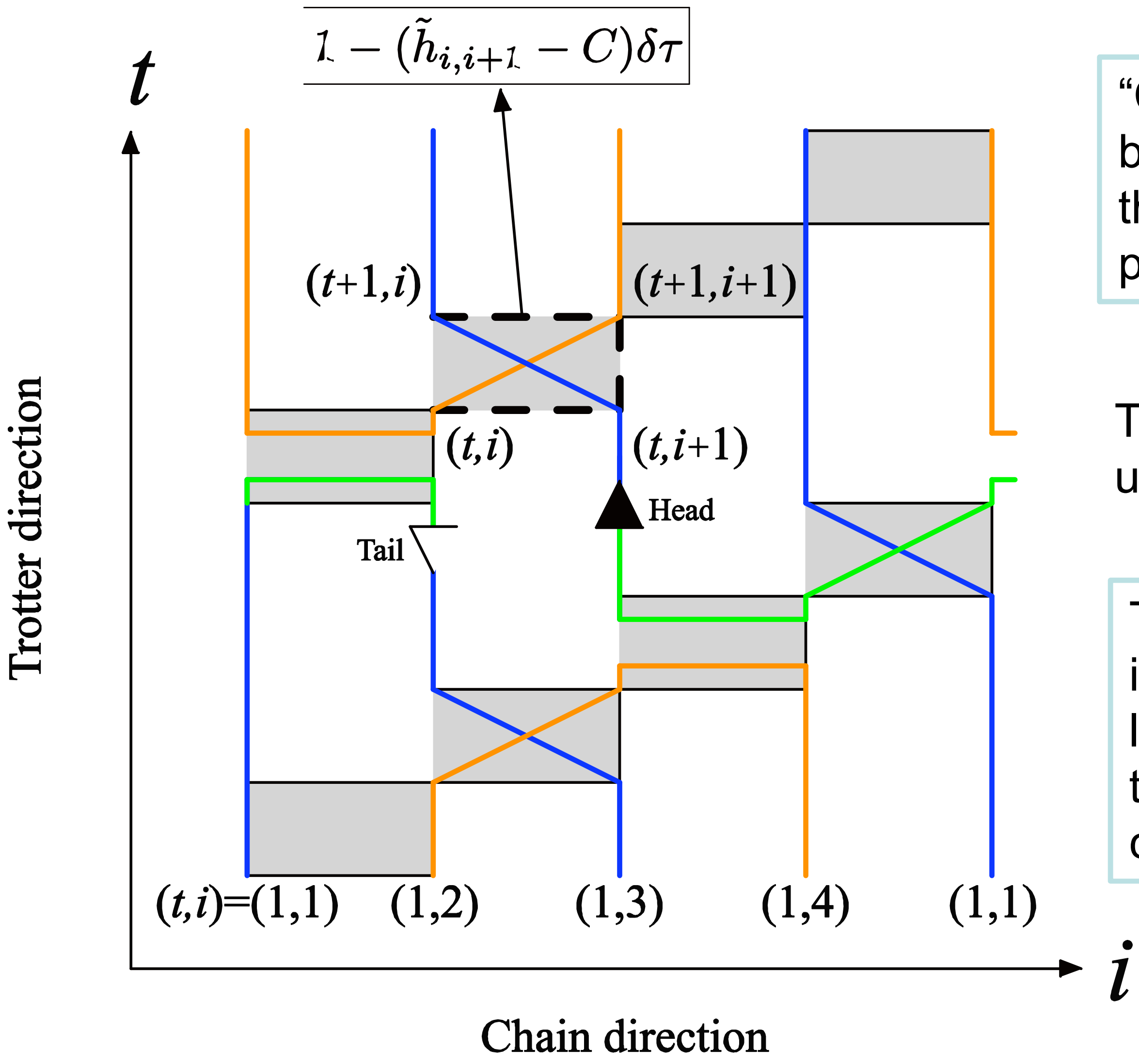
Generalized Jordan-Wigner

$$Q_{i,j} = diag(1,-1\cdots-1,\cdots1,\cdots1,-1\cdots-1,\cdots1,\cdots1)$$

$$\widetilde{h}_{i,i+1} = -\Gamma^c - (1-\alpha)\Gamma^h + \alpha\Gamma^r$$

The same diagram for “N- particle colors”

directed loop algorithm

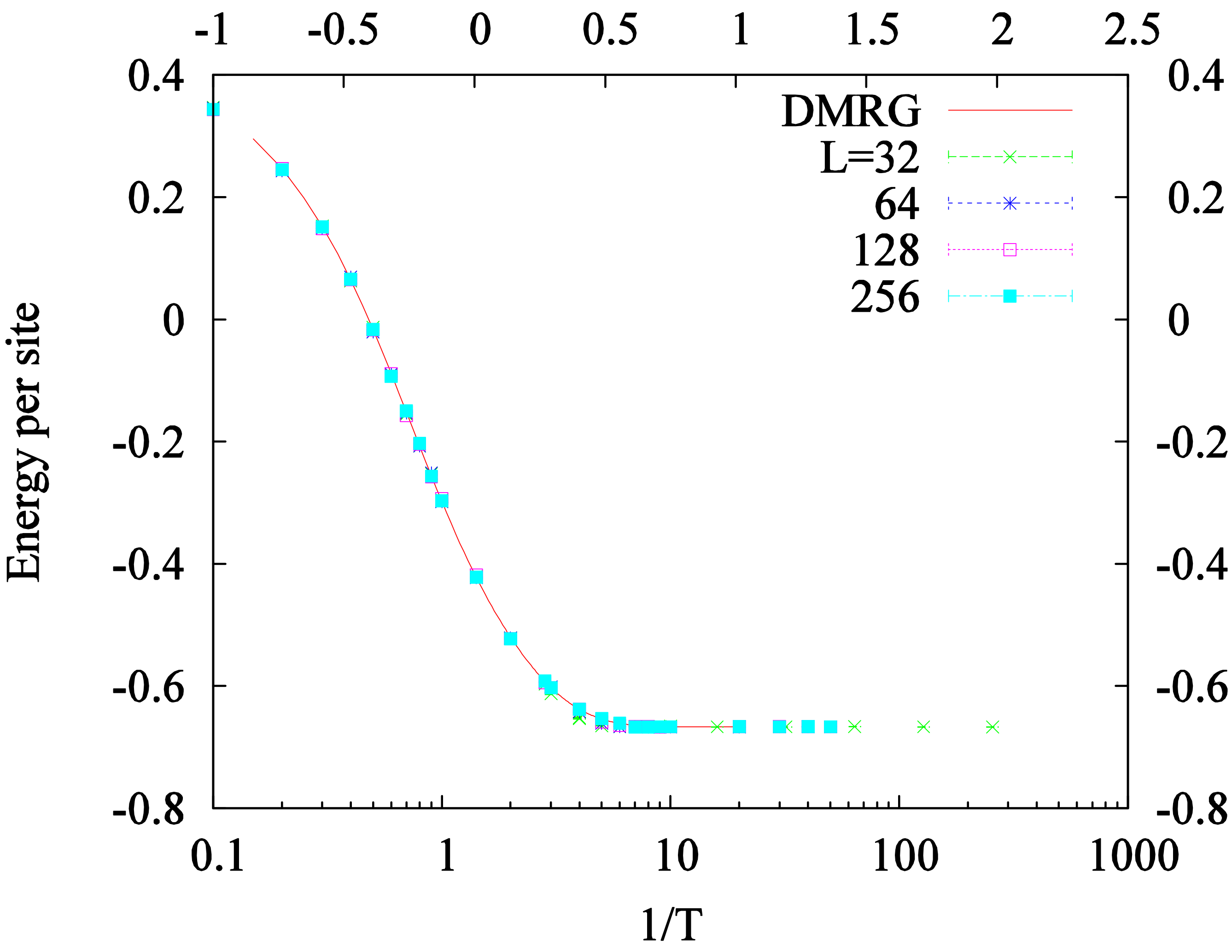


"C" controls the bounce rate, but it does not contribute to the expectation values of the physical quantities.

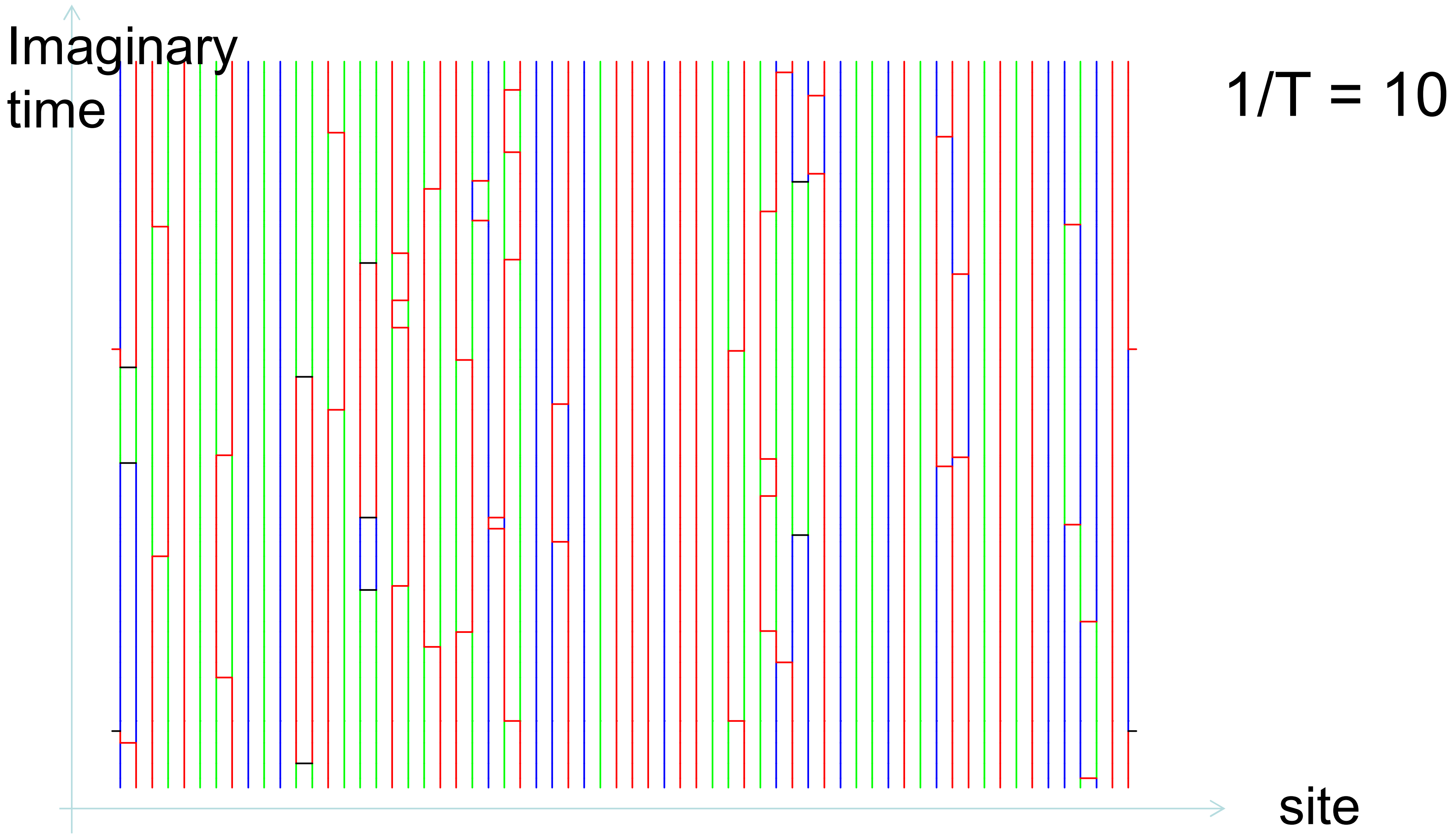
The head of the worm moves, until the head meets its tail.

The transition rate of a worm is determined, so that a world line without worm satisfies the detailed balance condition

Demonstration: AKLT point β=1/3



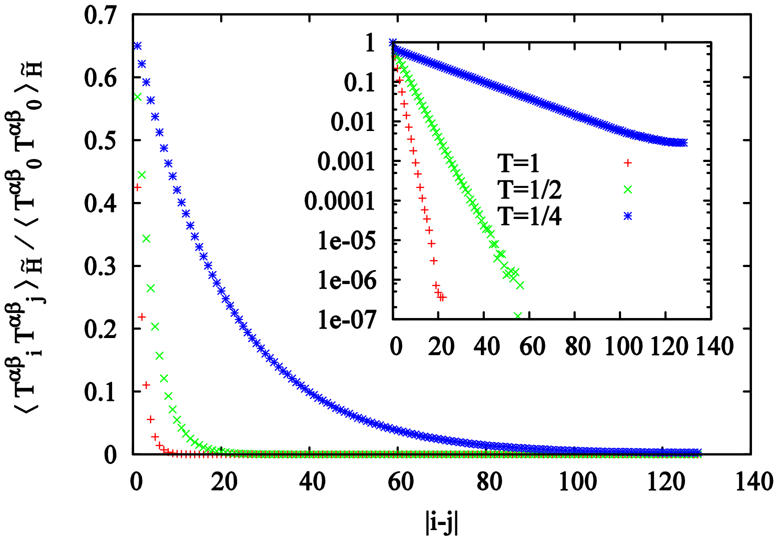
snap shot of world line: AKLT point β=1/3



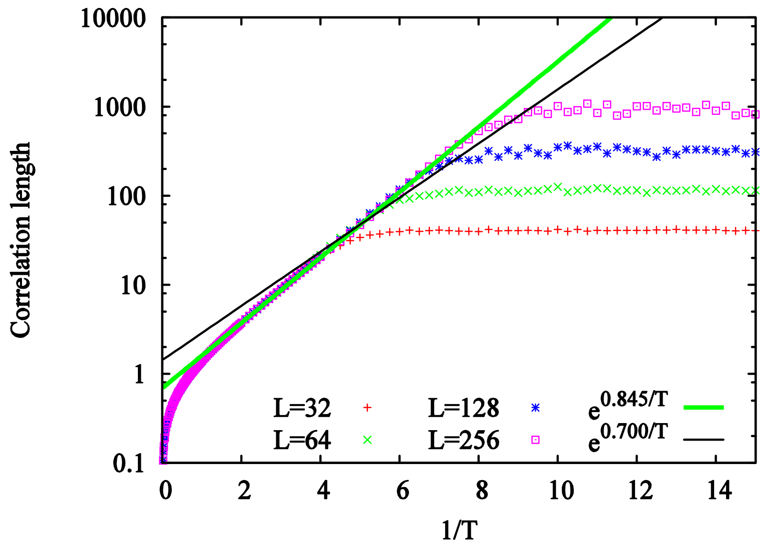
blue, red, green: color of particles corresponding to $n = 1,2,3$

String correlation

S=1 BLBQ chain/AKLT point



String correlation function



Correlation length

$$\xi(T) \propto \exp(\Delta_\xi / T)$$

$$\Delta_\xi \cong 0.875 (> \Delta = 0.700)$$

summary of part1

- SO(N)
  SPT entanglement can be disentangled by the KT or generalized JW transformations

  ⇨ Negative sign can be removed in the VBS phase.

- the number of the topological degeneracy corresponds to the number of the sign distributions in the negative-sign free representation

- Directed loop algorithm is actually formulated for the negative sign free N-color bosonic particle model.

Part 2

“Duality, criticality, anomaly, and topology in quantum spin-1 chains”
Phy. Rev B **107**, 125158 (2023)

with Hong Yang (U Tokyo)
Linhao Li (ISSP -> Ghent)
Hosho Katsura (U Tokoy)

$\mathcal{H}_{\mathrm{BLBQ}}$ — KT transformation — $\tilde{\mathcal{H}}_{\mathrm{BLBQ}}$

Z_2xZ_2 SPT — Z_2xZ_2 SSB

KT transformation and duality

Interpolation between the SPT and SSB Hamiltonians

$$\mathcal{H}(\lambda) = (1-\lambda)\mathcal{H}_{\mathrm{BLBQ}} + (1+\lambda)\tilde{\mathcal{H}}_{\mathrm{BLBQ}}$$

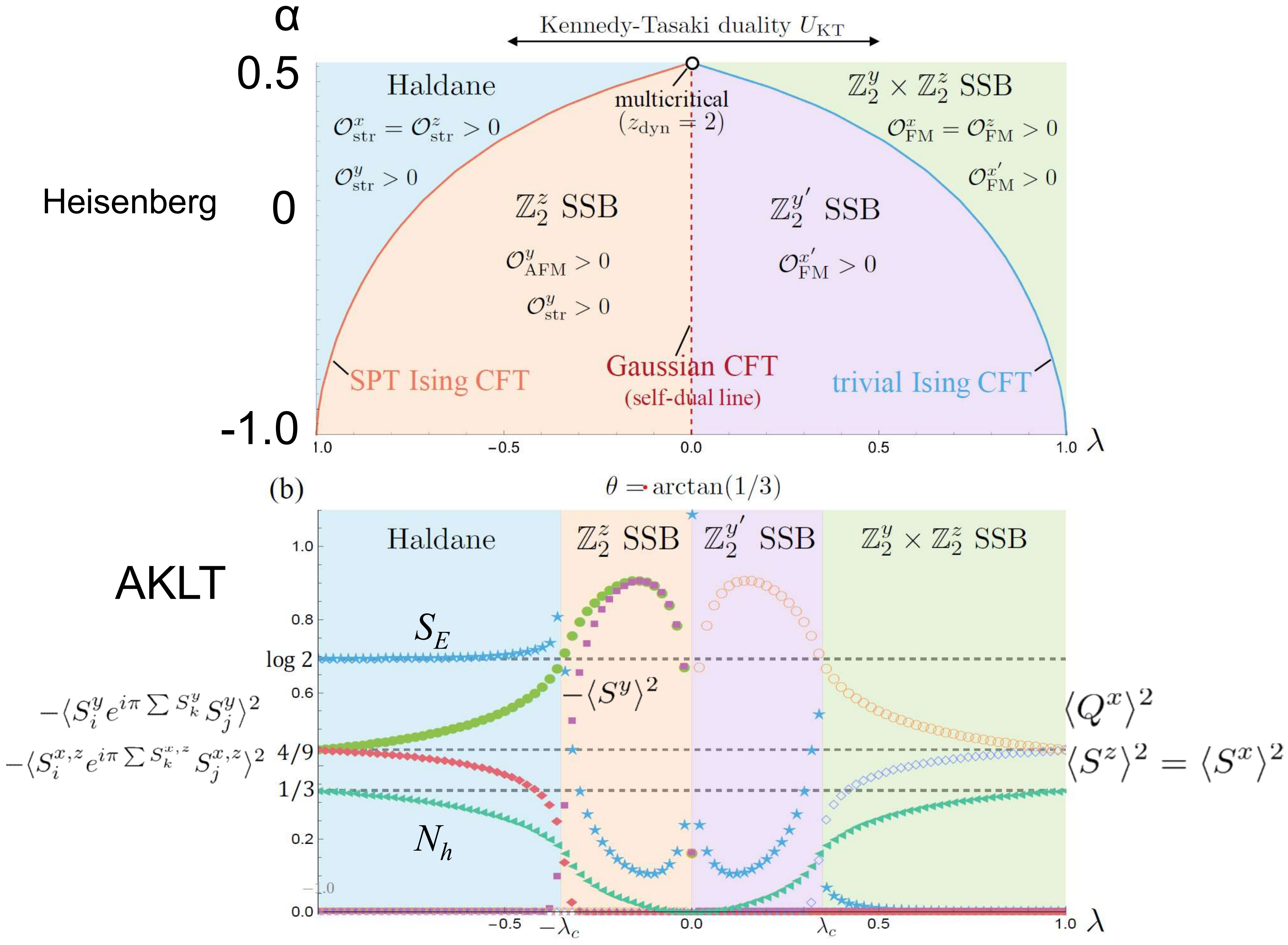
$$\left[\tilde{\mathcal{H}}_{\mathrm{BLBQ}} = U^\dagger \mathcal{H}_{\mathrm{BLBQ}} U\right]$$

KT = duality transformation $\quad \mathcal{H}(-\lambda) = U^\dagger \mathcal{H}(\lambda) U$

selfdual point $\quad \lambda = 0$

Question

How the SPT order is changed to the corresponding SSB order?



α
Kennedy-Tasaki duality $U_{\rm KT}$
0.5
Heisenberg
0
-1.0
Haldane
$\mathcal{O}^x_{\rm str} = \mathcal{O}^z_{\rm str} > 0$
$\mathcal{O}^y_{\rm str} > 0$
multicritical
$(z_{\rm dyn} = 2)$
$\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ SSB
$\mathcal{O}^x_{\rm FM} = \mathcal{O}^z_{\rm FM} > 0$
$\mathcal{O}^{x'}_{\rm FM} > 0$
$\mathbb{Z}_2^z$ SSB
$\mathcal{O}^y_{\rm AFM} > 0$
$\mathcal{O}^y_{\rm str} > 0$
$\mathbb{Z}_2^{y'}$ SSB
$\mathcal{O}^{x'}_{\rm FM} > 0$
SPT Ising CFT
Gaussian CFT
(self-dual line)
trivial Ising CFT
1.0
−0.5
0.0
0.5
1.0
λ
(b)
$\theta = \arctan(1/3)$
AKLT
Haldane
$\mathbb{Z}_2^z$ SSB
$\mathbb{Z}_2^{y'}$ SSB
$\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ SSB
1.0
0.8
log 2
0.6
4/9
1/3
0.2
0.0
S_E
$-\langle S^y \rangle^2$
$-\langle S_i^y e^{i\pi \sum S_k^y} S_j^y \rangle^2$
$-\langle S_i^{x,z} e^{i\pi \sum S_k^{x,z}} S_j^{x,z} \rangle^2$
N_h
$\langle Q^x \rangle^2$
$\langle S^z \rangle^2 = \langle S^x \rangle^2$
−0.5
$-\lambda_c$
0.0
λ_c
0.5
1.0
λ

$\lambda = 0$ selfdual point

decoupling of $|h\rangle = \frac{1}{\sqrt{2}}(|+1\rangle + |-1\rangle)$ states

⇒ effective XXZ chain

$$\mathcal{H}_{\mathrm{XXZ}} = (\cos\theta - \sin\theta)\sum_j (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \sin\theta \sum_j \sigma_j^z \sigma_{j+1}^z \qquad (\theta = \arctan\alpha)$$

For $-1 < \alpha < 0.5$, XY-like regime

⇒ gapless ground state

c=1 Gaussian CFT

(Z2-Ising × 2)

summary of part 2

- Selfdual BLBQ chain
- Relation between SPT and SSB orders
- Sequential phase transitions:
  Ising(Z2) criticality + c=1 CFT
  (selfdual point)
- Selfdual point:
  decoupling of hole degrees of freedom
- $\alpha=1/2$, $\lambda=0$：multicritial → incommensurate?