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# Symmetry-Protected topological entanglement and negative sign problem for the SO(N) biliner-biquadratic chains


Niigata University
新潟大学
Kouichi Okunishi
奥西巧一

Kyoto University
京都大学
Kenji Harada
原田健自

# Negative sign problem in QMC

D-dimensional quantum lattice model

↓ Suzuki-Trotter decomposition

D+1 dimensional classical model

Markov chain Monte-Carlo simulation for the mapped classical model

Transition probability

$$\langle s'_i\, s'_{i+1} | \exp(-\Delta\tau h_{i,i+1}) | s_i s_{i+1} \rangle$$

$|s_i s_{i+1}\rangle$ Naïve product state of the single particle bases

BUT, Frustrating systems/Ferimion systems

This transition probability becomes negative !

The serious problem in QMC

M. Troyer and U.-J. Wise, Phys. Rev. Lett. 94, 170201 (2005)

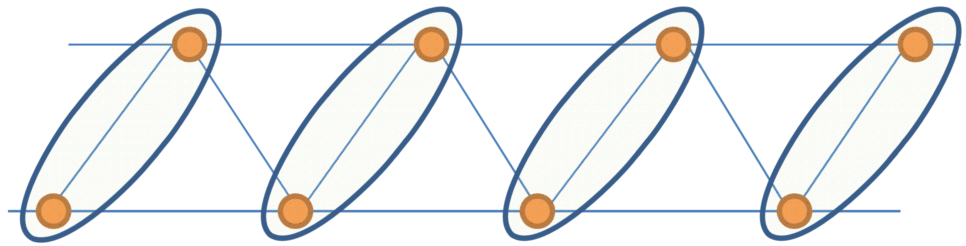
⇒ NP hard

Nontrivial and nonlocal entanglement structure of the world-lines based on the single particle bases.

Local basis change does not settle the problem.

# two exceptions

1D zigzag chain : T. Nakamura, PRB 57 R3197 (1998)



Negative sign is removed by Kennedy-Tasaki type transformation combined with dimer-R bases.

<u>Dimer-R bases</u>

$$|1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right) \qquad |3\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

$$|2\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle\right) \qquad |4\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

But, further extension has not been found

SU(N) chain :

L. Messio and F. Mila, PRL 109,205306 (2012)

B. Frischmuth, F.Mila and M. Troyer, PRL 82, 835 (1999)

Sing control of state vectors based on permutations

$$\left|\cdots s_i s_{i+1} \cdots\right\rangle \Rightarrow (-)^{n(P)} \left|\cdots s_i s_{i+1} \cdots\right\rangle$$

n(P): number of permutations of different colors.

if particles of different species are exchanged, assign a minus sign to a state vector.

No further extension....

SU(N) chain is Bethe ansatz soluble and the groundstate is gapless.

One may wonder if the vanishing mechanism relies on the integrability.

# S=1 bilinear-biquadratic chain

two sites Hamiltonian

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

$\alpha$=0 : Heisenberg chain, Haldane state

$\alpha$=1/3 : AKLT chain, exact matrix product groundstate

$\alpha$=1 : SU(3) point, Bethe ansatz solved

$\alpha$=-1 : Taktajian-Babujian point , Bethe ansatz solved

-1 <$\alpha$<1 Haldane phase, Z2xZ2 symmetry breaking

The ground state is also numerically well-understand by DMRG

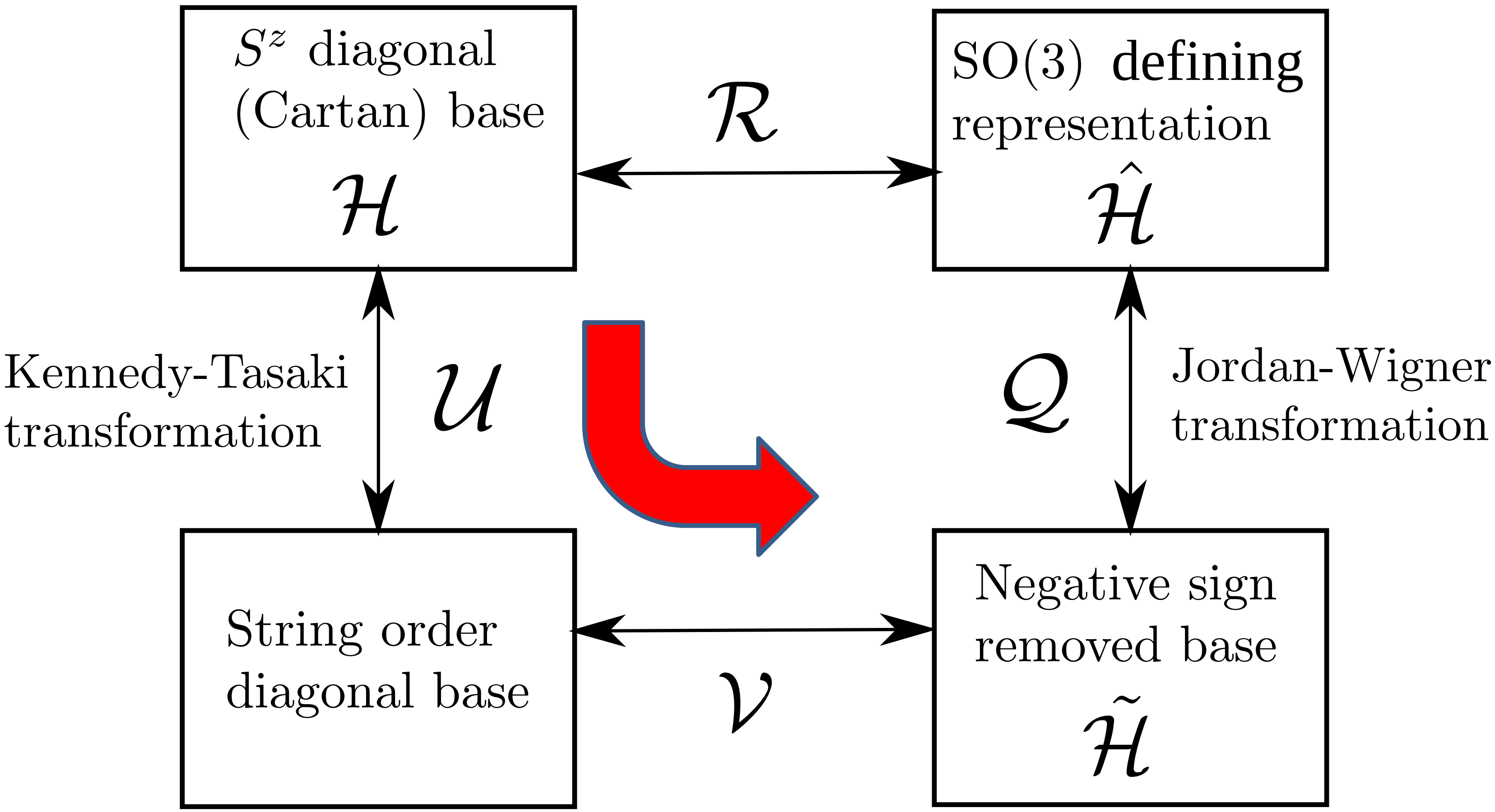
QMC : The region of $\alpha$>0 is dark side; negative sign problem

# Hamiltonian : matrix elements

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

$\alpha>0$ ; negative sign problem

# Summary of various transformations



# Idea for the bilinear-biquadratic chain

Kennedy-Tasaki Transformation $U$

+

Local unitary transformation $V$ (dimer-R)

KT transformation : MPS => classical ground state(disentangled)

T. Kennedy and H. Tasaki, PRB45, 304 (1992), K. Okunishi, PRB 83, 104411 (2011)

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

manifest Z2 x Z2 symmetry

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

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

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

# local unitary transformation : $V$

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

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

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

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

$$V^2 = I$$

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

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

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

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

T. Kennedy, J. Phys. condens matt. 6, 8015 (1994)

: Perron-frobenius theorem

# KT transformation + V transformation

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

Off diagonal elements of this Hamiltonian are negative for $\alpha <= 1$ .
(No negative sign problem of the Boltzmann weight)

# Physical meaning of the matrix elements

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

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

$\Gamma_c$ exchange of particles

$\Gamma_h$ pair creation & anihiration of particles

$\Gamma_r$ repulsion between particles of the same color (diagonal elements)

# SU(3) generators /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

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

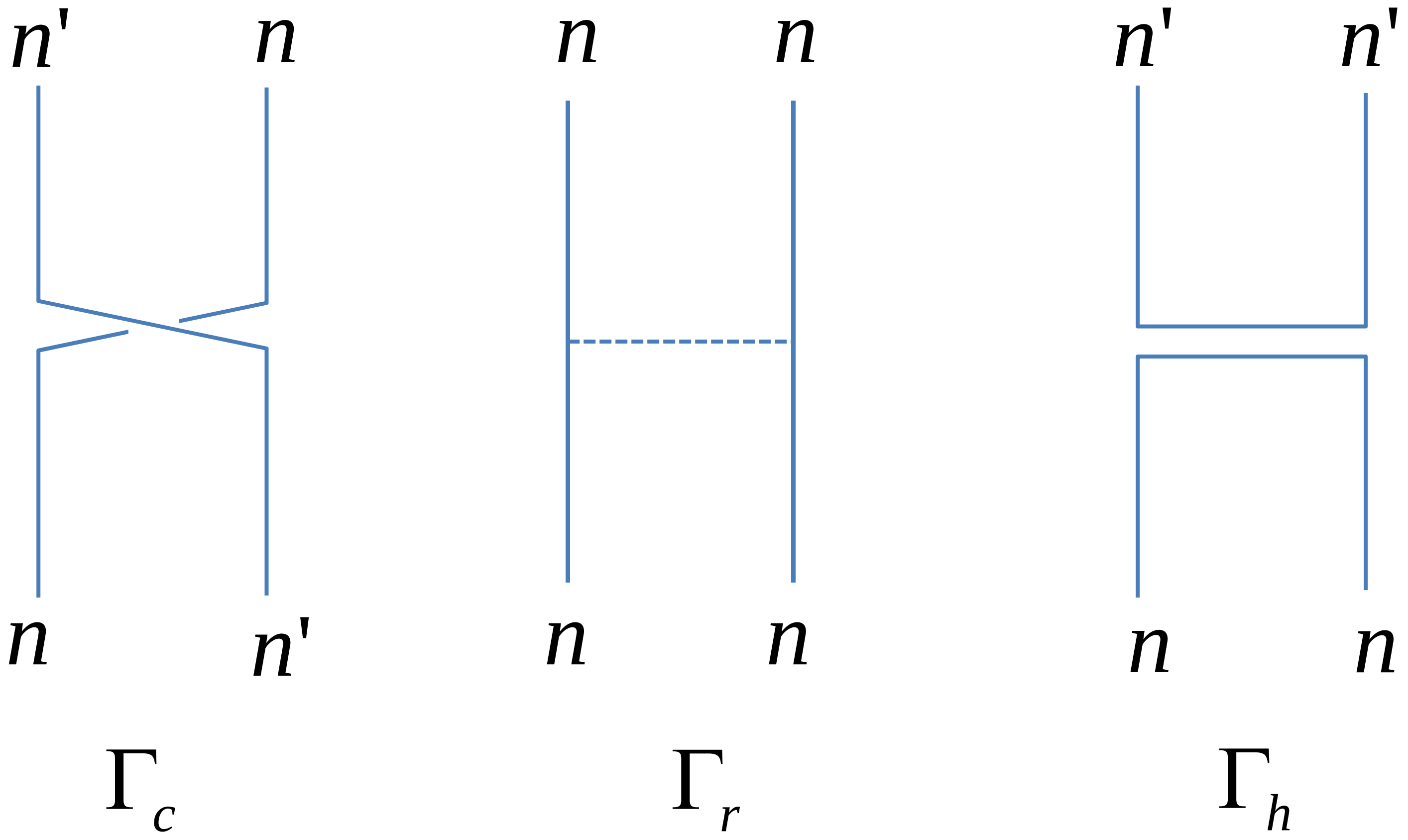
## Scwinger boson

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

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

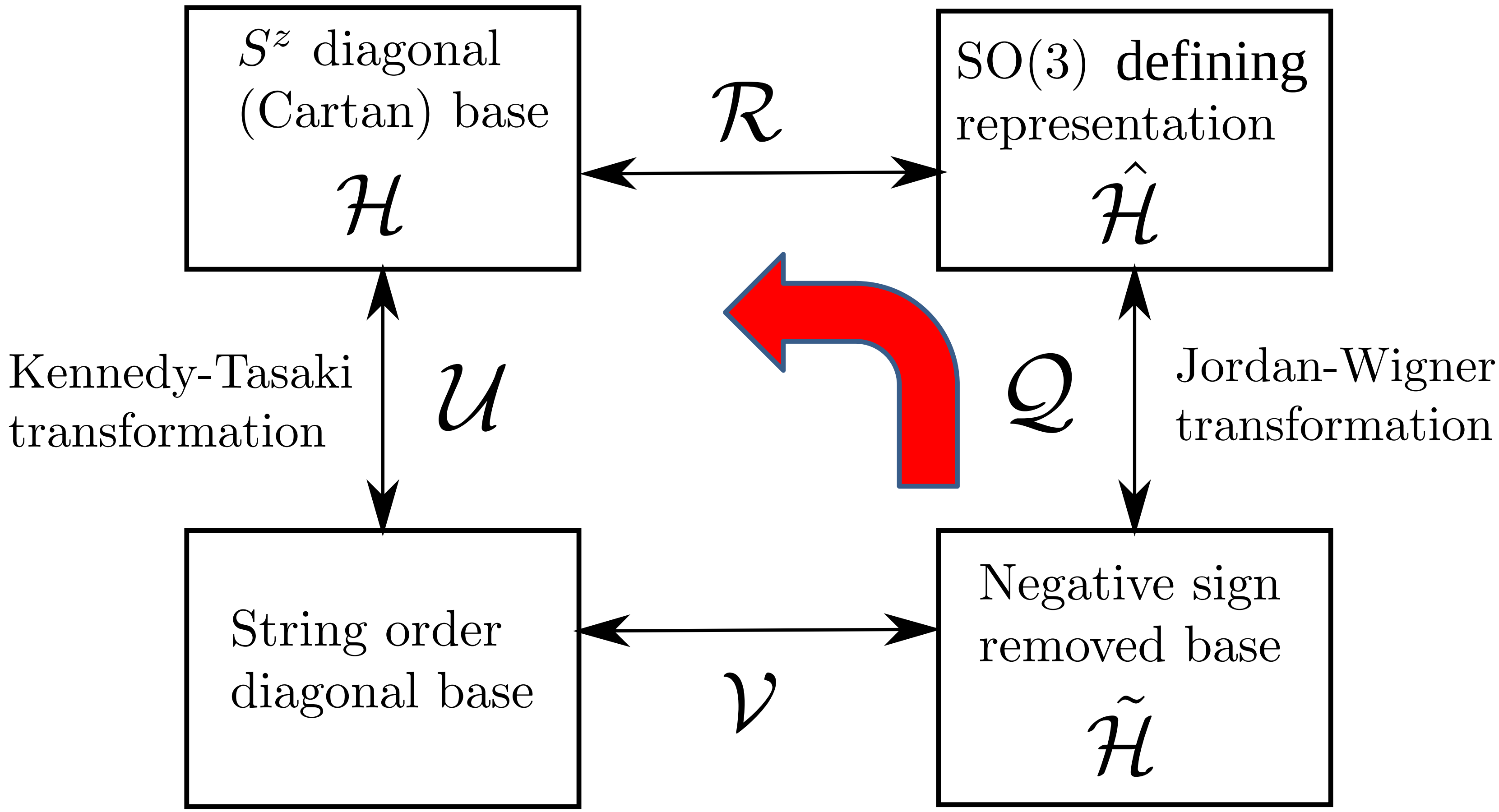
$\Gamma$ ⇨ scattering of bosonic particles

# diagrammatic representation




Continuous time worm type algorithm is possible

# Summary of various transformations



# 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).

⇒

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

# relation to SU(3) chains

Jordan -Wigner

$$Q\tilde{h}_{i,i+1}Q = \hat{h}^{[10]}_{i,i+1} + (\alpha - 1)\hat{h}^{[11]}_{i,i+1} = \hat{h}_{i,i+1}$$

$$\hat{h}^{[10]}_{i,i+1} = Q\tilde{h}^{[10]}_{i,i+1}Q = \Gamma^c + \Gamma^r$$

SU(3) fundamental representation

$$\hat{h}^{[11]}_{i,i+1} = Q\tilde{h}^{[11]}_{i,i+1}Q = \Gamma^h + \Gamma^r$$

SU(3) singlet

$$\Rightarrow \quad \hat{h}_{i,i+1} = \hat{h}^{[10]}_{i,i+1} + (\alpha - 1)\hat{h}^{[11]}_{i,i+1} = \Gamma^c + \alpha\Gamma^r + (\alpha - 1)\Gamma^h$$

What is this Hamiltonian?

# $H$ and $\hat{H}$

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

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

bilinear-biquadratic chain in the defining representation

$$R = \begin{pmatrix} -i/\sqrt{2} & 0 & i/\sqrt{2} \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \end{pmatrix} \qquad R^+ \vec{L} R = \vec{S}$$

# Operator form

Jordan-wigner

$$\mathcal{Q} L_i^x \mathcal{Q} = e^{i\pi \sum_{j<i} (L_j^y + 1)} L_i^x e^{i\pi \sum_{j>i} (L_j^z + 1)}$$
$$\mathcal{Q} L_i^y \mathcal{Q} = e^{i\pi \sum_{j<i} L_j^z} L_i^y e^{i\pi \sum_{j>i} L_j^x}$$
$$\mathcal{Q} L_i^z \mathcal{Q} = e^{i\pi \sum_{j<i} (L_j^x + 1)} L_i^z e^{i\pi \sum_{j>i} (L_j^y + 1)}.$$

KT transformation

$$\mathcal{V}\mathcal{U} S_i^x \mathcal{U}\mathcal{V}^\dagger = T_i^x e^{i\pi \sum_{j>i} T_j^x}$$
$$\mathcal{V}\mathcal{U} S_i^y \mathcal{U}\mathcal{V}^\dagger = e^{i\pi \sum_{j<i} T_j^z} L_i^y e^{i\pi \sum_{j>i} T_j^x}$$
$$\mathcal{V}\mathcal{U} S_i^z \mathcal{U}\mathcal{V}^\dagger = e^{i\pi \sum_{j<i} T_j^z} T_i^z$$

$$T^x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad T^x = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad T^x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

# 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) bilinear-biquadratic chain

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

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

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

The same diagram for “N- particle colors”

# VBS points $a = \frac{N-2}{N}$

Matrix product state (Cartan generator diagonalizing base )

H.-H. Tu, G.-M. Zhang, and T. Xiang, PRB 78 094404 (2009)

$$|\Psi\rangle = \mathrm{Tr}(g_1 g_2 \dots g_N)$$
$$= \sum_{a_1 \dots a_N} \mathrm{Tr}(\Gamma^{a_1}\Gamma^{a_2}\dots\Gamma^{a_N})|n^{a_1}n^{a_2}\dots n^{a_N}\rangle,$$

SO(5) VBS chain

$$g_j = \begin{pmatrix} |0\rangle_j & \sqrt{2}|-1\rangle_j & \sqrt{2}|-2\rangle_j & 0 \\ -\sqrt{2}|1\rangle_j & -|0\rangle_j & 0 & \sqrt{2}|-2\rangle_j \\ \sqrt{2}|2\rangle_j & 0 & -|0\rangle_j & -\sqrt{2}|-1\rangle_j \\ 0 & \sqrt{2}|2\rangle_j & \sqrt{2}|1\rangle_j & |0\rangle_j \end{pmatrix}$$

Topological entanglement $(Z_2 \times Z_2)^2$ # of edge states

$$R \,\&\, Q$$

disentangled $\left|\Phi^{\nu}\right\rangle = \prod_{i} \left|\phi_i^{\nu}\right\rangle$ product state of

$$\left|\phi_i^{\nu}\right\rangle = \frac{1}{\sqrt{N}} \sum_{n_i=1}^{N} \sigma^{\nu}(n_i) \left|n_i\right\rangle$$

# of degeneracy → distribution of "-" sign $\sigma^{\nu}(n_i) = \pm 1$

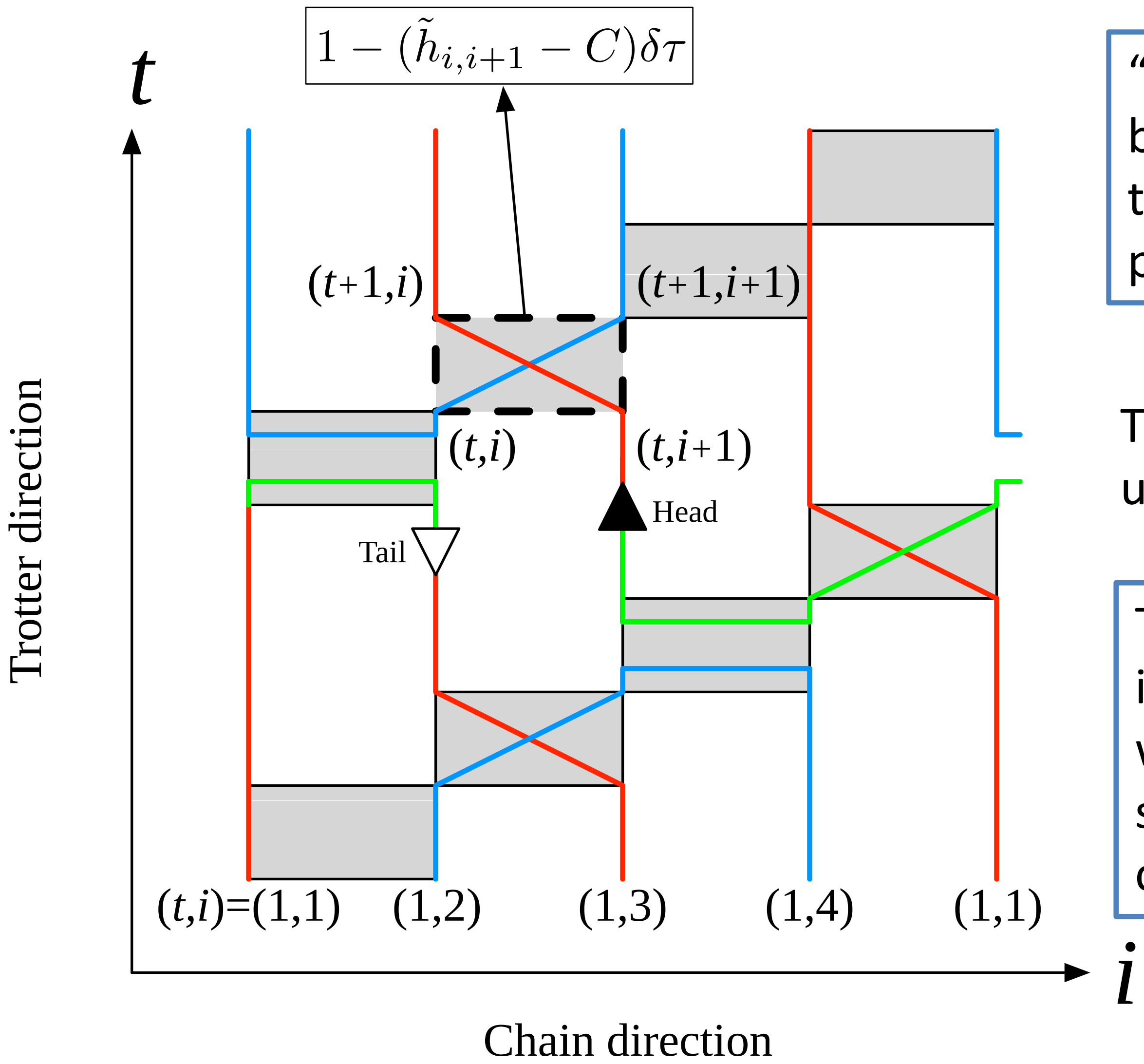
**degeneracy**

$(Z_2 \times Z_2)^l$ Edge degrees of feedom

$$l = \begin{cases} (N-1)/2 & odd \\ N/2 & even \end{cases}$$

→ $2^{N-1}$ distribution of "–" sign for N color particles without the overall sign

# directed loop algorithm

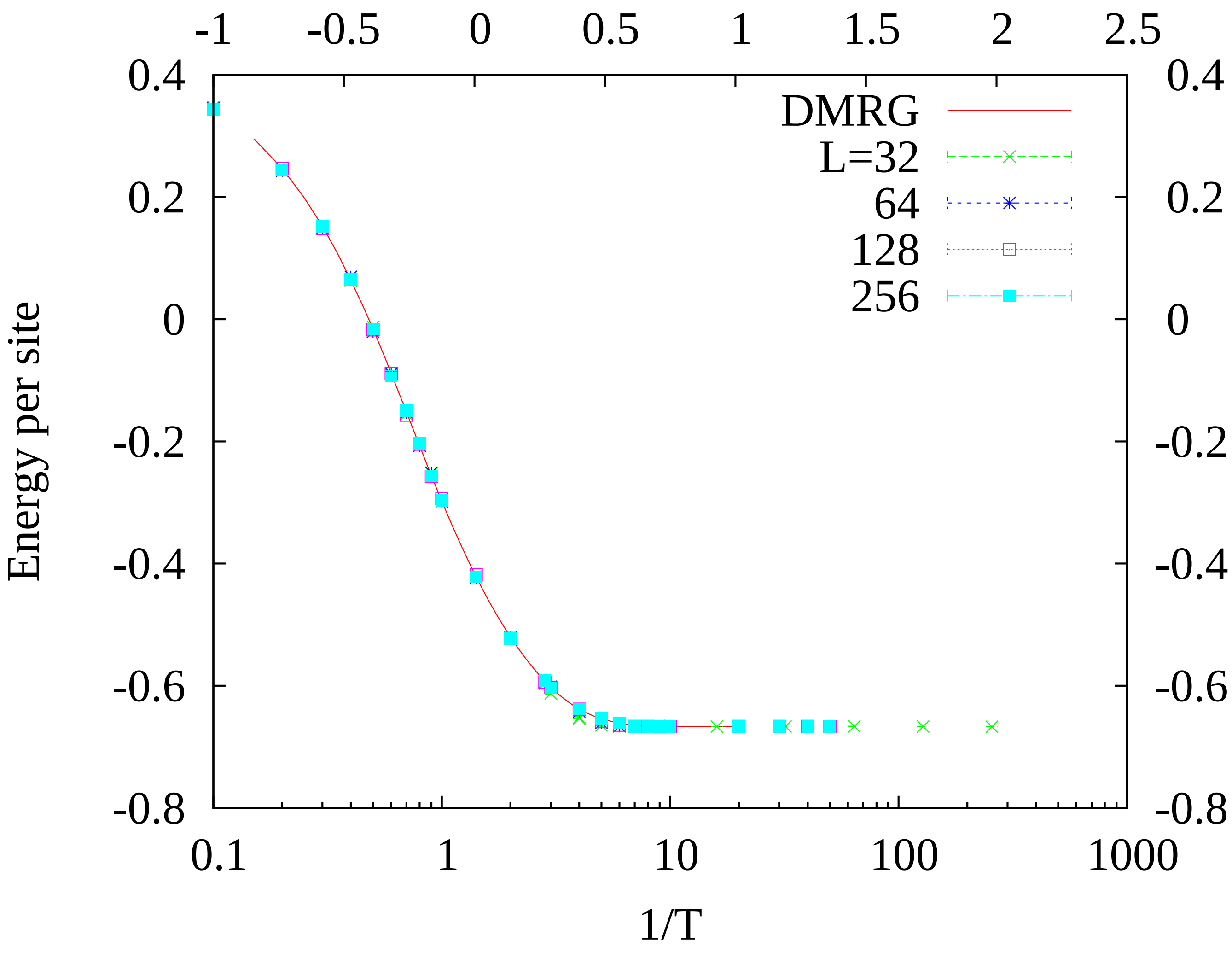



"C" controls the bounce rate, but it does not contribute to the expectation values of the physical quantities.

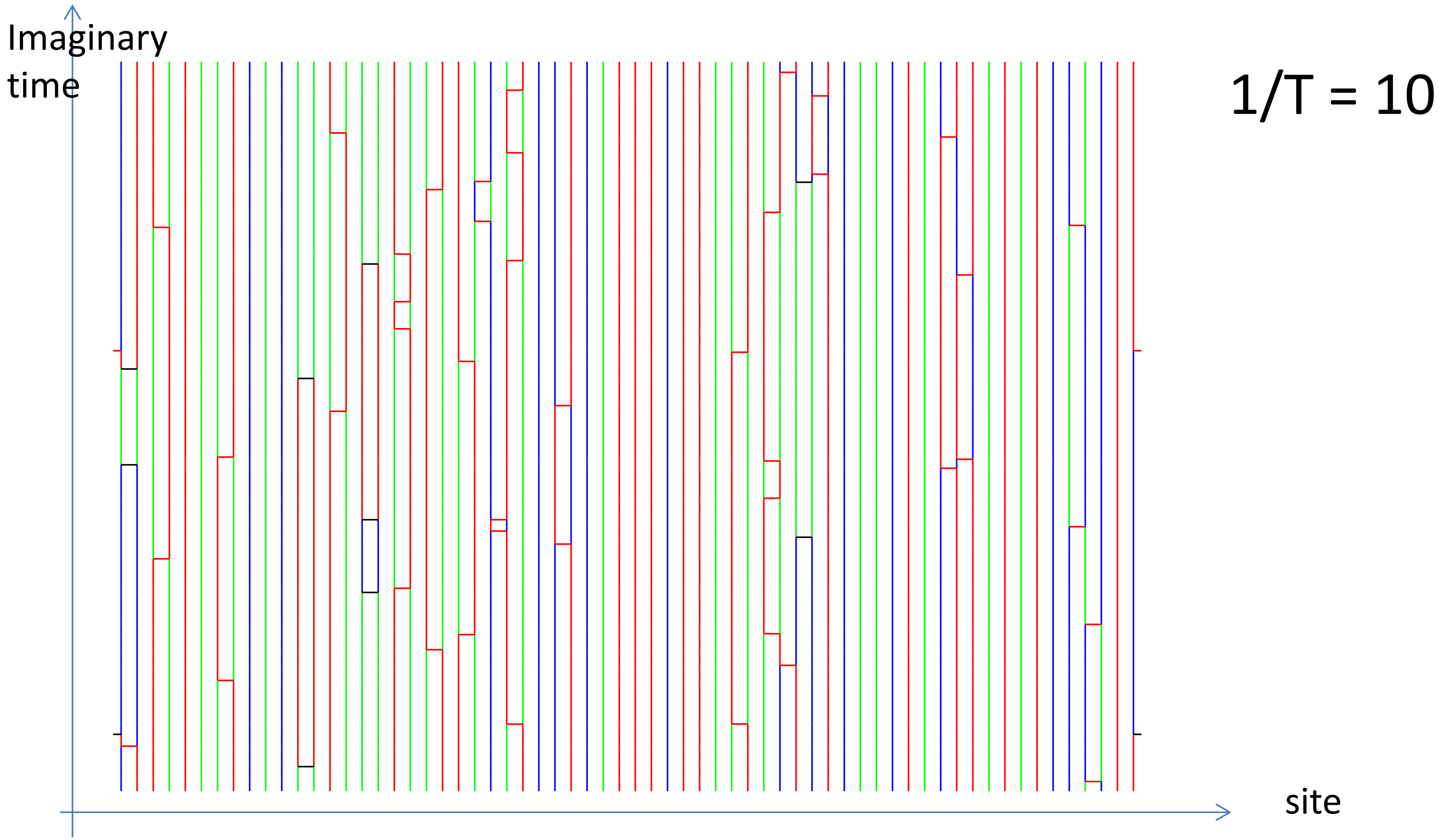
The head of the worm moves, until the head meets its tail.

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

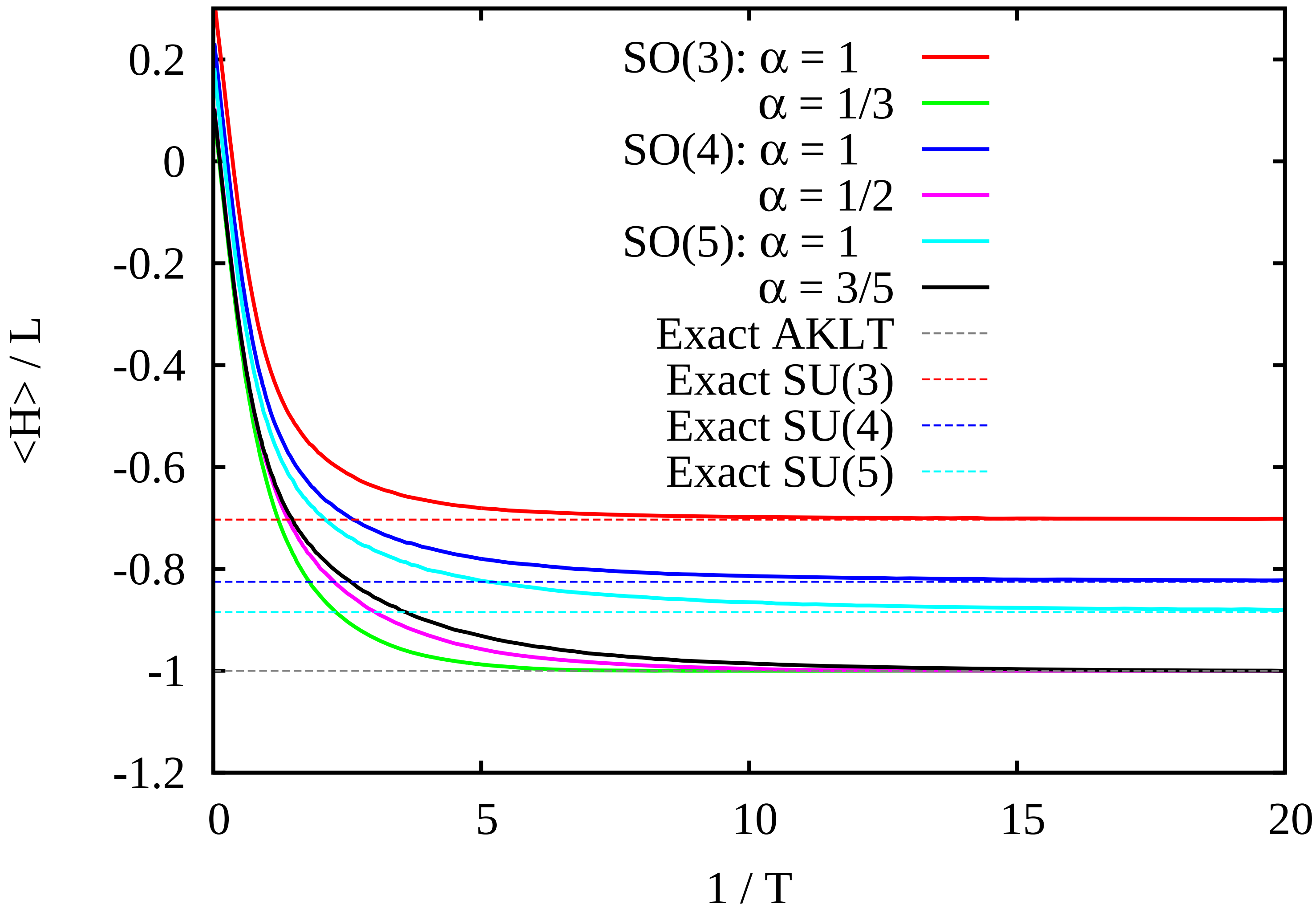


# snap shot of world line: AKLT point β=1/3



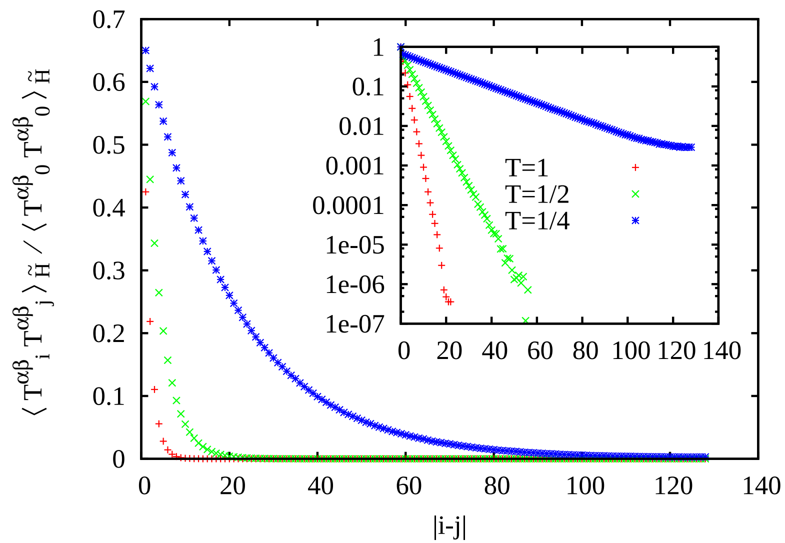

blue, red, green: color of particles corresponding to $n = 1,2,3$

# SO(N) VBS points & SU(N) points

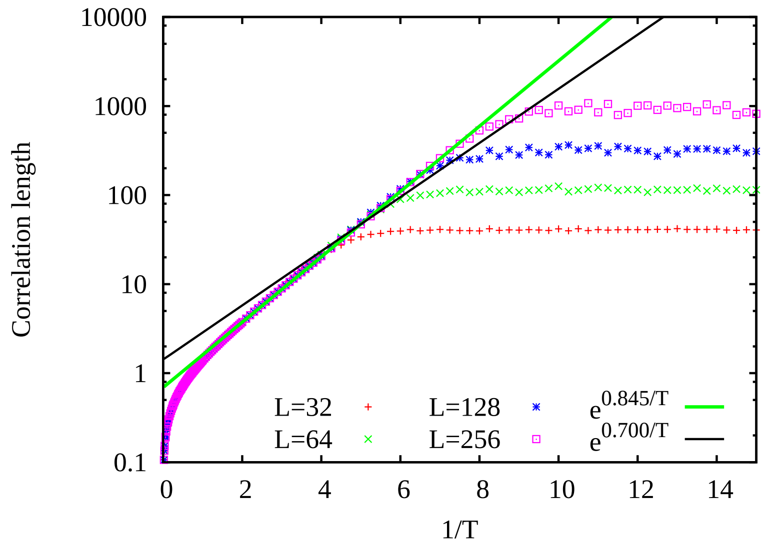


# String correlation

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

- SO(N)
  symmetry protected entanglement can be disentangled by the generalized Jordan-Wigner transformation on the basis of the defining representations.
  ⇒ Negative sign can be removed in the SPT 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.