Loop algorithm with non-binary loops

August 2, 2006

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History of quantum world-line Monte Carlo

- Path-integral representation of the partition function (Feynmann, Suzuki (1976))
- Cluster algorithm for classical Monte Carlo (Swendsen & Wang (1987))
- Loop algorithm for quantum Monte Carlo (Evertz, Lana & Marcu (1993))

Outline

I. Quantum world-line Monte Carlo

a. Path-integral representation
b. Loop algorithm

II. Non-binary loop algorithm
a. Non-binary loop
b. Applications

Coworker: Naoki Kawashima (ISSP, Univ. of Tokyo)

Canonical ensemble for a quantum system

Average

$$\langle A \rangle \equiv \frac{\mathbf{Tr} A \exp(-\beta \mathcal{H})}{Z}$$

Partition function

$$Z \equiv \mathbf{Tr} \exp(-\beta \mathcal{H}) = \mathbf{Tr} \rho(\beta)$$

Density operator

$$\rho(\beta) \equiv \exp(-\beta \mathcal{H})$$

Density operator

$$\rho(\beta) \equiv e^{-\beta(\mathcal{H}_0+V)} = e^{-\beta\mathcal{H}_0}\rho'(\beta)$$

➡ $$\frac{d\rho'(\beta)}{d\beta} = -V(\beta)\rho'(\beta)$$ (Bloch eq.)

Interaction picture $V(t) \equiv e^{t\mathcal{H}_0} V e^{-t\mathcal{H}_0}$

➡ $$\rho'(\beta) = I - \int_0^\beta dt\ V(t)\rho'(t)$$

Matsubara formula

$$\rho'(\beta) = I - \int_0^\beta dt_1 V(t_1) + \int_0^\beta dt_2 \int_0^{t_2} dt_1 V(t_2) V(t_1) - \cdots$$

If $V \equiv \sum_b V_b$, then

$$= I - \sum_{b_1} \int_0^\beta dt_1 V_{b_1}(t_1) + \sum_{b_1, b_2} \int_0^\beta dt_2 \int_0^{t_2} dt_1 V_{b_2}(t_2) V_{b_1}(t_1) - \cdots$$

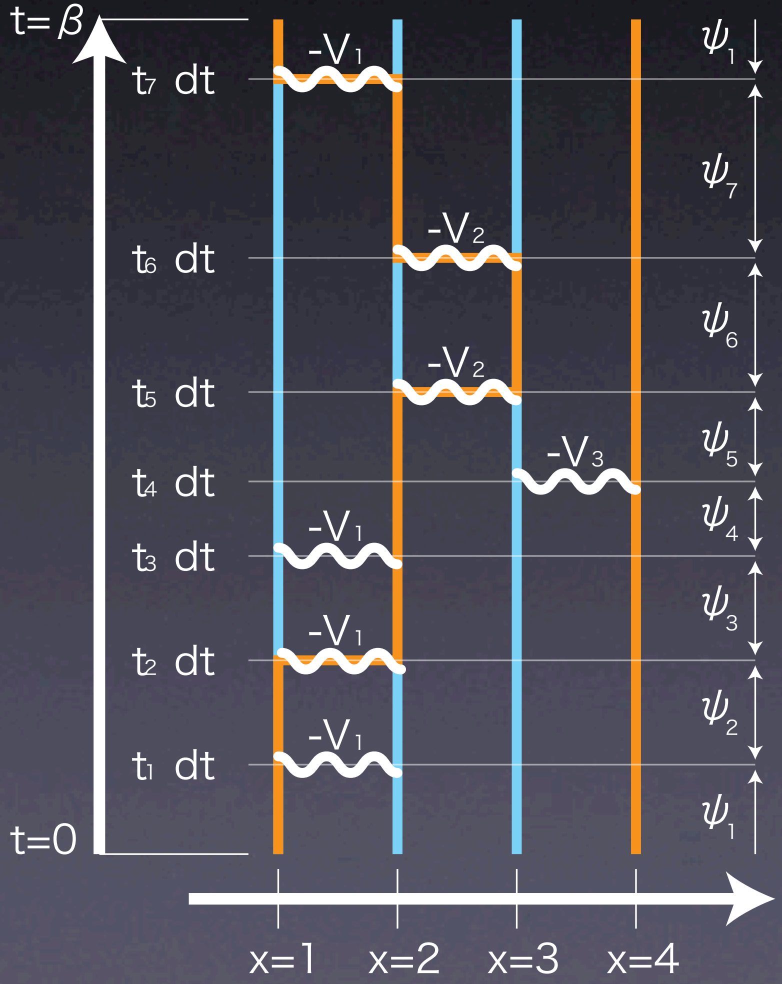
Path-integral representation

$$\langle\psi_1|\rho'(\beta)|\psi_1\rangle = \cdots + \sum_{(\{\psi_i\},\{b_i\},\{t_i\})} \prod_{i=1}^{n} \langle\psi_{i+1}|(-V_{b_i}(t_i))|\psi_i\rangle + \cdots$$

E.g. S=1/2 HAF model on a 4-sites chain

$$V_b \equiv J\vec{S}_{x=b}\cdot\vec{S}_{x=b+1}$$

$$|\psi\rangle \equiv |z_1 z_2 z_3 z_4\rangle \qquad \left(z_i = \pm\frac{1}{2}\right)$$



Path-integral representation of partition function

$$Z \equiv \mathrm{Tr}\rho(\beta) = \sum_{n=0}^{\infty} \left[\sum_{\psi_n,\cdots,\psi_1 (\psi_{n+1}=\psi_1)} \sum_{b_n,\cdots,b_1} \int_{\beta \geq t_n \geq \cdots \geq t_1 \geq 0} W_n(\{\psi_i\},\{b_i\},\{t_i\}) \right]$$

Weight of world-line configuration $(\{\psi_i\},\{b_i\},\{t_i\})_{i=1\ldots n}$

$$W_n \equiv e^{-\beta \mathcal{H}_0(\psi_1)} \prod_{i=1}^{n} \langle \psi_{i+1} | (-V_{b_i}(t_i)) | \psi_i \rangle dt_i$$

Quantum world-line Monte Carlo

- Canonical ensemble average

$$\langle A \rangle \equiv \frac{\mathbf{Tr} A \rho(\beta)}{Z} = \sum_{\{\psi_i\},\{b_i\},\{t_i\}} A(\psi_1) \frac{W_n(\{\psi_i\},\{b_i\},\{t_i\})}{Z}$$

- Monte Carlo sampling of world-line configurations with the probability

$$\mathbf{Prob}(\{\psi_i\},\{b_i\},\{t_i\}) = \frac{W_n(\{\psi_i\},\{b_i\},\{t_i\})}{Z}$$

Monte Carlo algorithm

- Markov chain

$$\cdots \to S_1 \to S_2 \to \cdots$$

- Metropolis's method
(local updates only before loop algorithm)

➡ Long correlation times in sequence of samples at low temperatures and quantum critical points

Loop algorithm

Evertz, et al. (1993)

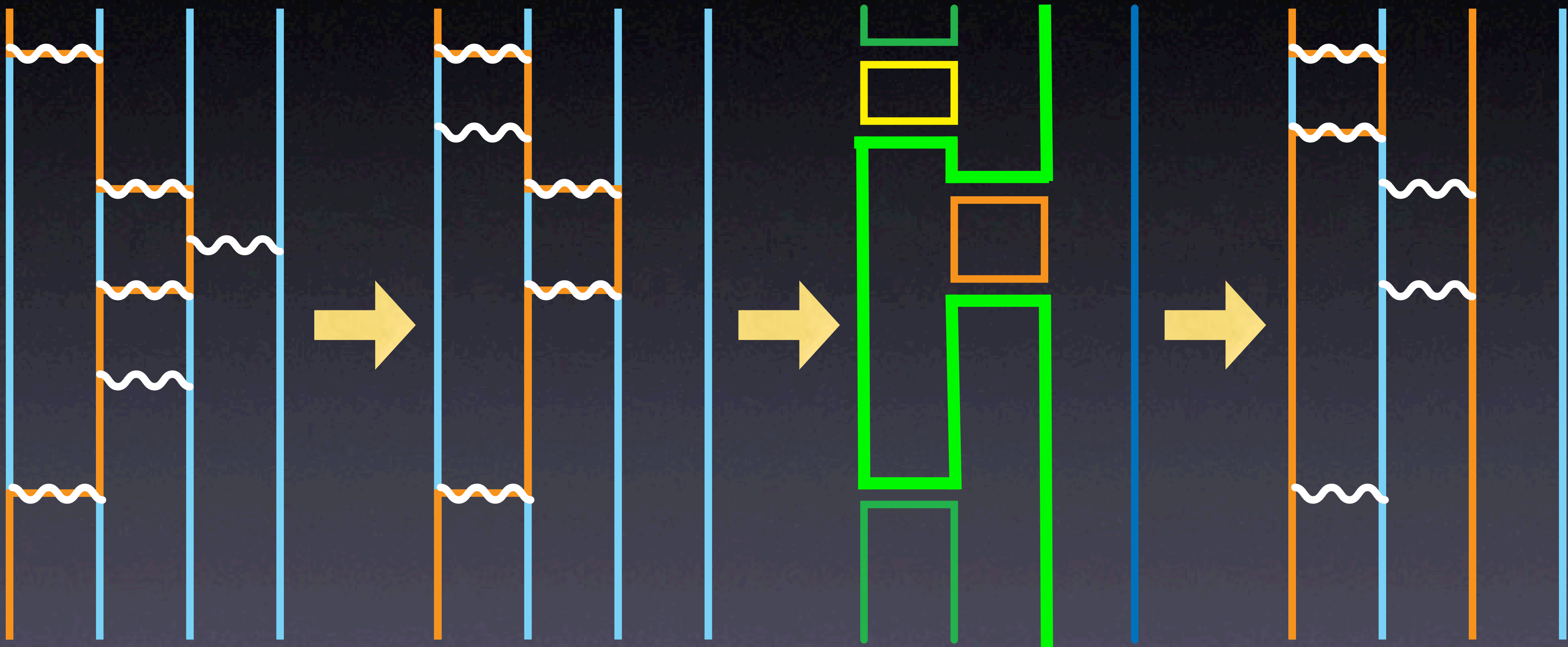
Global loop updating for world-line configurations

- Short correlation times at quantum critical points and low temperatures
- Grand canonical sampling

➡ Applicable to quantum critical phenomena for quantum spin and boson models

Procedure of loop algorithm

E.g. s=1/2 HAF model on a 4-sites chain

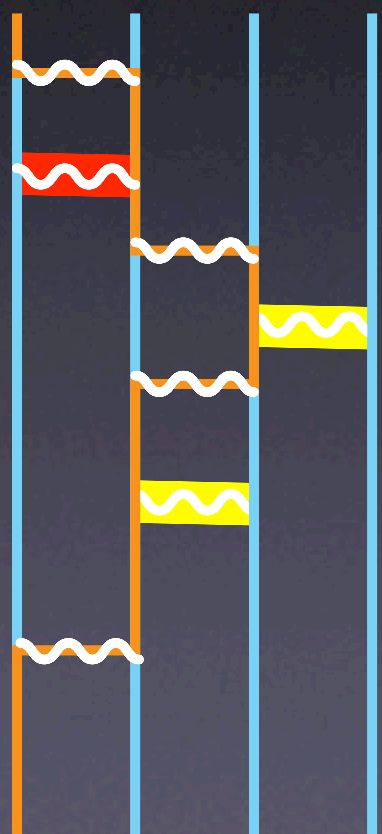


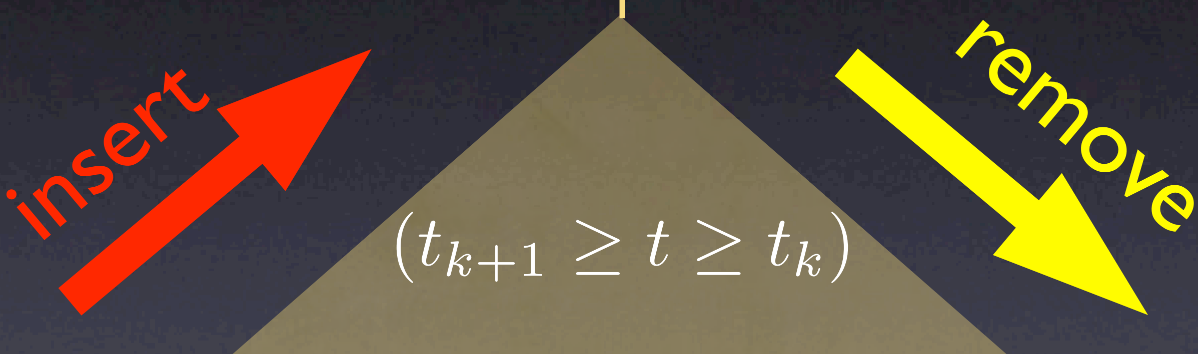
(1) Update vertexes
(2) Decompose spin variables into loops
(3) Flip each loop with a probability 1/2

Detail balance condition for updating a vertex: insert and remove

Weight of a world-line configuration

$$\cdots\{-V_{b_{k+1}}(t_{k+1})dt_{k+1}\}|\psi_{k+1}\rangle\langle\psi_{k+1}|\{-V_{b_k}(t_k)dt_k\}\cdots$$



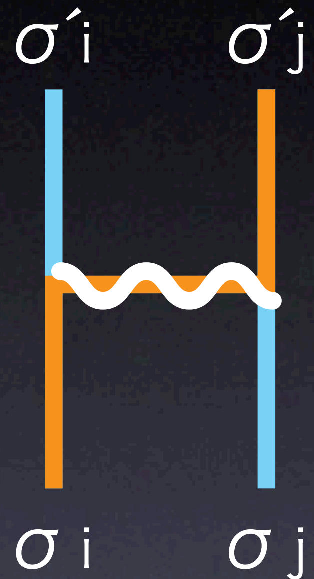


Poisson process

Always for a vertex on non-kink

$$\langle\psi_{k+1}|\{-V_b(t)\boxed{dt}\}|\psi_{k+1}\rangle$$

Delta operator



E.g. s=1/2 HAF interaction

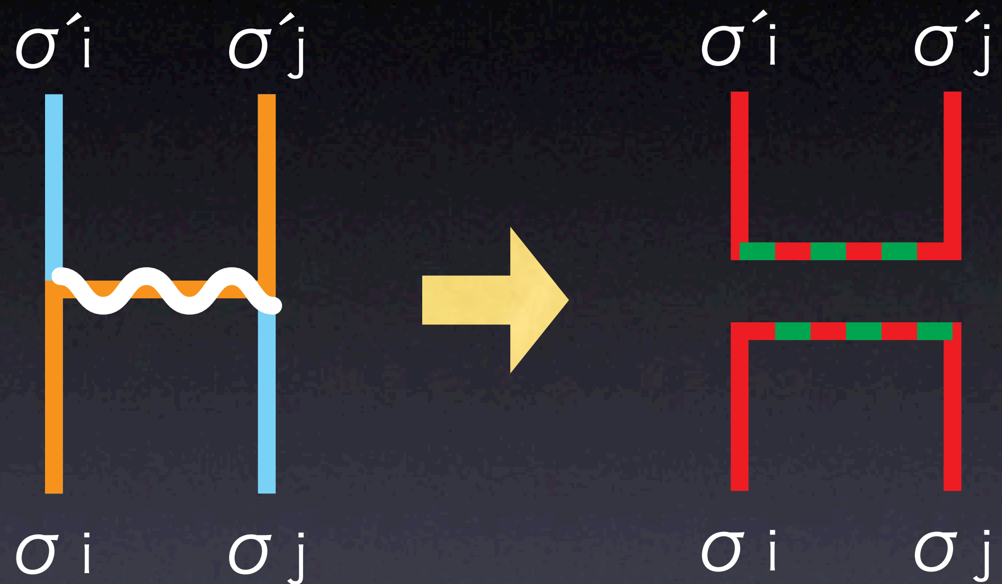
$$-\mathcal{H}_{ij}^{\mathrm{HAF}} \equiv -U^{-1}\left(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4}\right)U \qquad \left(U \equiv e^{-i\pi S_j^z}\right)$$

$$= \frac{1}{2}\hat{\Delta}(g_H)$$

$$\langle \sigma_i' \sigma_j' | \hat{\Delta}(g_H) | \sigma_i \sigma_j \rangle \equiv \begin{cases} 1 & (\text{if } \sigma_i + \sigma_j = 0 \text{ and } \sigma_i' + \sigma_j' = 0) \\ 0 & (\text{otherwise}) \end{cases}$$

$$S_i^z |\sigma_i\rangle = \sigma_i |\sigma_i\rangle \qquad \left(\sigma_i = \pm\frac{1}{2}\right)$$

Graph of delta operator

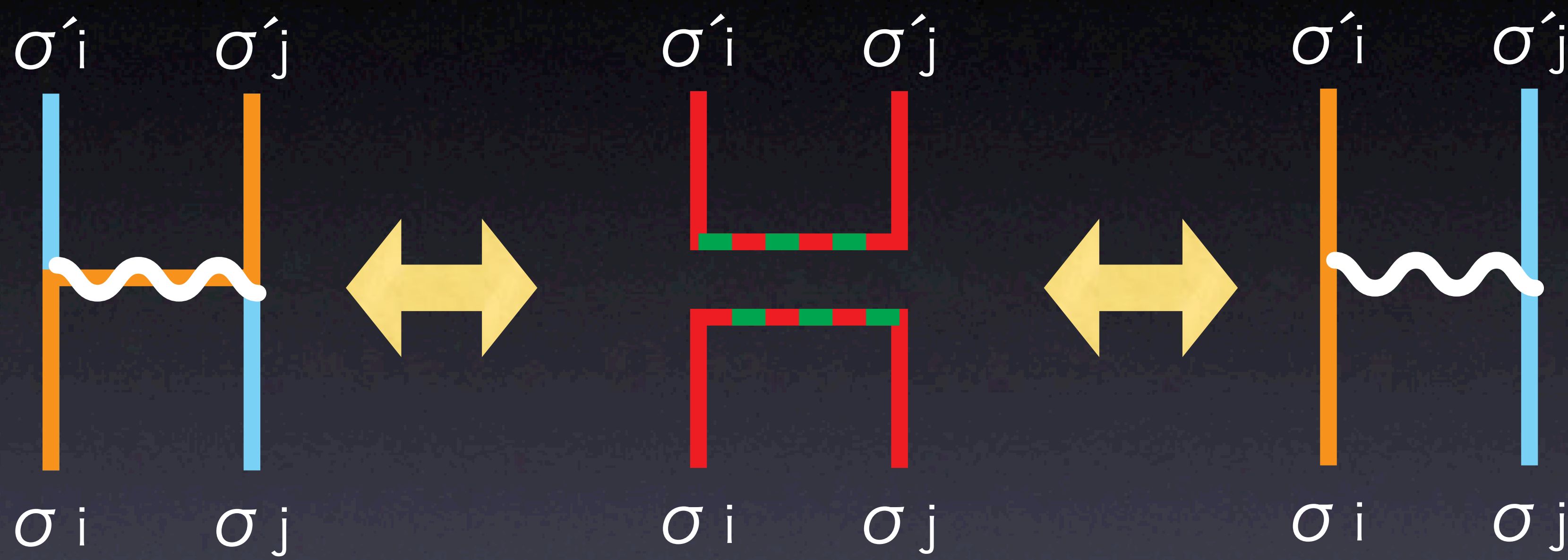


E.g.
Horizontal graph

$$\langle \sigma_i' \sigma_j' | \hat{\Delta}(g_H) | \sigma_i \sigma_j \rangle \equiv \begin{cases} 1 & (\text{if } \sigma_i + \sigma_j = 0 \text{ and } \sigma_i' + \sigma_j' = 0) \\ 0 & (\text{otherwise}) \end{cases}$$

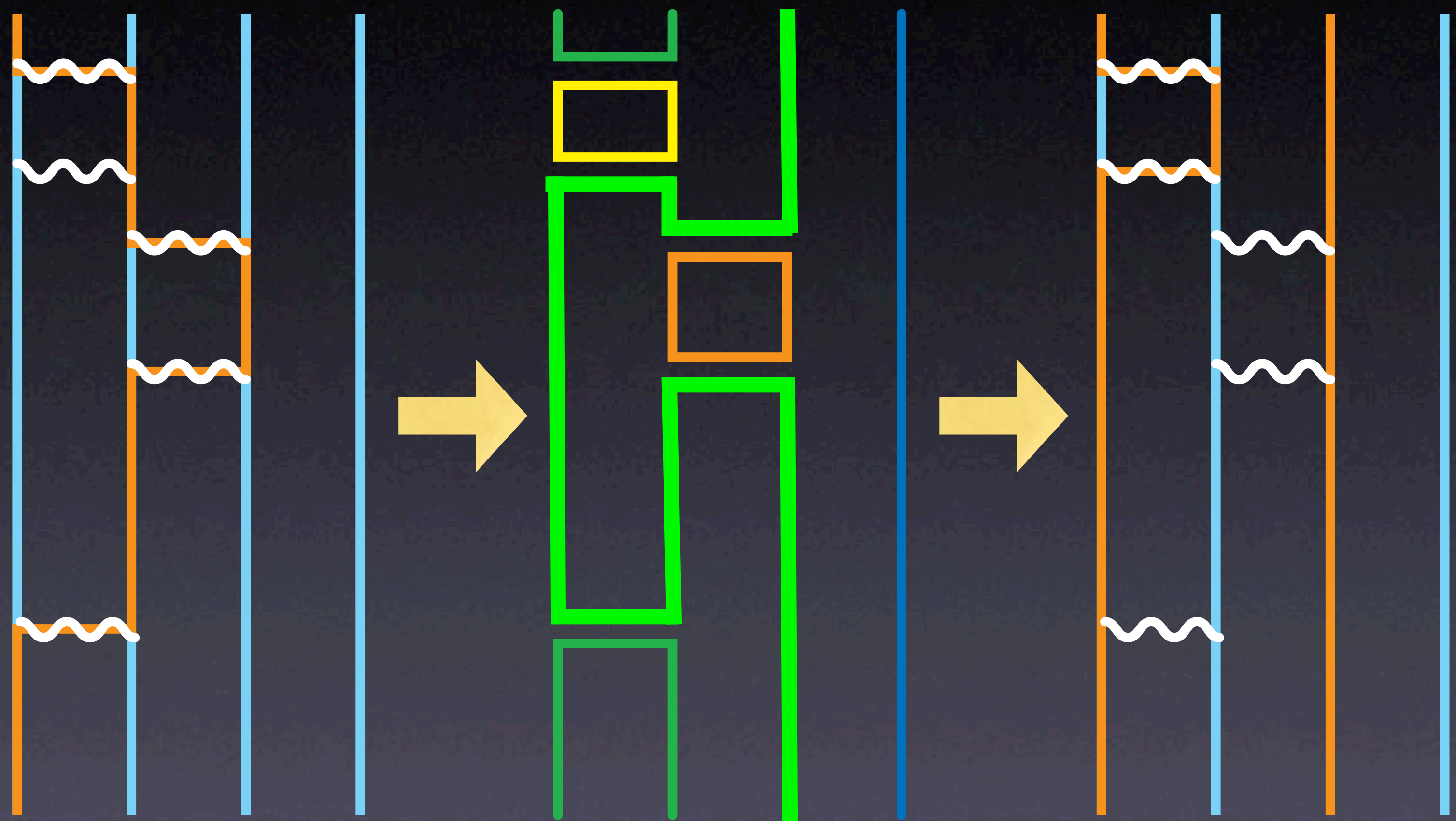
$$S_i^z |\sigma_i\rangle = \sigma_i |\sigma_i\rangle \qquad \left(\sigma_i = \pm \frac{1}{2}\right)$$

Graph of delta operator



The value of weight is not changed, as long as a modification of spin configuration matches the graph

Loop update



(i) Each vertex replaces the corresponding graph
(ii) Decompose spin variables into a set of loops
(iii) Flip each loop randomly with a probability 1/2

Loop algorithm

- Update vertexes by a Poisson process
- Update spin variables on each loop defined by graphs on vertexes, independently

➡ Very short correlation time between samples!

Applications for loop algorithm

- Quantum S>=1/2 XYZ model in magnetic field
- Hardcore and softcore boson model
- S=1 bilinear biquadratic model
- ...

Note: only not frustrated case!

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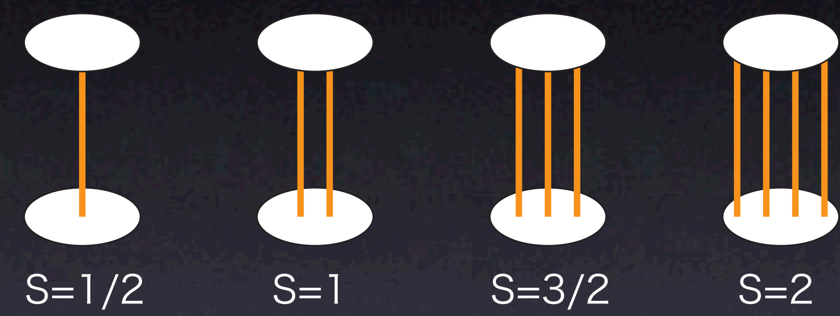
Split-spin technique for an s>1/2 case

(Kawashima & Gubernatis (1994))

S=m spin — 2m Pauli spins

$$S^{\alpha} \Rightarrow \tilde{S}^{\alpha} \equiv P^{-1}\left(\sum_{\mu} S^{\alpha}_{\mu}\right) P$$

Sum of permutations $P \equiv \sum_{\pi} P_{\pi}$



Map from an s=m spin to s=1/2 spins

⇒ Loop algorithm for s=1/2 model can be applied to s>=1/2 model

SU(N) model

SU(3) model (S=1)

$$H_{ij} = -(S_i \cdot S_j) - (S_i \cdot S_j)^2$$

$$H_{ij} = -(S_i \cdot S_j)^2$$

SU(4) model (S=3/2)

$$H_{ij} = -93(S_i \cdot S_j) + 20(S_i \cdot S_j)^2 + 16(S_i \cdot S_j)^3$$

$$H_{ij} = 81(S_i \cdot S_j) - 44(S_i \cdot S_j)^2 - 16(S_i \cdot S_j)^3$$

SU(4) model (Spin & Orbital)

$$H_{ij} = -\left(S_i \cdot S_j - \frac{1}{4}\right)\left(T_i \cdot T_j - \frac{1}{4}\right)$$

SU(N) model

$$H_{ij} = \frac{J}{N} S_{\alpha}^{\beta}(i) S_{\beta}^{\alpha}(j)$$

$$[S_{\alpha}^{\beta}(i), S_{\gamma}^{\delta}(j)] = \delta_{i,j}[\delta_{\gamma}^{\beta} S_{\alpha}^{\delta}(i) - \delta_{\alpha}^{\delta} S_{\gamma}^{\beta}(i)]$$

where $S_{\alpha}^{\beta}(i)$ are the generators of SU(N)

N.Read and S.Sachdev, Physical Review B 42, 4568 (1990)

Symmetry of a model

- S=1/2 HAF model → SU(2)

  → Graph with binary (+1/2, -1/2)

- S=1 bi-quadratic model $H_{ij} = -(S_i \cdot S_j)^2$

  → SU(3)

  → Graph with non-binary (+1, 0, -1)?

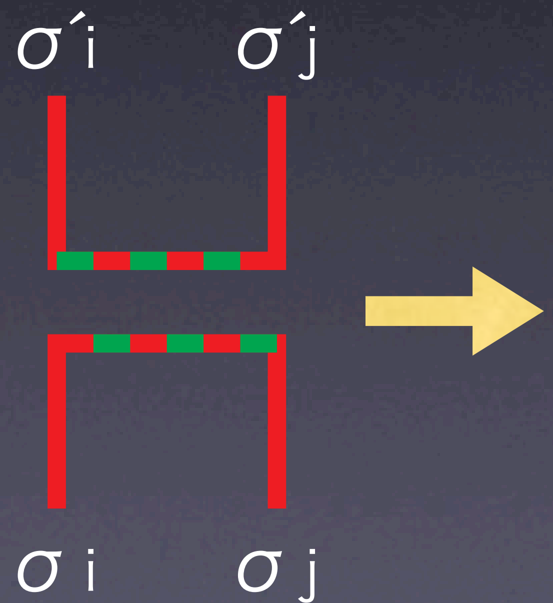
Yes

N. Kawashima & K. Harada, JPSJ 73 (2004) 1379

Graph for bi-quadratic interaction

$$(S_i \cdot S_j)^2 - I = U^t \hat{\Delta}(g_H) U \qquad \text{(S=1)}$$

$$\langle \sigma'_i \sigma'_j | \hat{\Delta}(g_H) | \sigma_i \sigma_j \rangle \equiv \begin{cases} 1 & (\text{if } \sigma_i + \sigma_j = 0 \text{ and } \sigma'_i + \sigma'_j = 0) \\ 0 & (\text{otherwise}) \end{cases}$$

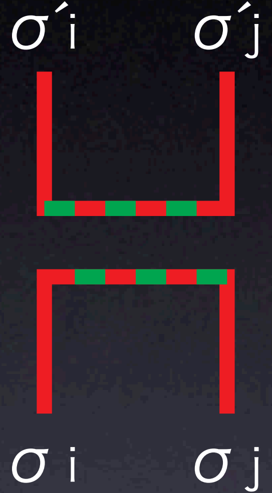


$$(\sigma_i = -1, 0, 1)$$

If the number of states is 3, then Horizontal graph has SU(3) symmetry

N. Kawashima & K. Harada, JPSJ 73 (2004) 1379

Graph for SU(N)



$$\langle \sigma'_i \sigma'_j | \hat{\Delta}(g_H) | \sigma_i \sigma_j \rangle \equiv \begin{cases} 1 & (\text{if } \sigma_i = -\sigma_j \text{ and } \sigma'_i = -\sigma'_j) \\ 0 & (\text{otherwise}) \end{cases}$$

$$(\sigma_i = (-N+1)/2, \ldots, (N-1)/2)$$

$$\langle \sigma'_i \sigma'_j | \hat{\Delta}(g_C) | \sigma_i \sigma_j \rangle \equiv \begin{cases} 1 & (\text{if } \sigma_i = \sigma'_j \text{ and } \sigma'_i = \sigma_j) \\ 0 & (\text{otherwise}) \end{cases}$$

$$(\sigma_i = (-N+1)/2, \ldots, (N-1)/2)$$

Proof of SU(N) symmetry

$$\langle z_i' z_j' | U_i^t U_j^t \hat{\Delta}(g_C) U_i U_j | z_i z_j \rangle = \sum_{\sigma_i', \sigma_j'} \sum_{\sigma_i, \sigma_j} \langle z_i' z_j' | U_i^t U_j^t | \sigma_i' \sigma_j' \rangle$$

$$\times \langle \sigma_i' \sigma_j' | \hat{\Delta}(g_C) | \sigma_i \sigma_j \rangle \langle \sigma_i \sigma_j | U_i U_j | z_i z_j \rangle$$

$$= \sum_{\sigma_i, \sigma_j} \langle z_i' z_j' | U_i^t U_j^t | \sigma_j \sigma_i \rangle \langle \sigma_i \sigma_j | U_i U_j | z_i z_j \rangle$$

$$= \sum_{\sigma_i, \sigma_j} \langle z_i' | U_i^t | \sigma_j \rangle \langle \sigma_j | U_j | z_j \rangle \langle z_j' | U_j^t | \sigma_i \rangle \langle \sigma_i | U_i | z_i \rangle$$

$$= \begin{cases} 1 & (\text{if } z_i' = z_j \text{ and } z_j' = z_i) \\ 0 & (\text{otherwise}) \end{cases}$$

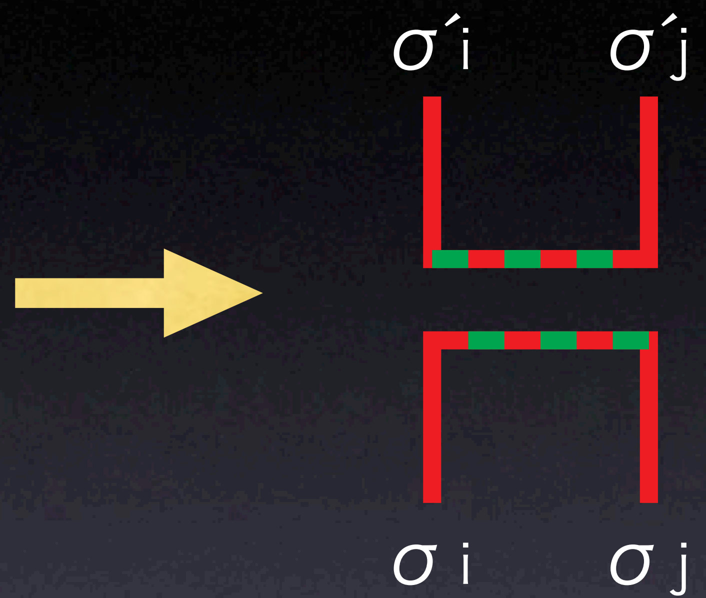
→ The cross graph operator does not change under any uniform SU(3) rotation

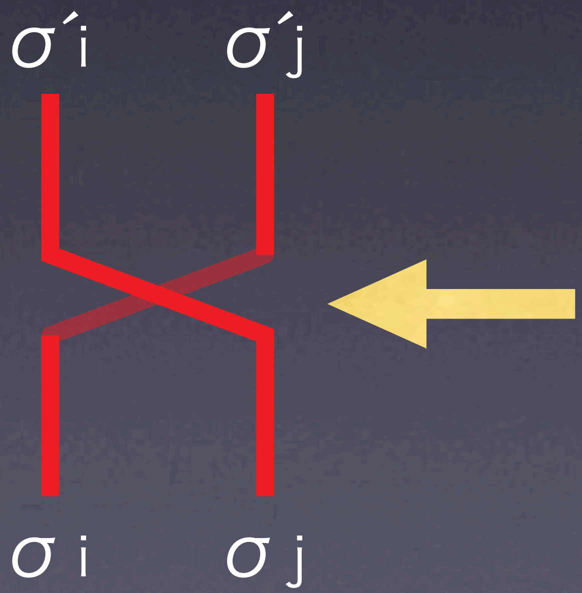
SU(N) model

$$H_{ij} = -(S_i \cdot S_j)^2$$

$$H_{ij} = 81(S_i \cdot S_j) - 44(S_i \cdot S_j)^2 - 16(S_i \cdot S_j)^3$$

$$H_{ij} = -\left(S_i \cdot S_j - \frac{1}{4}\right)\left(T_i \cdot T_j - \frac{1}{4}\right)$$





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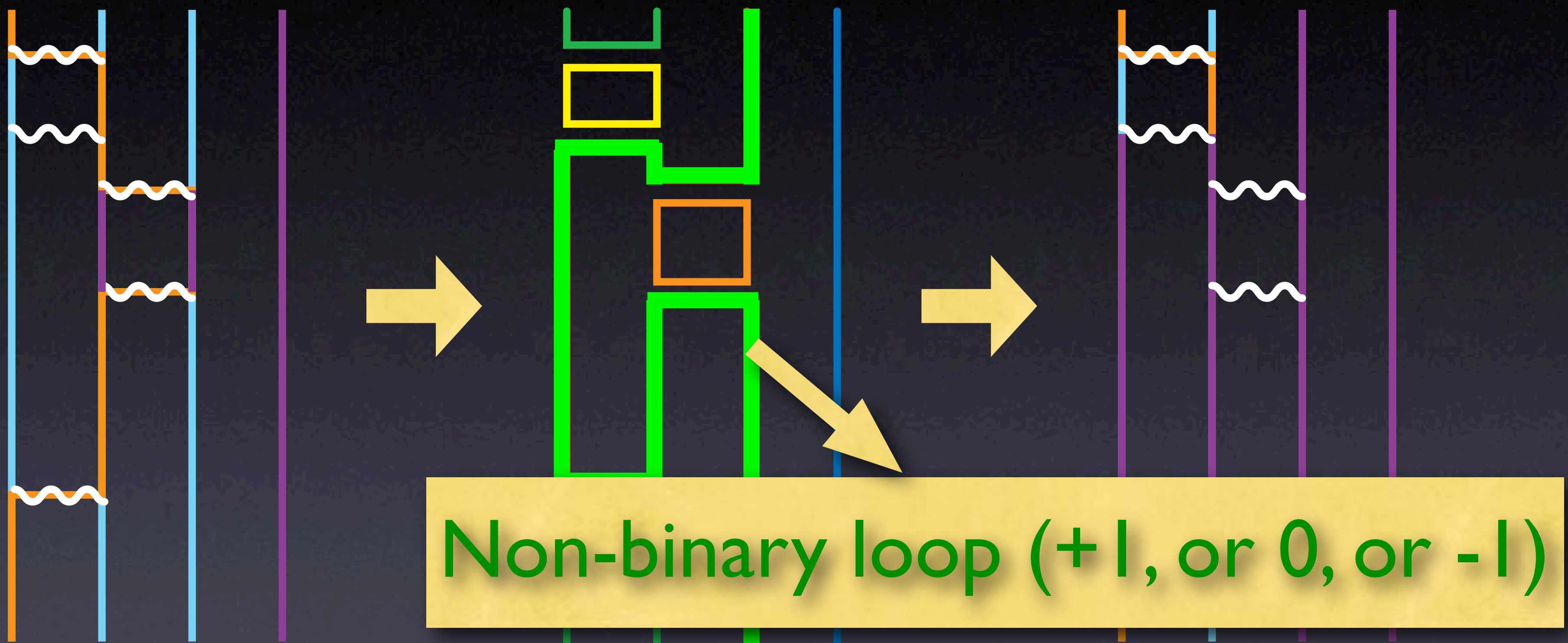
N. Kawashima & K. Harada, JPSJ 73 (2004) 1379

Non-binary loop update



(i) Each vertex replaces a corresponding graph

(ii) Decompose spin variables into a set of loops

(iii) Choose one of the N possible states
for each loop with equal probability

Applications

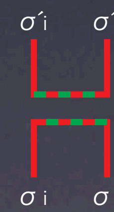
- SU(N) quantum antiferromagnets
- S=1 bi-linear bi-quadratic model

S=1 bi-linear bi-quadratic model

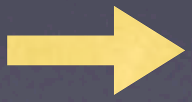
$$H_{ij} \equiv J_{ij}\left[(\cos\theta)(S_i \cdot S_j) + (\sin\theta)(S_i \cdot S_j)^2\right]$$

SU(3) points : θ/π=-3/4 and -1/2 on bipartite lattice

which correspond to 

and 

, respectively

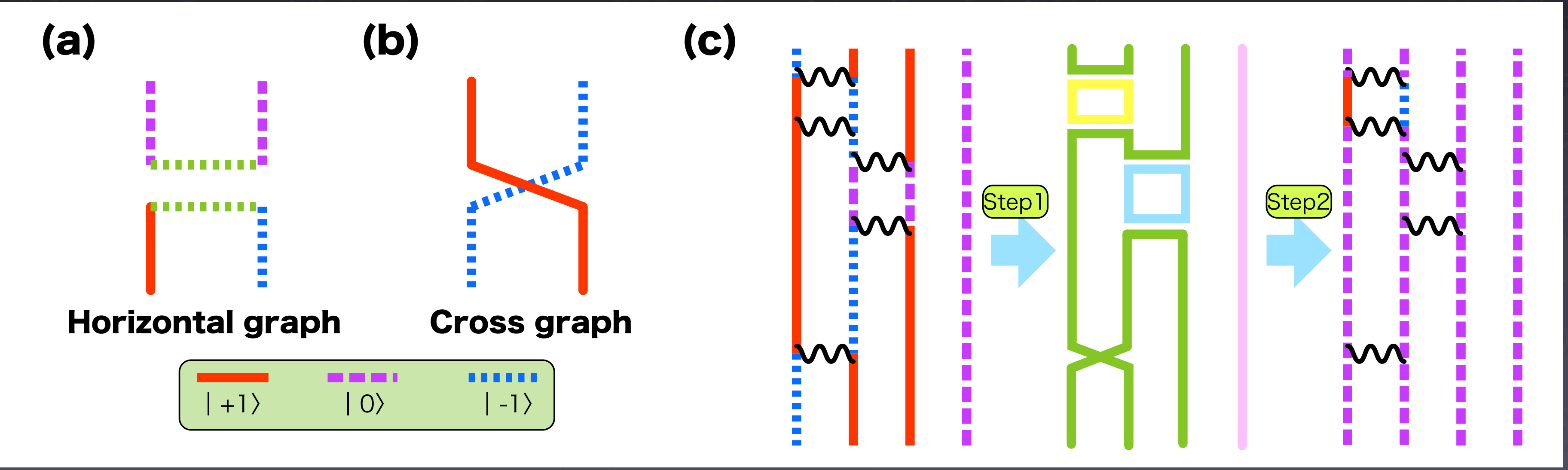


We can calculate not only at two special points, but also between these points!

Non-binary loop algorithm for $-\frac{3}{4} \leq \frac{\theta}{\pi} \leq -\frac{1}{2}$

Decomposition to graph operators

$$H_{ij} = (\cos\theta)\hat{\Delta}(g_C) + (\sin\theta - \cos\theta)\hat{\Delta}(g_H)$$

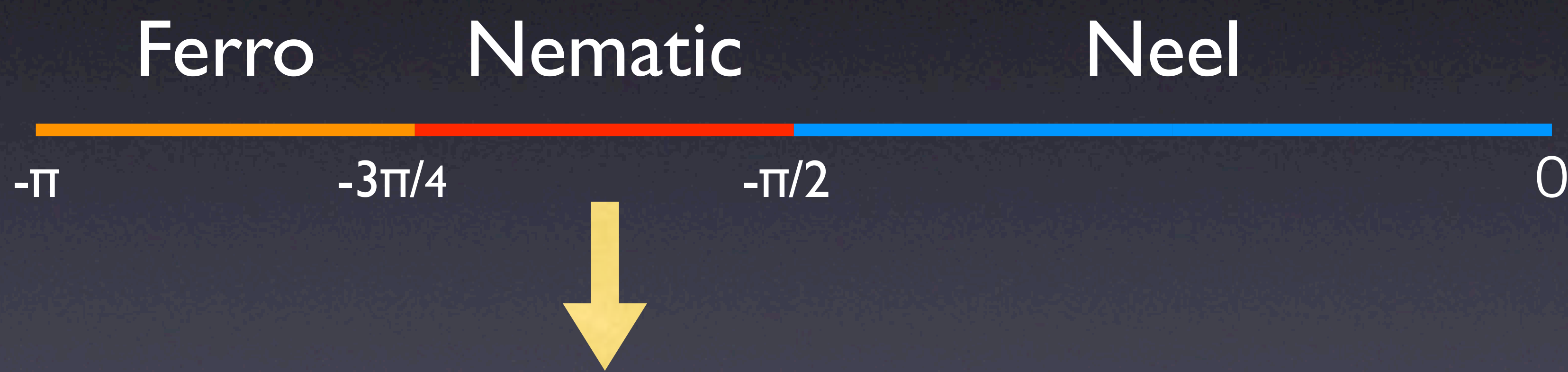


→ loop algorithm with 3-state loop

cf. loop algorithm for s=1/2 XXZ model

Ground states in higher dimensions with S=1

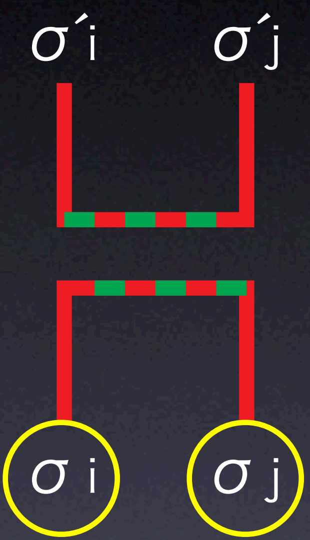
From mean-field theory



Quadrupolar order

$$Q_z \equiv \sum_i \left[(S_i^z)^2 - \frac{2}{3} \right]$$

Relation between quadrupole and loop correlations



Horizontal graph

$$Q_z(\sigma_i) = Q_z(\sigma_j)$$
$$Q_z(\sigma'_i) = Q_z(\sigma'_j)$$

Cross graph

$$Q_z(\sigma_i) = Q_z(\sigma'_j)$$
$$Q_z(\sigma'_i) = Q_z(\sigma_j)$$

$$\Rightarrow \quad \langle Q_z(\sigma) Q_z(\sigma') \rangle = \frac{4}{9} \langle \delta_{\ell(\sigma), \ell(\sigma')} \rangle$$

$\ell(\sigma)$: loop ID

Improved estimator

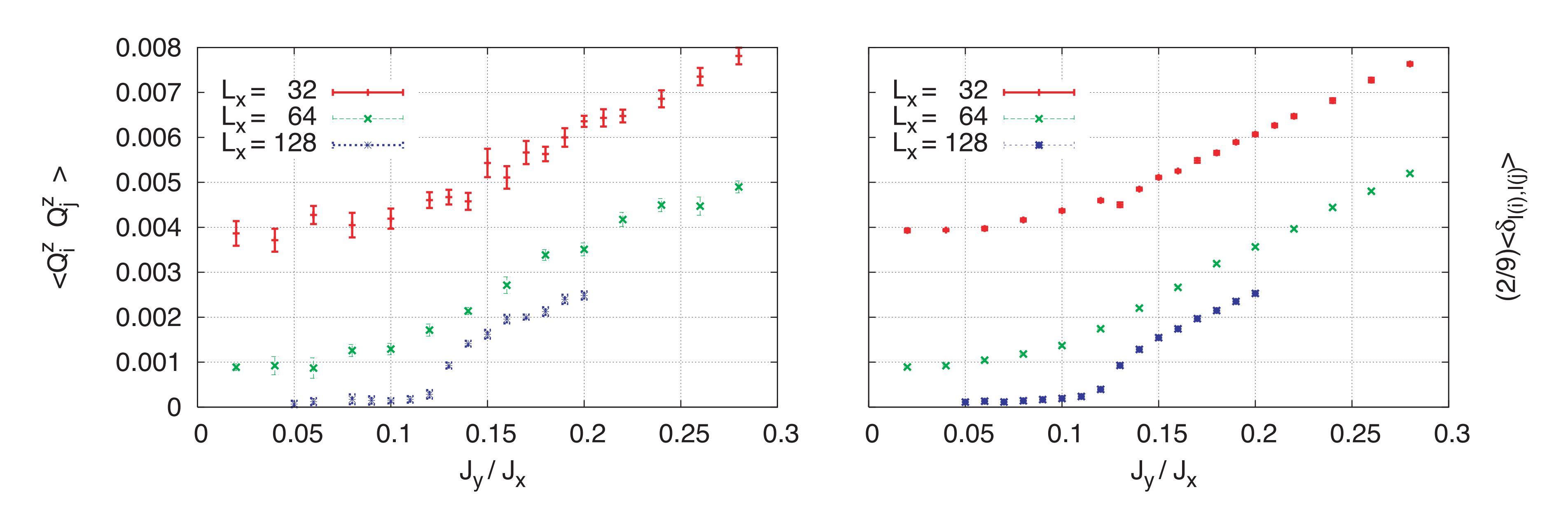


Figure: Comparison of a conventional and an improved measurement at θ=-π/2 with an aspect ratio Ly/Lx=1/4.

Efficiency of loop update

The loop correlation between two sites
is equal to the quadrupolar one

↓

Update scale equals to the one of quadrupolar order region

↓

No critical slowing down near quadrupolar transition point

Summary

I. Non-binary loop algorithm
   a. SU(N) graph with non-binary states
   b. Non-binary loop update
   c. SU(N) quantum antiferromagnetic on 2D
      i. "Emerging spatial structures in SU(N) Heisenberg model" by N. Kawashima in symposium
   d. S=1 bi-linear bi-quadratic model
      i. "Quantum Phase Transition between Two Ordered Phases with Unrelated Symmetries" by KH in symposium