Quantum Monte Calro Algorithms Based on World-Lines

Naoki Kawashima (ISSP)

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Mapping D-dimensional quantum system to (D+1)-dimensional classical system

$$H = \sum_b H_b \quad \left(b \equiv (ij) \ldots \text{"bond"}\right)$$

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \sum_{\psi_1} \left\langle \psi_1 \middle| e^{-\beta H} \middle| \psi_1 \right\rangle$$

$$= \sum_{\{\psi^k\}} \left\langle \psi^1 \middle| e^{-\Delta\tau H} \middle| \psi^L \right\rangle \left\langle \psi^L \middle| e^{-\Delta\tau H} \middle| \psi^{L-1} \right\rangle \cdots \left\langle \psi^2 \middle| e^{-\Delta\tau H} \middle| \psi^1 \right\rangle \quad \left(\Delta\tau \equiv \frac{\beta}{L}\right)$$

$$= \sum_{\{\psi^k\}} \prod_{k=1}^{L} \left\langle \psi^{k+1} \middle| e^{-\Delta\tau H} \middle| \psi^k \right\rangle$$

Factorizing by time

$$= \sum_{\{\psi^k\}} \prod_{k=1}^{L} \prod_b \left\langle \psi_b^{k+1} \middle| e^{-\Delta\tau H_b} \middle| \psi_b^k \right\rangle$$

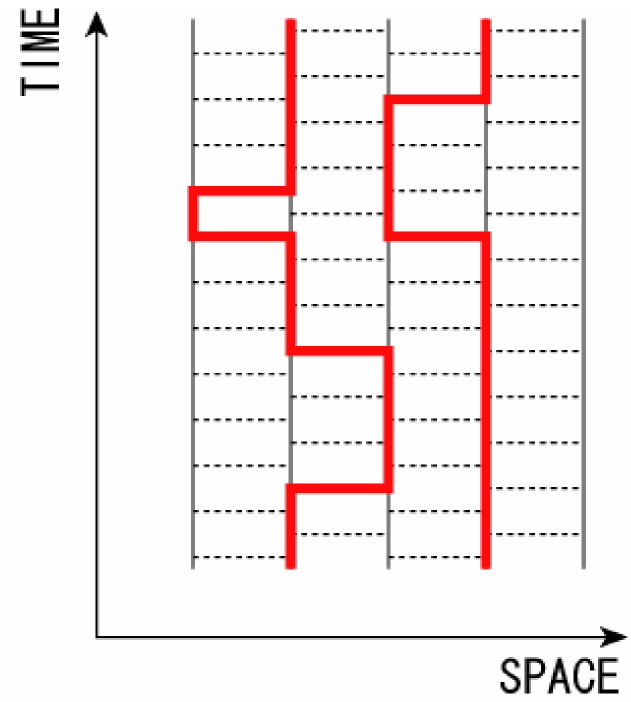
Factorizing by space

$$= \sum_S \prod_u w_u(S_u) \quad \left(S = \{\psi^k\},\ \ u = (i, j, k),\ \ S_u = \left(\psi_{ij}^{\mathrm{k+1}}, \psi_{ij}^{\mathrm{k}}\right)\right)$$

global state (worldline config.) local unit local state

Monte Carlo sampling of world-lines

Suzuki 1976



local interaction "u"

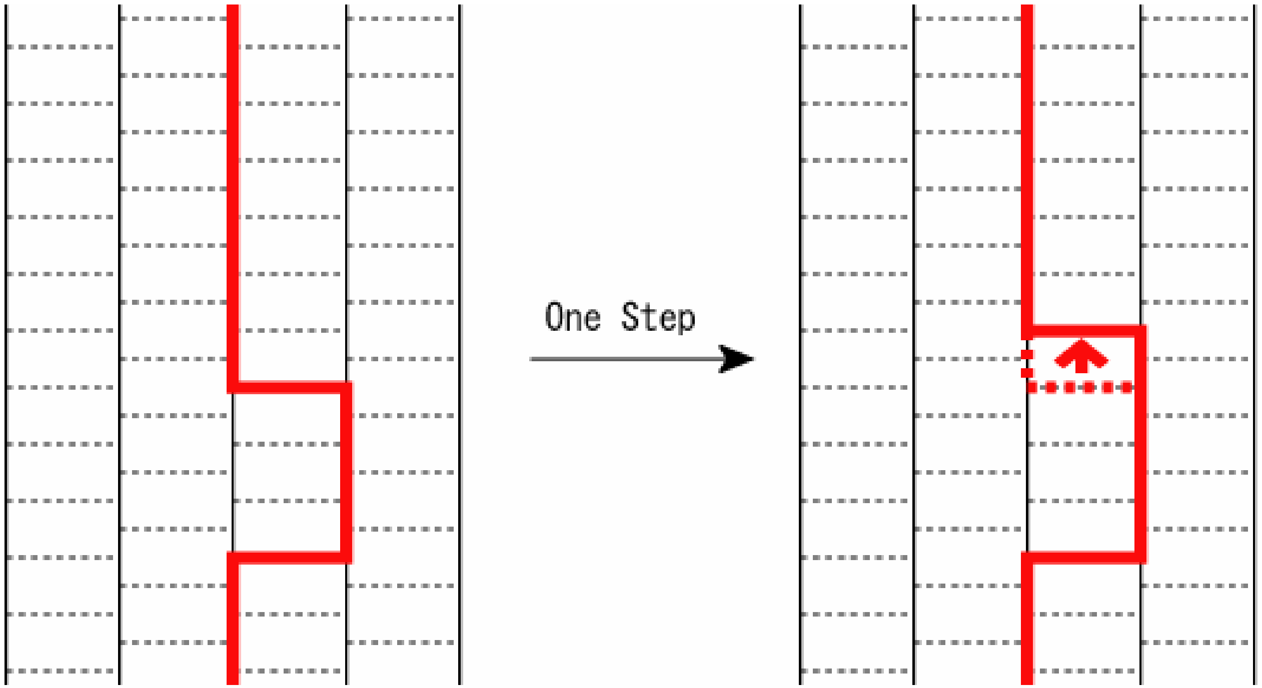
world-line

$$Z = \sum_S W(S)$$

$$\left(W(S) \equiv \prod_u w_u(S_u) \right)$$

S : world-line configuration

The method used before 1993



A lot of problems

Problems with the old method

1. critical slowing-down
2. systematic error due to time-discretization
3. slowing-down due to time-discretization
4. off-diagonal Green's function
5. grand canonical average
6. artificial conservation (winding number, etc)
7. negative sign problem

Fortuin-Kasteleyn Formulation

$$Z = \sum_S W(S) \qquad \left(W(S) \equiv \prod_{(ij)} w_{ij}(S_i, S_j) \right)$$

$$w_{ij}(S_i, S_j) = \begin{cases} e^K & (\text{if } S_i = S_j) \\ e^{-K} & (\text{if } S_i \neq S_j) \end{cases}$$

$$= e^{-K}\,\Delta(0; S_i, S_j) + \left(e^K - e^{-K}\right)\Delta(1; S_i, S_j)$$

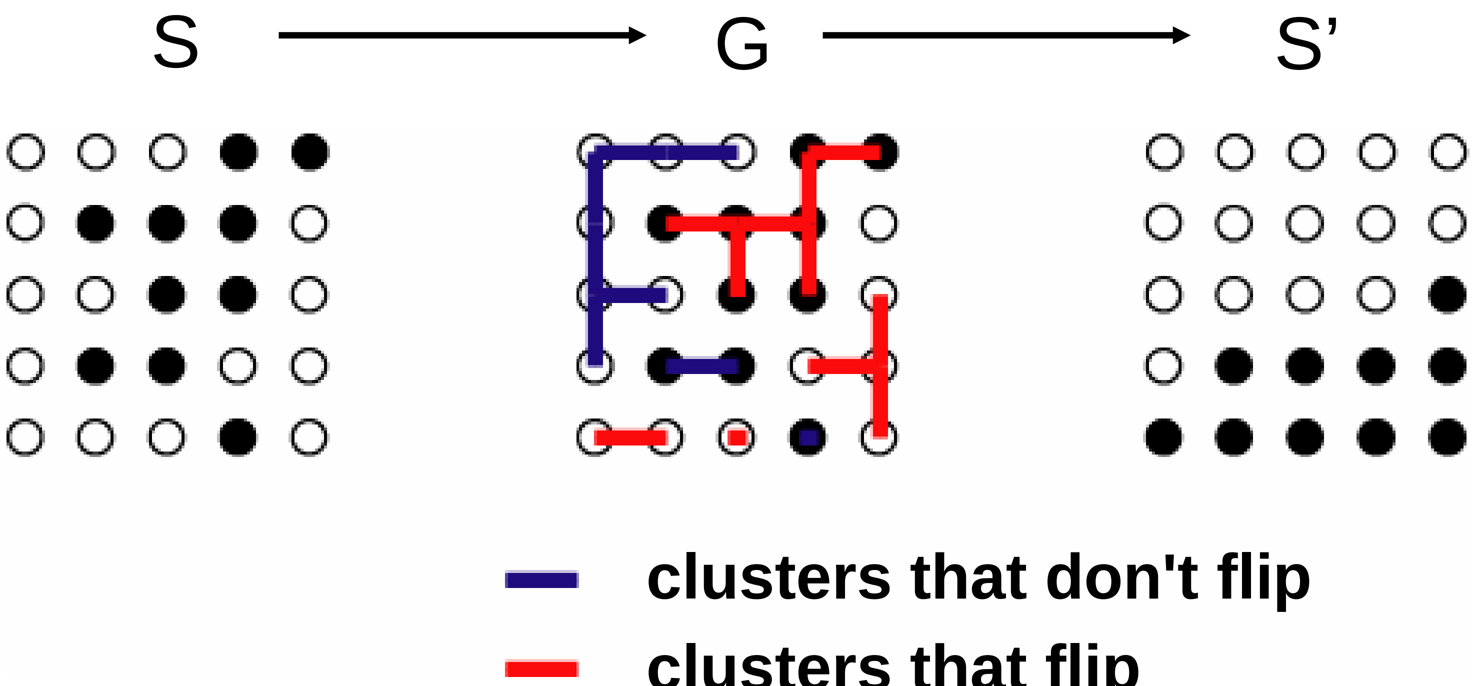
$$= \sum_{G_{ij}=0,1} v(G_{ij})\,\Delta(G_{ij}\,; S_i, S_j)$$

Introducing "auxiliary field" G_b

$$\longrightarrow \qquad Z = \sum_S W(S) = \sum_{S,G} W(S,G)$$

Swendsen-Wang Algorithm

Swendsen-Wang 1987



$$\mathrm{Prob}(S \to G) = \frac{W(S,G)}{\sum_{G} W(S,G)}, \quad \mathrm{Prob}(G \to S) = \frac{W(S,G)}{\sum_{S} W(S,G)}$$

Updating by Loops

Generalization of FK Formulation

$$H = \sum_b H_b$$

e.g. $H_{XY} = \sum_{b=(ij\alpha)} H_b$

$$H_{ij0} = \frac{J}{2}\left(-S_i^x S_j^x - S_i^y S_j^y + S_i^z S_j^z\right), \quad H_{ij1} = \frac{J}{2}\left(-S_i^x S_j^x - S_i^y S_j^y - S_i^z S_j^z\right)$$

$$Z = \sum_{\{\psi^k\}} \prod_{k=1}^{L} \prod_b \left\langle \psi_b^{k+1} \right| e^{-\Delta\tau H_b} \left| \psi_b^k \right\rangle$$

$$\approx \sum_{\{\psi^k\}} \prod_{k=1}^{L} \prod_b \left\langle \psi_b^{k+1} \right| 1 - \Delta\tau H_b \left| \psi_b^k \right\rangle$$

linear approximation

$$= \sum_{\{\psi^k\}} \prod_{k=1}^{L} \prod_b \sum_{G_b=0,1} \left\langle \psi_b^{k+1} \right| \left(-\Delta\tau H_b\right)^{G_b} \left| \psi_b^k \right\rangle$$

"auxiliary field" G_b introduced

$$= \sum_{S=\{\psi^k\}} \sum_{G=\{G_b\}} \prod_{u=(k,b)} w(S_u, G_u)$$

$$\longrightarrow \quad Z = \sum_S W(S) = \sum_{S,G} W(S,G)$$

Series Expansion Formulation

$$Z = \mathrm{Tr}\left(\sum_{n=0}^{\infty}\frac{\beta^n}{n!}(-H)^n\right) \approx \mathrm{Tr}\left(\sum_{n=0}^{L}\frac{\beta^n}{n!}(-H)^n\right) + O\left(e^{-aL/\beta V}\right)$$

cut-off L

$$= \mathrm{Tr}\left(\sum_{n=0}^{L}\frac{\beta^n}{n!}\frac{1}{{}_L C_n}\times\sum_{\substack{\{G_k=0,1\}\\ \left(\sum G_k=n\right)}}\prod_{k=1}^{L}(-H)^{G_k}\right) + O\left(e^{-aL/\beta V}\right)$$

Introducing L "boxes" and filling variable G_k=0,1

$$= \sum_G \beta^{n(G)}\frac{(L-n(G))!}{L!}\,\mathrm{Tr}\left(\prod_{k=1}^{L}(-H)^{G_k}\right) + O\left(e^{-aL/\beta V}\right)$$

G={G_k}...graph

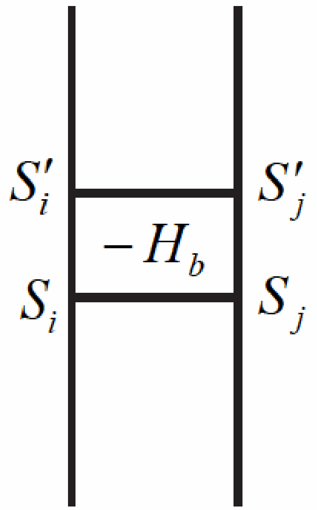
$$= \sum_{S,G}\left(\frac{\beta}{L}\right)^{n(G)}\prod_u\left\langle \psi_b^{k+1}\right|(-H_b)^{G_k}\left|\psi_b^k\right\rangle + O\left(L^{-c}\right)$$

Tr is replaced by a sum over "world-line" configurations

$$= \sum_{S=\{\psi^k\}}\sum_{G=\{G_b\}}\prod_{u=(k,b)} w(S_u,G_u) + O\left(L^{-c}\right)$$

arrived at the same expression!

The Simplest Example



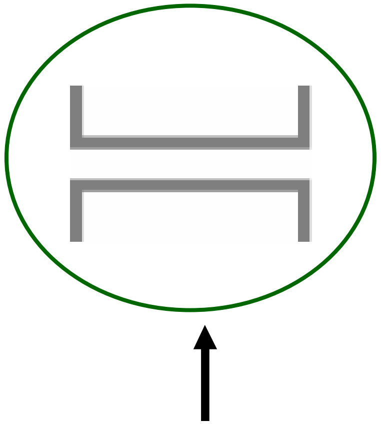
S=1/2 Antiferromagnetic Heisenberg Model

$$-H_b = \begin{pmatrix} 0 & & & \\ & 1/2 & 1/2 & \\ & 1/2 & 1/2 & \\ & & & 0 \end{pmatrix} = \delta_{S'_i,-S'_j}\delta_{S_i,-S_j} = \Delta\left(\quad \right)$$

Loop Algorithm

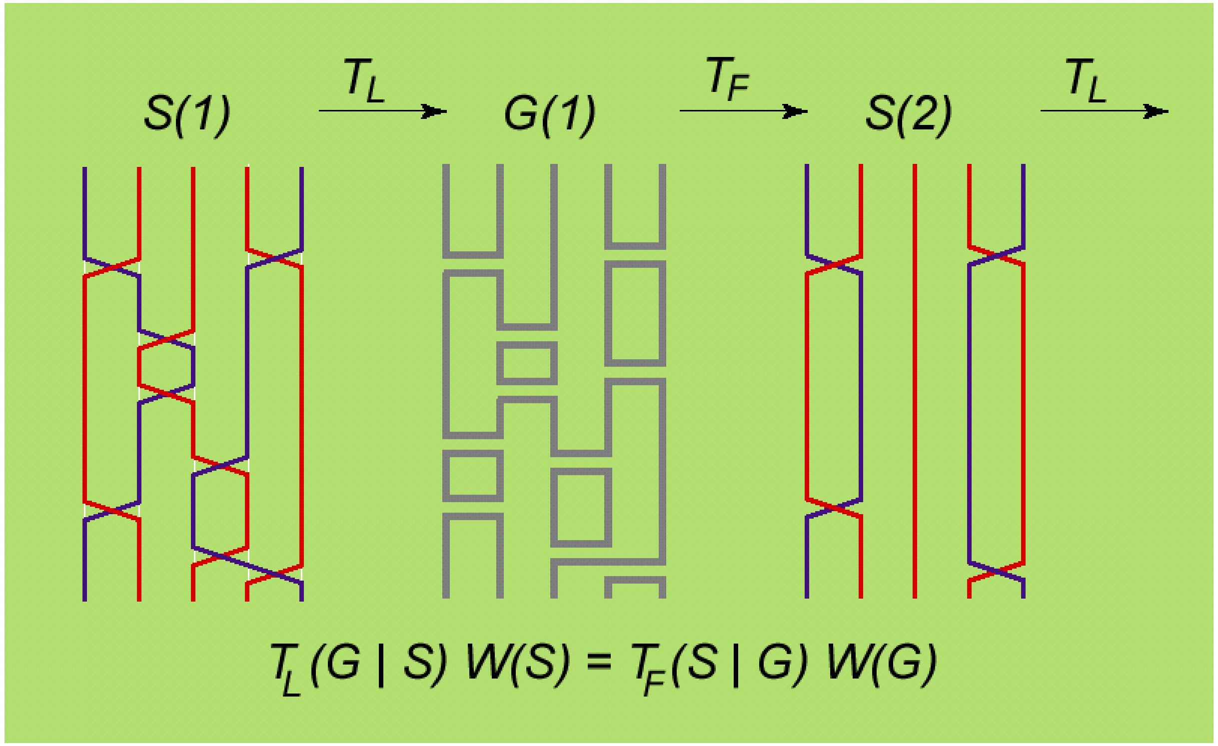
Evertz-Lana-Marcu 1993

Cluster algorithm with path-integral representation



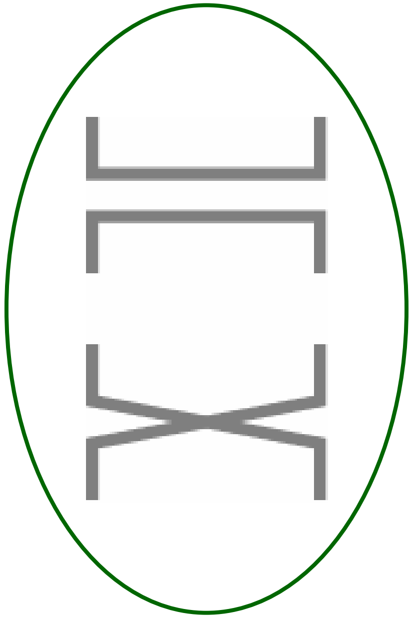
A graph element

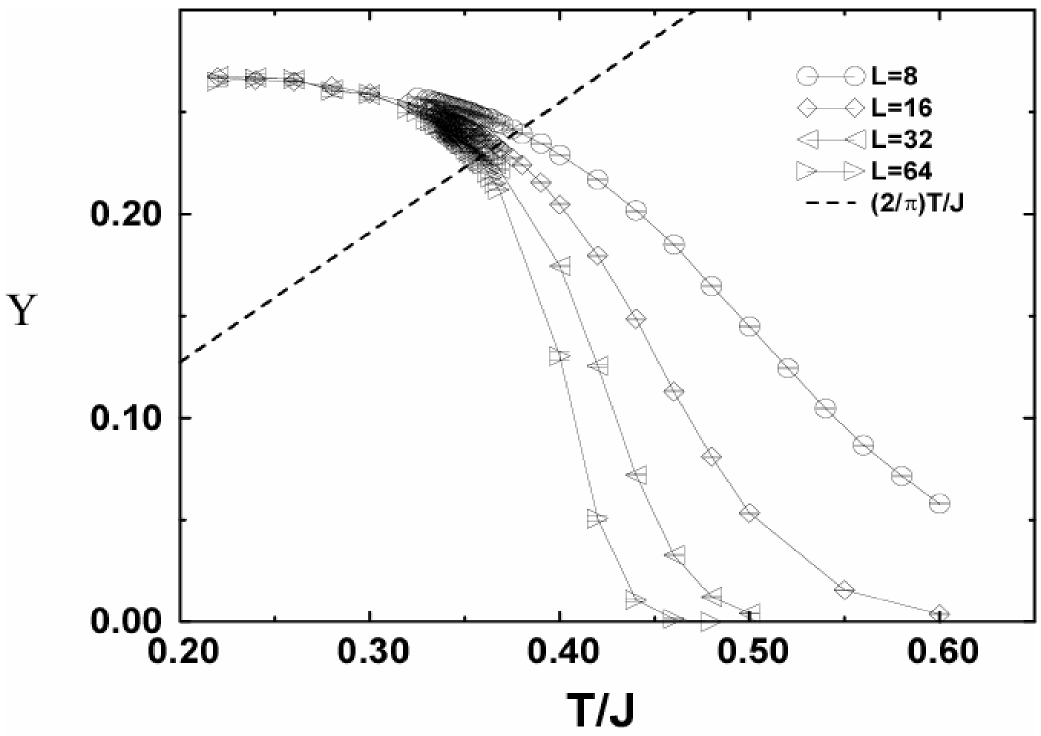
(The building block of graphs)



S＝1／2 XY model

Harada-Kawashima 1998





Tc = 0.34271(5)J

S＞1／2 problems in 1D

S-dependence of 1D antiferromagnetic Heisenberg model

S.Todo and K.Kato 2001

S	L	T	MCS	E/L	χ_s	ξ_x	Δ
1	128	0.0156250	2×10^7	-1.401481(4)	18.4048(7)	6.0153(3)	0.41048(6)
2	724	0.0055249	2×10^6	-4.761249(6)	1164.0(2)	49.49(1)	0.08917(4)
3	5792	0.0010359	3×10^4	-10.1239(1)	158000(310)	637(1)	0.01002(3)

SU(N) model

A general extension of the S＝1／2 Heisenberg model

$$H = \frac{J}{N} \sum_{(r,r')} J^{\alpha}_{\beta}(r)\, J^{\beta}_{\alpha}(r')$$

$$\left[J^{\alpha}_{\beta} \,,\, J^{\gamma}_{\delta} \right] = \delta^{\alpha}_{\delta} J^{\gamma}_{\beta} - \delta^{\gamma}_{\beta} J^{\alpha}_{\delta} \qquad \alpha, \beta, \gamma, \delta = 1, 2, \cdots, N$$

（Fundamental repl. for A sublattice and its conjugate for B sublattice） $\longrightarrow$ **N dimensions for each site**

non-binary loops ... Harada (Aug. 3)

... Kawashima (Aug. 9)

Off Diagonal Green's Function

Brower, Chandrasekharan and Wiese 1998

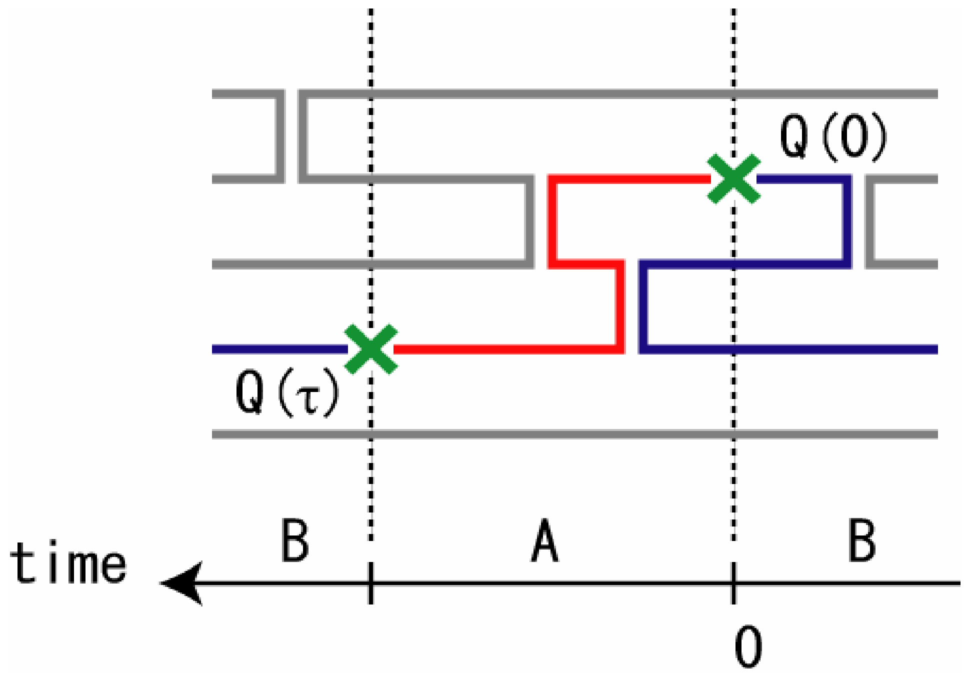
$$\mathrm{Tr}\left(e^{-\beta H} Q'(\tau) Q(0)\right)$$

$$= \sum_{S} \sum_{G} V(G) \Delta(S_B, G_B) Q'(S_B, S_A) \Delta(S_A, G_A) Q(S_A, S_B)$$

$$= \sum_{G} V(G) \chi_{Q'Q}(G)$$

$$\downarrow$$

$$\langle Q'(\tau) Q(0) \rangle = \langle \chi_{Q'Q} \rangle_g$$



Meron Algorithm

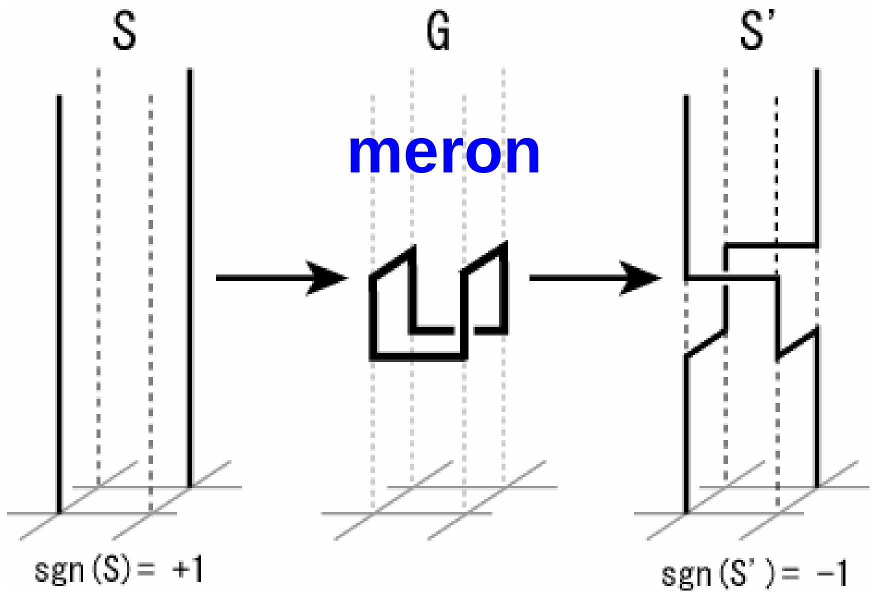
Chandrasekharan and Wiese 1999

$$Z = \sum_S \left[\mathrm{sgn}(S) \times W(S)\right]$$

$$= \sum_S \sum_G \left[\mathrm{sgn}(S) \times V(G) \times \Delta(S,G)\right]$$

$$= \sum_G \left[V(G) \sum_{\{\sigma_l\}} \prod_{l:\text{meron}} (-1)^{\sigma_l} \right]$$

$$= \sum_{G:\text{no meron}} V(G)$$



The condition for the meron algorithm to work:

1）The global sign can be factorized into local signs.

2）Graphs with meron has no contribution to Z.

3）Graphs with no meron has positive contributions to Z.

Negative sign problem for spinless fermion can be removed.

Updating by Worms

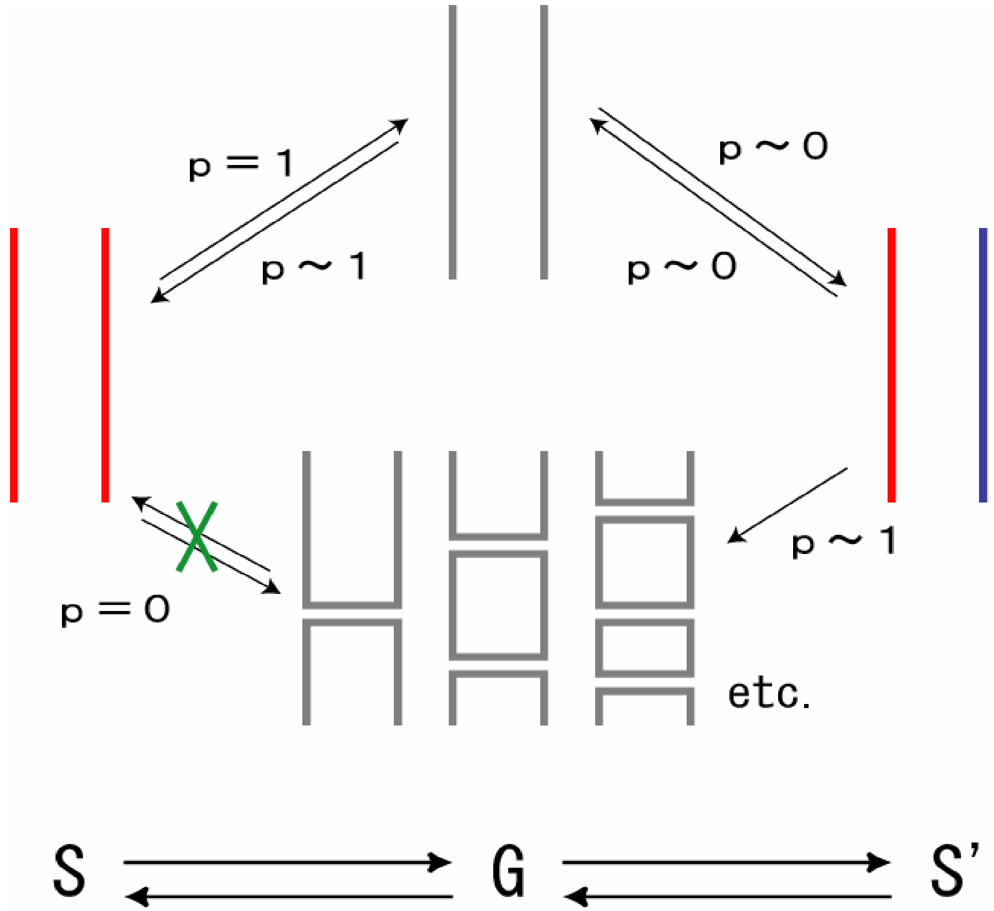
Problem with Loop Algorithm

— Magnetic field that competes against exchange interaction —

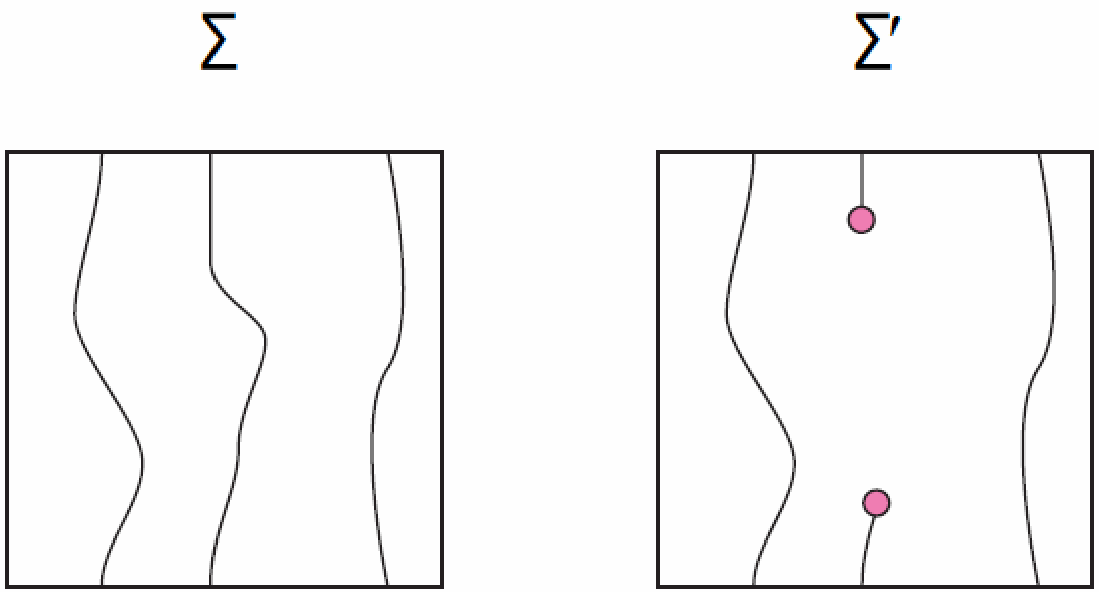
$$H = J\,\mathbf{S}_i \cdot \mathbf{S}_j - B\left(S_i^z + S_j^z\right)$$

A bottle neck appears in the phase space

Effect of magnetic field is not taken into account in graph construction



Introducing Discontinuities to Worldlines



"Worm algorithm" = "A Markov process in Σ' "

Weight: $$W(S)=\left[\prod_u w(S_u')\right]\times w_{head}(S_{head})\times w_{tail}(S_{tail})$$

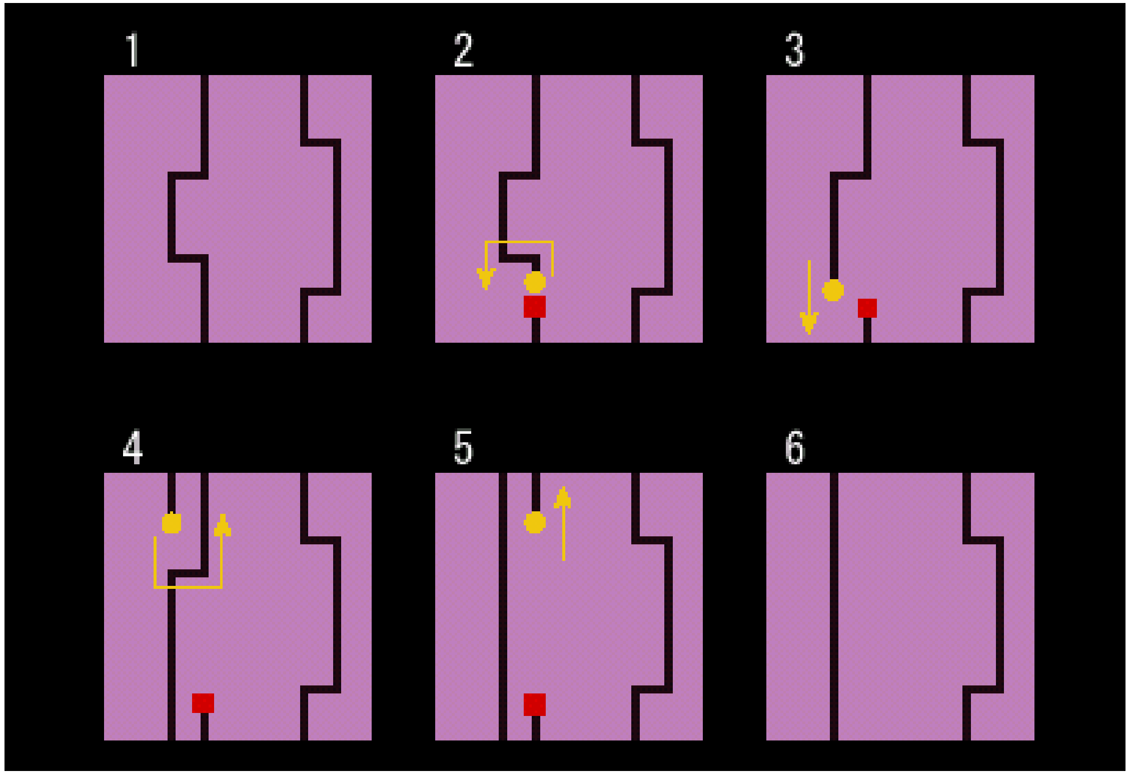
$$e.g.,\ \ w_{head}(S_{head})=\left\langle \psi' \middle| S^+ + S^- \middle| \psi \right\rangle$$

Updating with Worms

Prokofiev-Svistunov-Tupitsyn 1996

See Prokof'ev (Aug. 8)

[Worm] = [Discontinuity point on world lines]



The worm *feels* its environment while moving around.

Syljuasen-Sandvik Framework

Syljuasen-Sandvik 2002 **See Sandvik (Tomorrow!)**

Vertices (=graph elements) are placed before world-line configuration is altered like the loop algorithm.

World-line configuration is updated by worms, but the worm head can hop to the neighboring site only at a vertex.

Worm update reduces to the single-spin update for Ising-like XXZ model

If applied to the Ising model, the worm head cannot hop to the neighboring site. It just goes up and down along the same vertical line. Therefore, the best it can do in a single cycle is just flipping a single spin.

On the other hand, when the loop algorithm is applied to the Ising model, it reduces to the Swendsen-Wang algorithm, which is nice. But it cannot be generalized to the systems with frustrations.

Loop vs. Worm

GOODS and BADS

- LOOP
  - The size of clusters is just right
  - Critical slowing-down is reduced
  - Cannot handle the field competing with exchange interactions

- WORM
  - Robust (Competing fields are OK)
  - Reduces to local update in some cases

Improvements Achieved Since 1993

- No need for time-discretization
- Critical slowing-down is reduced
- Grand canonical averages and winding number fluctuation can be computed
- Some off-diagonal Green's functions can be computed
- Solvable negative-sign problem was found
- General algorithm applicable to a broad class of quantum system has been developed.
- Bose systems can be handled
- Can be fit in the extended ensemble method

Future Problems

- Crystalline field (tetragonal, cubic, etc)
- Generalization of worm update to cover the Ising like XXZ model
- Negative sign problem

  (Does the general solution exist?)
- Frustration with no negative signs

  --- Extended ensemble methods

Extended Ensemble Method

There are cases, such as the frustrated Ising like XXZ model,
in which the worm update reduces to the single-spin update.
In order to overcome the critical slowing-down, therefore,
we need to use some other techniques.

... Extended ensemble methods are promising candidates.

- ◇ Multi canonical ensemble method (Berg & Neuhaus (1991))
- ◇ Broad histogram method (Oliveira et al (1996))
- ◇ Replica exchange method (Hukushima & Nemoto (1996))
- ◇ Simulated tempering (Marinari & Parisi (1992))
- ◇ Wang-Landau method (F. Wang & Landau (2001))

etc.

There are many possible implementations.