Quantum Monte Carlo Algorithms Based on World-Lines

Naoki Kawashima (ISSP)

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

\[ H = \sum_{b} H_b \quad (b \equiv (ij) \ldots "\text{bond}"
\]

\[ Z = \text{Tr}(e^{-\beta H}) = \sum_{\psi_1} \langle \psi_1 | e^{-\beta H} | \psi_1 \rangle
\]

\[ = \sum_{\psi^k} \left( \sum_{\psi^{k+1}} \langle \psi^1 | e^{-\Delta \tau H} | \psi^L \rangle \cdot \langle \psi^L | e^{-\Delta \tau H} | \psi^{L-1} \rangle \cdot \ldots \cdot \langle \psi^2 | e^{-\Delta \tau H} | \psi^1 \rangle \right) \left( \Delta \tau = \frac{\beta}{L} \right)
\]

\[ = \sum_{\psi^k} \prod_{k=1}^{L} \langle \psi^{k+1} | e^{-\Delta \tau H_b} | \psi^k \rangle \]

Factorizing by time

Factorizing by space

\[ = \sum_{S} \prod_{u} w_u (S_u) \quad (S = \{\psi^k\}, \quad u = (i, j, k), \quad S_u = (\psi^k_{ij}, \psi^k_{ij}))
\]

global state (worldline config.)

local unit

local state
Monte Carlo sampling of world-lines

\[ Z = \sum_{S} W(S) \]

\[
W(S) = \prod_{u} w_u(S_u)
\]

\( S \) : world-line configuration

Suzuki 1976

local interaction "u"
world-line
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

\[ Z = \sum_{S} W(S) \quad \left( W(S) \equiv \prod_{(ij)} w_{ij}(S_i, S_j) \right) \]

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

\[ = e^{-K} \Delta(0; S_i, S_j) + (e^K - e^{-K}) \Delta(1; S_i, S_j) \]

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

Introducing "auxiliary field" \( G_b \)

\[ Z = \sum_{S} W(S) = \sum_{S,G} W(S, G) \]
Swendsen-Wang Algorithm

Swendsen-Wang 1987

\[ \text{clusters that don't flip} \]
\[ \text{clusters that flip} \]

\[ \text{Prob}(S \rightarrow G) = \frac{W(S, G)}{\sum_{G} W(S, G)}, \quad \text{Prob}(G \rightarrow S) = \frac{W(S, G)}{\sum_{S} W(S, G)} \]
Updating by Loops
Generalization of FK Formulation

\[ H = \sum_{b} H_{b} \]

\[ e.g. \quad H_{xy} = \sum_{b=(xy)} H_{b} \]

\[ H_{ij0} = \frac{J}{2} \left( -S_i^z S_j^z - S_i^x S_j^y + S_i^y S_j^z \right) \]

\[ H_{ij1} = \frac{J}{2} \left( -S_i^z S_j^z - S_i^y S_j^y - S_i^x S_j^x \right) \]

\[ Z = \sum_{\{\psi^k\}_{k=1}^{L}} \prod_{b} \left\langle \psi_{b}^{k+1} \left| e^{-\Delta\tau H_{b}} \right| \psi_{b}^{k} \right\rangle \]

\[ \approx \sum_{\{\psi^k\}_{k=1}^{L}} \prod_{b} \left\langle \psi_{b}^{k+1} \left| 1 - \Delta\tau H_{b} \right| \psi_{b}^{k} \right\rangle \quad \text{linear approximation} \]

\[ = \sum_{\{\psi^k\}_{k=1}^{L}} \prod_{b} \sum_{G_{b}=0,1} \left\langle \psi_{b}^{k+1} \left| (-\Delta\tau H_{b})^{G_{b}} \right| \psi_{b}^{k} \right\rangle \quad \text{"auxiliary field" } G_{b} \text{ introduced} \]

\[ = \sum_{S=\{\psi^k\}} \sum_{G=\{G_{b}\}} \prod_{u=(k,b)} w(S_{u}, G_{u}) \]

\[ Z = \sum_{S} W(S) = \sum_{S,G} W(S,G) \]
Series Expansion Formulation

\[ Z = \text{Tr} \left( \sum_{n=0}^{\infty} \beta^n \frac{(-H)^n}{n!} \right) \approx \text{Tr} \left( \sum_{n=0}^{L} \beta^n \frac{(-H)^n}{n!} \right) + O(e^{-aL/\beta}) \quad \text{cut-off } L \]

Introducing \( L \) "boxes" and filling variable \( G \)

\[ \sum_{n=0}^{L} \frac{\beta^n}{n!} \times \prod_{k=1}^{L} (-H)^{G_k} + O(e^{-aL/\beta}) \]

\[ = \sum_{G} \beta^{n(G)} \frac{(L-n(G))!}{L!} \text{Tr} \left( \prod_{k=1}^{L} (-H)^{G_k} \right) + O(e^{-aL/\beta}) \quad G=\{G_k\}...graph \]

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

\[ = \sum_{S=\psi^k} \sum_{G=\{G_b\}} \prod_{u=(k,b)} w(S_u, G_u) + O(L^{-c}) \quad \text{arrived at the same expression!} \]
The Simplest Example

**S=1/2 Antiferromagnetic Heisenberg Model**

\[ -H_b = \begin{pmatrix} 0 & 1/2 & 1/2 \\ 1/2 & 1/2 & 0 \end{pmatrix} = \delta_{s'_i,-s'_j} \delta_{s_i,-s_j} = \Delta \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \]
Loop Algorithm

Evertz-Lana-Marcu 1993

Cluster algorithm with path-integral representation

A graph element
(The building block of graphs)

\[ T_L(G \mid S) \, \mathcal{W}(S) = T_F(S \mid G) \, \mathcal{W}(G) \]
$S = \frac{1}{2} XY$ model

Harada-Kawashima 1998

$T_c = 0.34271(5)J$
S > 1/2 problems in 1D

S-dependence of 1D antiferromagnetic Heisenberg model

S. Todo and K. Kato 2001

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<th>$S$</th>
<th>$L$</th>
<th>$T$</th>
<th>MCS</th>
<th>$E/L$</th>
<th>$\chi_S$</th>
<th>$\xi_S$</th>
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<td>158000(310)</td>
<td>637(1)</td>
<td>0.01002(3)</td>
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SU(N) model

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

\[ H = \frac{J}{N} \sum_{(r,r')} J^\alpha_\beta (r) J^\beta_\alpha (r') \]

\[ [J^\alpha_\beta , J^\gamma_\delta ] = \delta^\alpha_\delta J^\gamma_\beta - \delta^\gamma_\beta J^\alpha_\delta \quad \alpha, \beta, \gamma, \delta = 1, 2, \ldots, N \]

(Fundamental repl. for A sublattice and its conjugate for B sublattice) \rightarrow \text{N dimensions for each site}

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

... Kawashima (Aug. 9)
Off Diagonal Green's Function

Brower, Chandrasekharan and Wiese 1998

\[
\text{Tr}\left(e^{-\beta H} Q'(\tau)Q(0)\right) \\
= \sum_{S} \sum_{G} V(G) \Delta(S_B, G_B) Q'(S_B, S_A) \Delta(S_A, G_A) Q(S_A, S_B) \\
= \sum_{G} V(G) \chi_{Q'Q}(G) \\
= \langle Q'(\tau)Q(0) \rangle = \langle \chi_{Q'Q} \rangle_g
\]
Meron Algorithm

Chandrasekharan and Wiese 1999

\[ Z = \sum_S [\text{sgn}(S) \times W(S)] \]
\[ = \sum_S \sum_G [\text{sgn}(S) \times V(G) \times \Delta(S, G)] \]
\[ = \sum_G \left[ V(G) \sum_{\{\sigma_i\} l: \text{meron}} \prod (-1)^{\sigma_i} \right] \]
\[ = \sum_{G: \text{no meron}} V(G) \]

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 —

\[ H = J S_i \cdot S_j - B\left(S_i^z + S_j^z\right) \]

A bottle neck appears in the phase space

Effect of magnetic field is not taken into account in graph construction
Introducing Discontinuities to Worldlines

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

"Worm algorithm" = "A Markov process in $\Sigma'$"

e.g., \[ w_{\text{head}}(S_{\text{head}}) = \langle \psi' | S^+ + S^- | \psi \rangle \]
Updating with Worms

[Worm] = [Discontinuity point on world lines]

The worm *feels* its environment while moving around.
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))

etc.

There are many possible implementations.