WORM ALGORITHM

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Why bother with algorithms?

Efficiency
- PhD while still young
- Better accuracy
- Large system size
- More complex systems
- Finite-size scaling
- Critical phenomena
- Phase diagrams
- Reliably!

New quantities, more theoretical tools to address physics
- Grand canonical ensemble $N(\mu)$
- Off-diagonal correlations $G(r, \tau)$
- “Single-particle” and/or condensate wave functions $\varphi(r)$
- Winding numbers and $\rho_s$

Examples from: superfluid-insulator transition, spin chains, helium solid & glass, deconfined criticality, resonant fermions, holes in the t-J model, …
Consider:

- configuration space = arbitrary closed loops

- each cnf. has a weight factor $W_{cnf}$

- quantity of interest $A_{cnf} \quad \rightarrow \quad \langle A \rangle = \frac{\sum_{cnf} A_{cnf} W_{cnf}}{\sum_{cnf} W_{cnf}}$
“conventional” sampling scheme:

**local shape change**

Add/delete small loops

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No sampling of topological classes (non-ergodic)

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Critical slowing down (large loops are related to critical modes)

\[ \left( \frac{N_{\text{updates}}}{L^d} \right) \sim L^z \]

dynamical critical exponent \( z \approx 2 \) in many cases
Worm algorithm idea

- Draw and erase:

- Topological are sampled (whatever you can draw!)

- No critical slowing down in most cases

Disconnected loops are related to correlation functions and are not merely an algorithm trick!
High-T expansion for the Ising model

\[-\frac{H}{T} = K \sum_{\langle ij \rangle} \sigma_i \sigma_j \quad (\sigma = \pm 1)\]

\[Z = \sum_{\{\sigma_i\}} e^{-H_i/T} \equiv \sum_{\{\sigma_i\}} \prod_{b=\langle ij \rangle} e^{K \sigma_i \sigma_j} \equiv \sum_{\{\sigma_i\}} \prod_{b=\langle ij \rangle} \cosh K (1 + \tanh K \sigma_i \sigma_j)\]

\[\sim \sum_{\{\sigma_i\}} \prod_{b=\langle ij \rangle} \sum_{N_b=0,1} \left( \tanh K \sigma_i \sigma_j \right)^{N_b} = \sum_{\{N_b=0,1\}} \left( \prod_{b=\langle ij \rangle} \tanh^{N_b} K \right) \prod_i \left( \sum_{\sigma_i=\pm 1} \sigma_i^{M_i} \right)\]

\[\sim \sum_{\{N_b\}=\text{loops}} \left( \prod_{b=\langle ij \rangle} \tanh^{N_b} K \right)\]

Graphically:

\[M_i = \sum_{\langle ij \rangle} N_b = \text{even}\]

\[N_b = \text{number of lines; continuity (enter/exit)} \quad \rightarrow M_i = \text{even}\]
Spin-spin correlation function:

\[ g_{IM} = \frac{G_{IM}}{Z}, \quad G_{IM} = \sum_{\{\sigma_i\}} e^{-H/T} \sigma_I \sigma_M \]

\[ G \equiv \sum_{\{N_b\}} \left( \prod_{b=\langle ij \rangle} \tanh^{N_b} K \right) \prod_i \left( \sum_{\sigma_i=\pm 1} \sigma_i^{M_i+\delta_{il}+\delta_{im}} \right) \sim \sum_{\{N_b\}=\text{loops} + IM \text{ worm}} \left( \prod_{b=\langle ij \rangle} \tanh^{N_b} K \right) \]

Worm algorithm cnf. space = \( Z \quad G \)

Same as for generalized partition

\[ Z_W = Z + \kappa G \]
Complete algorithm:

- If $I = M$, select a new site for $I, M$ at random

- select direction to move $M$, let it be bond $b$

- If $N_b = \begin{cases} 0 & \text{accept} \\ 1 & \end{cases}$ $N_b \rightarrow \begin{cases} 1 & \text{with prob.} \\ 0 & \end{cases}$ $R = \begin{cases} \min(1, \tanh(K)) & \\ \min(1, \tanh^{-1}(K)) & \end{cases}$

Easier to implement then single-flip!
Correlation function: \[ g(i) = G(i) / Z \]

Magnetization fluctuations: \[ \langle M^2 \rangle = \langle \left( \sum_i \sigma_i \right)^2 \rangle = N \sum_i g(i) \]

Energy: either

\[ E = -JNd \langle \sigma_1 \sigma_2 \rangle = -JNd g(1) \]

or

\[ E = -J \tanh(K) \left[ dN + \langle N_{bonds} \rangle \sinh^2(K) \right] \]

MC estimators

\[ G(I - M) = G(I - M) + 1 \]

\[ Z = Z + \delta_{I,M} \]

\[ N_{bonds} = N_{bonds} + \left( \sum_b N_b \right) \]
Ising → lattice field theory

\[-\frac{H}{T} = t \sum_{i, \nu = \pm(x, y, z)} \psi_{i+\nu}^* \psi_i + \mu \sum_i |\psi_i|^2 - U \sum_i |\psi_i|^4\]

\[Z = \prod_i \int d\psi_i \ e^{-H/T} \quad \text{expand} \quad e^{i\psi_{i+\nu}^* \psi_i} = \sum_{N=0}^{\infty} \frac{t^N (\psi_{i+\nu}^* \psi_i)^N}{N!}\]

\[Z = \sum_{\{N_{i,\nu}\}} \left( \prod_{i, \nu} \frac{t^{N_{i,\nu}}}{N_{i,\nu}!} \right) \prod_i \left( \int d\psi_i \ \psi_i^{M_{i,i}} (\psi_i^*)^{M_{2,i}} e^{\mu |\psi_i|^2 - U |\psi_i|^4} \right) \]

\[e^{i\varphi(M_1 - M_2)} \rightarrow M_1 = M_2 = M\]

\[\prod_i Q(M_i)\]

where \(Q(M) = \begin{cases} 0 & \text{if } M_1 \neq M_2 \quad \rightarrow \quad \text{closed oriented loops} \\ \pi \int_0^\infty dx \ x^M e^{\mu x - U x^2} & \text{tabulated numbers} \end{cases} \]
\[ \psi_i \sum_v N_{i,v} (\psi_i^*) \sum_v N_{i+v,-v} \]

Flux in = Flux out \( \rightarrow \) closed oriented loops of integer N-currents

\[ g(I - M) = \frac{G(I - M)}{Z} = \left\langle \psi_i \psi_i^* \right\rangle \]

(one open loop)

Worm algorithm cnf. space = \( Z \ G \)
Same algorithm:

- \( Z \leftrightarrow G \) sectors, prob. to accept \( R_{z \rightarrow G} = \min \left[ 1, \frac{Q(M_t + 1)}{Q(M_t)} \right] \)

- \( N_{M,v} \rightarrow N_{M,v} + 1 \) draw \( R = \min \left[ 1, \frac{t Q(M_{M_t} + 1)}{(N_{M,v} + 1)Q(M_{M_t})} \right] \)

- \( N_{M^+, \neg v} \rightarrow N_{M^+, \neg v} - 1 \) erase \( R = \min \left[ 1, \frac{(N_{M^+, \neg v}) Q(M_{M_t} - 1)}{t Q(M_{M_t})} \right] \)

Keep drawing/erasing …
Multi-component gauge field-theory
(deconfined criticality, XY-VBS and Neel-VBS quantum phase transitions…)

\[-\frac{H}{T} = t \sum_{a;i\nu} \psi^*_a e^{iA_\nu(i)} + \nu \sum_{a;i} |\psi_{a,i}|^2 - \sum_{ab;i} U_{ab} |\psi_{a,i}|^2 |\psi_{b,i}|^2 - \kappa \sum [\nabla \times A_\nu(i)]^2\]

\[U_{11} = U_{22} \neq U_{12} \quad \text{XY-VBS transition} \]
no DCP, always first-order

\[U_{11} = U_{22} = U_{12} \quad \text{Neel-VBS transition, unknown!}\]
\[ H = H_0 + H_1 = \sum_{ij} U_{ij} n_i n_j - \sum_i \mu_i n_i - \sum_{<ij>} t(n_i, n_j) b_j^+ b_i \]

Lattice path-integrals for bosons and spins are "diagrams" of closed loops!

\[ Z = \text{Tr} \ e^{-\beta H} \equiv \text{Tr} \ e^{-\beta H_0} e^{-\int_0^\beta H_1(\tau) d\tau} \]

\[ = \text{Tr} \ e^{-\beta H_0} \left\{ 1 - \int_0^\beta H_1(\tau) d\tau + \int_0^\beta \int_0^\beta H_1(\tau) H_1(\tau') d\tau d\tau' + \ldots \right\} \]

\[ |n_i = 0, 1, 2, 0 \rangle \]
Diagrams for

\[ Z = \text{Tr} \ e^{-\beta H} \]

Diagrams for

\[ G_{IM} = \text{Tr} \ T_{\tau} b_M^{\dagger} (\tau_M) b_I (\tau_I) e^{-\beta H} \]

The rest is conventional worm algorithm in continuous time

(there is no problem to work with arbitrary number of continuous variables as long as an expansion is well defined)
Diagrammatic Monte Carlo (not in this lecture)

\[ A(\vec{y}) = \sum_{n=0}^{\infty} \sum_{\xi} \int \int \int d\vec{x}_1 d\vec{x}_2 \ldots d\vec{x}_n D_n(\xi; \vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n, \vec{y}) \]

Diagram order

Same-order diagrams

Integration variables

Contribution to the answer or the diagram weight (positive definite, please)
Path-integrals in continuous space are consist of closed loops too!

\[ H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V(r_i - r_j) \]

\[ Z = \int\int\int dR_1 ... dR_P \exp \left\{ -\frac{p=\beta/\tau}{\sum_{i=1}^p} \left( \frac{m(R_{i+1} - R_i)^2}{2\tau} + U(R)\tau \right) \right\} \]

\[ R_i = (r_{i,1}, r_{i,2}, \ldots, r_{i,N}) \]
diagrammatic expansion for $V(r) < 0$
Not necessarily for closed loops!

Feynman (space-time) diagrams for fermions with contact interaction (attractive)

\[ \bullet = -U \]

Pair correlation function

\[ \left\langle a_{i\uparrow}^+ (r_1, \tau_1) a_{i\downarrow}^+ (r_1, \tau_1) a_{i\downarrow} (r_2, \tau_2) a_{i\uparrow} (r_2, \tau_2) \right\rangle \]

connect vortexes with \( G_\downarrow \) and \( G_\uparrow \)

\[ D_n = (-U)^n G_\uparrow \cdots G_\uparrow G_\downarrow \cdots G_\downarrow (d^r d\tau)^n (-1)^{\text{perm}} \]

sum over all possible \( (n!)^2 \) connections

\[ \sum_\xi D_n (\xi) = (-U)^n \det^2 G_\uparrow (\vec{x}_i, \vec{x}_j) (d^r d\tau)^n \geq 0 \]
Domain walls in 2D Ising model are loops!

Disconnected loop is unphysical!

Worm cnf. space = $Z \cdot (G \Rightarrow \text{disconnected loop})$
Quantum spin chains magnetization curves, gaps, spin wave spectra

$$H = -\sum_{<ij>} \left[ J_x (S_x S_{ix} + S_y S_{iy}) + J_z S_z S_{iz} \right] - H \sum_i S_{iz}$$

S=1/2 Heisenberg chain

MC data

Bethe ansatz (M. Takahashi)
Line is for the effective fermion theory with spectrum

\[ \varepsilon(p = 2\pi n/L) = \sqrt{\Delta^2 + cp^2} \]

\[ \Delta = 0.4105(1) \]

\[ c = 2.48(1) \]

deviations are due to magnon-magnon interactions

Lou, Qin, Ng, Su, Affleck '99
Energy gaps: One dimensional S=1 chain with $J_z / J_x = 0.43$

$$G(p, \tau) = \int e^{ipx} dx \left\langle T_x S^+(x, \tau) S^-_I(0) \right\rangle$$

$$= \sum_{\alpha'} \left| (S^{+}_{p})_{G\alpha'} \right|^2 e^{(E_G - E_{\alpha'})\tau} \quad \tau J \ll 1 \rightarrow Z e^{-\Delta \tau}$$

Spin gap $\Delta = 0.02486(5)$

$Z$ -factor $Z = 0.980(5)$
Spin waves spectrum: One dimensional S=1 Heisenberg chain

\[ \Delta = 0.4105 \]
\[ c = 2.48 \]

- \[ E(p) = (\Delta^2 + c^2 p^2)^{1/2} \]
- \[ E(p) = \Delta + c^2 p^2 / 2\Delta \]
Conclusions:

Worm algorithm  = cnf. space of $Z \ G$ + updates based on

Can be formulated for:

- classical and quantum models (Bose/Fermi/Spin)
- different representations (path-integrals, Feynman diagrams, SSE)
- non-local solutions of balance Eqn. (clusters, directed loops, geom. worm)
Winding numbers

Homogeneous gauge in x-direction: \( t \to te^{iA} \), \( A_x(r) = \varphi/L \), \( \int A_x(r) \, dx = \varphi \)

\[
Z = \sum_{W_x} e^{i\varphi_{W_x}} Z_{W_x}
\]

\[
F = -T \ln Z = F(0) + L^d \, \Lambda_S \left( \frac{\varphi}{L} \right)^2 \frac{2}{2}
\]

\[
W_x = \sum_i (N_{i,x} - N_{i+\lambda,x}) / L = 1
\]

\[
\Lambda_S = L^{d-2} \frac{\partial^2 F}{\partial \varphi^2} = \frac{T \langle W_x^2 \rangle}{L^{d-2}}
\]

Ceperley Pollock '86