Worm Algorithm and Diagrammatic Monte Carlo

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(Pseudo-) classical representations of quantum statistics

$Z = \text{Tr} e^{-\beta H}, \quad \beta = 1 / T \quad (\hbar = k_B = 1)$

$e^{-\beta H} \equiv e^{-\epsilon H} e^{-\epsilon H} \cdots e^{-\epsilon H}$  \hspace{1cm} \text{An extra dimension—the “imaginary time”—appears.}

$\text{Tr} e^{-\beta H} = \langle \{\psi_0\} | e^{-\epsilon H} | \{\psi_1\} \rangle \langle \{\psi_1\} | e^{-\epsilon H} | \{\psi_2\} \rangle \cdots \langle \{\psi_m\} | e^{-\epsilon H} | \{\psi_0\} \rangle$

(a) Feynman’s path integrals: mapping onto polymers in $(d+1)$ dimensions

(b) Functional integrals: mapping onto classical/grassmanian fields in $(d+1)$

(c) Some other $(d+1)$-representations along qualitatively similar lines
Feynman’s path integral (worldline) representation of quantum statistics

\[ Z = \text{Tr} e^{-\beta H} \]
Single-particle Matsubara Green’s Function

\[ \hat{\Psi}_\alpha(\tau, \mathbf{r}) = e^{\tau H} \hat{\psi}_\alpha(\mathbf{r}) e^{-\tau H}, \quad \hat{\Psi}_\alpha(\tau, \mathbf{r}) = e^{\tau H} \hat{\psi}_\alpha(\mathbf{r}) e^{-\tau H} \]

\[ G_{\alpha\beta}(\tau_1, \mathbf{r}_1; \tau_2, \mathbf{r}_2) = -\langle T_\tau \hat{\Psi}_\alpha(\tau_1, \mathbf{r}_1) \hat{\Psi}_\beta(\tau_2, \mathbf{r}_2) \rangle \]

\[ \langle (...) \rangle \equiv Z^{-1} \text{Tr} \ e^{-\beta H} (...) \]

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

\[ G_{\alpha\beta}(\tau_1, \mathbf{r}_1; \tau_2, \mathbf{r}_2) \equiv G_{\alpha\beta}(\tau, \mathbf{r}, \mathbf{r}), \quad \tau = \tau_1 - \tau_2 \]

\[ n(\mathbf{r}) = \pm \sum_\alpha G_{\alpha\alpha}(\tau = 0, \mathbf{r}, \mathbf{r}), \quad p(\mu, T) = \int_{-\infty}^{\mu} n(\mu', T) \, d\mu' \]

fermions/bosons
Two sectors of the configuration space

\[ G(r_1, \tau_1; r_2, \tau_2) = \left\langle T_\tau \Psi^\dagger (r_2, \tau_2) \Psi (r_1, \tau_1) \right\rangle = \frac{\text{Tr} T_\tau \Psi^\dagger (r_2, \tau_2) \Psi (r_1, \tau_1) e^{-\beta H}}{\text{Tr} e^{-\beta H}} \]

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

\[ \text{Tr} T_\tau \Psi^\dagger (r_2, \tau_2) \Psi (r_1, \tau_1) e^{-\beta H} \]
By Diagrammatic Monte Carlo we mean:

1. Metropolis-Hastings-type Monte Carlo sampling of series of (similar) integrals with *variable number of integration variables*.

2. The above technique applied to *Feynman’s diagrams* in the thermodynamic limit, and especially in *combination with analytic diagrammatic tricks* (e.g., Dyson’s and ladder, summation, skeleton diagrams, etc.) and general re-summation techniques.
Traditional Quantum Monte Carlo:

1. Map a $d$-dimensional quantum system onto a $(d+1)$-dimensional classical counterpart.

2. Simulate the latter by Monte Carlo.

Diagrammatic Monte Carlo (DiagMC):

Samples diagrammatic series.

If applied to Feynman’s diagrammatics, DiagMC simulates an answer in thermodynamic limit.
Feynman diagrams

Generic structure of diagrammatic expansions:

\[ Q(y) = \sum_{m=0}^{\infty} \sum_{\xi_m} \int D(\xi_m, y, x_1, x_2, \ldots, x_m) \, dx_1 \, dx_2 \cdots dx_m \]

These functions are visualized with diagrams.

Example:

\[ Q(y) \text{ can be sampled by Monte Carlo} \]
Diagrammatic MC: Random walk in the diagrammatic space

*Not to be confused with the diagram-by-diagram evaluation!*

The space = **diagram order** + **topology** + **internal/external continuous variables**
Principles of stochastic sampling
Metropolis-Hastings Algorithm


Markov-type chain of updates transforming system configurations
Balancing: Metropolis Algorithm

For details, see, e.g.: http://people.umass.edu/~bvs/Metr_alg.pdf

\[ \sum_b \left( N_a P_{a \rightarrow b} - N_b P_{b \rightarrow a} \right) = 0 \]  \textit{generic balance equation for a Markovian process}

We want \( \{ P_{a \rightarrow b} \} \) such that: \( N_a \propto W_a \).

Continuum of solutions for \( \{ P_{a \rightarrow b} \} \).

Confine ourselves with \textit{detailed balance}: \( W_a P_{a \rightarrow b} = W_b P_{b \rightarrow a} \)

Still continuum of solutions for \( \{ P_{a \rightarrow b} \} \), with a very natural one being:

\[ P_{a \rightarrow b} = \begin{cases} 1, & \text{if } W_b \geq W_a , \\ W_b / W_a , & \text{if } W_b < W_a . \end{cases} \]
Metropolis-Hastings Algorithm

\[ W_a P_{a \rightarrow b} = W_b P_{b \rightarrow a} \]

\[ P_{a \rightarrow b} = P^{(propose)}_{a \rightarrow b} P^{(accept)}_{a \rightarrow b} \]

\[ W_a P^{(propose)}_{a \rightarrow b} P^{(accept)}_{a \rightarrow b} = W_b P^{(propose)}_{b \rightarrow a} P^{(accept)}_{b \rightarrow a} \]

\[ P^{(accept)}_{a \rightarrow b} = \begin{cases} 
1, & \text{if } R_{a \rightarrow b} \geq 1, \\
R_{a \rightarrow b}, & \text{if } R_{a \rightarrow b} < 1,
\end{cases} \quad R_{a \rightarrow b} = \frac{W_b P^{(propose)}_{b \rightarrow a}}{W_a P^{(propose)}_{a \rightarrow b}} \]
The updates related to changing the number of continuous variables always come as (complementary) pairs $A$-$B$. Update $A$ involves creating new variables, and update $B$ involves eliminating them. For update $A$, the proposal probability is a product of probability $P^{(addr)}_A$ to address the update $A$ and the probability $\Omega(\bar{X})d\bar{X}$ to seed the new variables in a given element of corresponding space.

Here $\Omega(\bar{X})$ is an arbitrary distribution function for generating particular values of new continuous variables in the update $A$.

Acceptance ratios for the updates $A$ and $B$

$$R_A(\bar{X}) = \frac{\text{New Diagram}}{\text{Old Diagram}} \frac{p^{(addr)}_B}{p^{(addr)}_A} \frac{1}{\Omega(\bar{X})}$$

$$R_B(\bar{X}) = \frac{\text{New Diagram}}{\text{Old Diagram}} \frac{p^{(addr)}_A}{p^{(addr)}_B} \Omega(\bar{X})$$

For a tutorial, see:

http://people.umass.edu/~bvs/Metropolis_walk.pdf

http://people.umass.edu/~bvs/Scattering_length.pdf
Diagrammatic Monte Carlo for fermions: Sign blessing rather than sign problem.

DiagMC simulates the answer in thermodynamic limit rather than a \((d+1)\)-dimensional object.
Q. How can a series with *factorially* growing number of diagrams within a given order converge?

A. *Fermionic sign blessing*: Factorially accurate cancellation of different diagrams within a given order.

*But why should we expect the sign blessing?*...

*... Because of the absence of Dyson's collapse (for discrete and some other special systems).*
Dyson’s collapse

**Dyson’s argument (1952):** A perturbative series has zero convergence radius if changing the sign of interaction renders the system pathological.

A conjecture: **Finite convergence radius if no Dyson’s collapse.**

*Pauli principle protects lattice and momentum-truncated fermions from Dyson’s collapse.*
Q. Why necessarily fermions—how about, say, spins (also protected from collapse)?

A. For Feynman diagrammatics, we need Gaussian non-perturbed action. That’s why fermions and fermionization.

More generally, Grassmannization.

Looks like one can fermionize/Grassmannize essentially any lattice system!

Computational complexity of diagrammatic Monte Carlo

Rossi, Prokof'ev, Svistunov, Van Houcke, and Werner, EPL 118, 10004 (2017)

t(\varepsilon) \sim \varepsilon^{-\#\ln(\ln\varepsilon^{-1})} \quad \text{with standard DiagMC: quasi-polynomial}

t(\varepsilon) \sim \varepsilon^{-\alpha} \quad \text{with Rossi’s determinant trick: polynomial}

Rossi, PRL, 119, 045701 (2017)
Diagrammatic Monte Carlo for fermions: Illustrative results
Model of Resonant Fermions
(from ultra-cold atoms to neutron stars)

No explicit interactions—just the boundary conditions:

\[ \forall i, j \text{ at } |r_{\uparrow i} - r_{\downarrow j}| \to 0: \quad \Psi(r_{\uparrow 1}, \ldots, r_{\uparrow N}, r_{\downarrow 1}, \ldots, r_{\downarrow N}) \to \frac{A}{|r_{\uparrow i} - r_{\downarrow j}|} + B, \quad \frac{B}{A} = c = \text{const} \]

(In the two-body problem, the parameter \( c \) defines the s-scattering length: \( a = -1/c \).)

\[ c \gg n^{1/3} \sim k_F \quad \Rightarrow \quad \text{BCS regime} \]

\[ -c \gg n^{1/3} \sim k_F \quad \Rightarrow \quad \text{BEC regime} \]

\[ |c| \sim n^{1/3} \sim k_F \quad \Rightarrow \quad \text{the crossover} \]

\[ c = 0 \quad \Rightarrow \quad \text{unitarity point: scale invariance} \]
Resonant fermipolaron

One (spin-down) particle interacting resonantly with an ideal (spin-up) Fermi sea.

The ground state:
A polaron, or a molecule (bound spin-up + spin-down state)
Resonant Fermi polaron: energy and effective mass

Energy

Effective Mass

Prokof'ev and BS, 2008
Unitary Fermi gas: Number density equation of state

Unitary Fermi gas: Momentum distribution and contact

Ground-State Phase Diagram of 2D Fermi-Hubbard Model in the Emergent BCS Regime

\[ H = -t \sum_{\langle ij \rangle} a_{\sigma i}^+ a_{\sigma j} + U \sum_i n_{\uparrow i} n_{\downarrow i}, \quad n_{\sigma i} = a_{\sigma i}^+ a_{\sigma i} \]
Extended crossover from Fermi liquid to quasi-antiferromagnet in the half-filled 2D Hubbard model

Graphene-type systems: RG flow in Dirac liquids

Effective Coulomb coupling constant in 2D: \( \alpha[l] = e^2/v_F \)

Q: How \( \alpha[l=ln(L)] \) renormalizes with the scale of distance \( l=ln(L/a) \)?

Conclusion: In the infrared limit, the system is asymptotically free with divergent Fermi velocity.

Interacting topological materials: Phase diagram of the Haldane-Hubbard-Coulomb model

Haldane-Hubbard model

Approximate and finite-size methods strongly disagree
(T.I. Vanhala et al, PRL 116, 225305 (2016))

Diagrammatic result

Coulomb tail effect

\( V(r) = U\delta_{r,0} + U_C(b/r) \)

Haldane-Hubbard

I.S. Tupitsyn and N.V. Prokof’ev, PRB 99, 121113(R) (2019)
Fermionized spins
Popov-Fedotov fermionization trick

Heisenberg model

\[ H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \]

Dynamical--but not statistical--equivalent

\[ H' = J \sum_{\langle ij \rangle} \left( f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta} \right) \cdot \left( f_{j\gamma}^\dagger \vec{\sigma}_{\gamma\delta} f_{j\delta} \right) \]

Dynamical and statistical equivalent

\[ H_{PF} = J \sum_{\langle ij \rangle} \left( f_{i\alpha}^\dagger \vec{\sigma}_{\alpha\beta} f_{i\beta} \right) \cdot \left( f_{j\gamma}^\dagger \vec{\sigma}_{\gamma\delta} f_{j\delta} \right) - \mu \sum_{j\alpha} (n_{j\alpha} - 1), \quad \mu = i\pi T / 2 \]
Spin-1/2 on triangular lattice by BDMC

Kulagin, Prokof'ev, Starykh, BS, and Varney, PRL 110, 070601 (2013); PRB 87, 024407 (2013).
Static magnetic response

\[ \chi(q,0) \]

- \( T/J = 0.375 \)
- \( T/J = 0.5 \)
- \( T/J = 1 \)
- \( T/J = 2 \)

[BZ]

\( \Gamma \rightarrow K \rightarrow M \rightarrow \Gamma \)
Quantum-to-classical correspondence of the static magnetic response

\[ \frac{\chi(r)}{\chi(0)} \]

\[ T/J = 1.0 \]
\[ T_{cl}/J = 1.45 \]

\[ |\chi(r)| \]
\[ \frac{|\chi(0)|}{|\chi(0)|} \]

\[ T_{cl}/J = 0.375 \]
\[ T_{cl}/J = 0.675 \]

\[ y = 4x/3 \]
\[ y = \frac{(4x^2 + Ax + B)}{(3x + C)} \]

for square lattice
Quantum-to-classical correspondence in the Heisenberg model on kagome lattice

$T_Q/J = 1$

Worm Algorithm
Feynman’s path integral (worldline) representation of quantum statistics

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

\( \beta = 1/T \)

spatial coordinate
Worldline winding numbers and superfluidity

$W = 0$

$W = +1$

$\beta = 1/T$

Superfluid density:

$$\rho_s \propto \frac{\langle W^2 \rangle}{\beta L^{d-2}}$$

Two sectors of the configuration space

\[ G(r_1, \tau_1; r_2, \tau_2) = \left< T_\tau \Psi^\dagger(r_2, \tau_2) \Psi(r_1, \tau_1) \right> = \frac{\text{Tr} \, T_\tau \Psi^\dagger(r_2, \tau_2) \Psi(r_1, \tau_1) e^{-\beta H}}{\text{Tr} e^{-\beta H}} \]

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

\[ \text{Tr} T_\tau \Psi^\dagger(r_2, \tau_2) \Psi(r_1, \tau_1) e^{-\beta H} \]
Worm algorithm: the idea

1. Combine both sectors into a single configuration space.

2. Use G-sector for efficient updates.

Prokof'ev, Svistunov, and Tupitsyn, JETP 87, 310 (1998)
Worm algorithm updates

Prokof’ev, Svistunov, and Tupitsyn, JETP 87, 310 (1998) [worm for lattice models]

Prokof’ev and Svistunov, PRL 87, 160601 (2001) [worm for classical models]

Boninsegni, Prokof’ev, and Svistunov, PRL 96, 070601 (2006) [worm for continuous space]

For a pedagogic introduction see:


Prokof’ev and B. Svistunov, Worm Algorithm for Problems of Quantum and Classical Statistics,
Inserting/removing a short worldline piece
Opening/closing a worldline gap
Shifting the worm
Reconnection: the most efficient update

Instructive fact:
The (generic) worm algorithm for Ising-type models in 3D overperforms system-specific cluster algorithms.
Worm algorithm: illustrative applications
Superfluidity in the core of a screw dislocation in He-4 crystal

Robert Hallock’s UMass Sandwich

Temperature gradient in Vycor rods does the job!

Observation of Unusual Mass Transport in Solid hcp $^4$He

M. W. Ray and R. B. Hallock

**discovery:**
isochoric compressibility (aka syringe effect)

UMass sandwich

**theory**

Underlying Mechanism for the Giant Isochoric Compressibility of Solid $^4$He: Superclimb of Dislocations

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PRL 100, 235301 (2008)
First validation of optical-lattice quantum emulator experiment with ultracold atoms in optical lattice

simulation by worm algorithm

Suppression of the critical temperature for superfluidity near the Mott transition

S. Trotzky¹*, L. Pollet²,³†, F. Gerbier⁴, U. Schnorrberger¹, I. Bloch¹,⁵, N. V. Prokof'ev²,⁶, B. Svistunov²,⁶ and M. Troyer³
Bose Hubbard model with bounded disorder at a commensurate filling

\[ H = -t \sum_{\langle i,j \rangle} a_i^+ a_j + \frac{U}{2} \sum_i n_i (n_i - 1) + \sum_i \epsilon_i n_i \]

\( \epsilon_i \in [-\Delta, \Delta] \) random on-site potential

\( \nu \equiv \bar{n}_i = 1 \) (or other integer)

Superfluid (SF)

Mott insulator (MI) gapped insulator

Bose glass (BG) compressible insulator

Q1: Does disorder change the phase diagram at \( \Delta \ll U, t \) ?

Q2: Is disorder a relevant perturbation for SF-insulator transition?


3D and 2D: Essentially complete theoretical control

(Theorem of inclusions + worm algorithm simulations)

Gurarie, Pollet, Prokof'ev, Svistunov, and Troyer, PRB 80, 214519 (2009)

Soyler, Kiselev, Prokof'ev, and Svistunov, PRL 107, 185301 (2011)
1D case

New universality class: “scratched 2D XY.”
Can preempt BKT-type transitions.

Pollet, Prokof’ev, and Svistunov, PRB 89, 054204 (2014)

Bose Hubbard model: Emergent relativistic physics in the vicinity of the Mott transition

\[ H = -t \sum_{\langle i,j \rangle} a_i^+ a_j + \frac{U}{2} \sum_i n_i (n_i - 1) \]

\( \nu \equiv \bar{n}_i = 1 \)

Emergence of particle-hole symmetry on the approach to the critical point from the Mott-insulator side

The Halon: a quasiparticle featuring critical charge fractionalization

A static impurity in O(2) Wilson-Fisher conformal field theory in (2+1)

By particle-vortex duality, the theory also describes the net magnetic flux induced by a solenoid introduced into 3D superconductor at the critical temperature.

size of the halo: \( r_0 \sim |V - V_c|^{-\tilde{\nu}}, \quad \tilde{\nu} = 2.33(5) \)

The halo charge \( \pm 1/2 \) is guaranteed by emergent particle-hole symmetry.

Huang, Chen, Deng, and Svistunov, PRB 94, 220502(R) (2016); see also PRB 98, 214516 (2018) and PRB 98, 140503(R) (2018).