Representations of Partition Functions and the Loop Algorithm

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- Representations of $\text{tr} \ e^{-\beta H}$, and mapping between them
- Loop algorithm (with extension to infinite lattice size)
- QMC method for coupled spins and bosons

Representations of $\exp(-\beta \hat{H})$: Discrete time

1D Heisenberg:

$$H = \sum_{\langle ij \rangle} \frac{J_x}{2} (S_i^+ S_j^- + S_j^+ S_i^-) + J_z S_i^z S_j^z$$

similar to tV-model:

$$H = \sum_{\langle ij \rangle} t (c_i^\dagger c_j + c_j^\dagger c_i) + V n_i n_j$$

Trotter decomposition:

$$Z = \text{tr} \ e^{-\beta H} = \lim_{M \to \infty} \text{tr} (e^{-\Delta \tau H_{\text{even}}} e^{-\Delta \tau H_{\text{odd}}})^M \quad \Delta \tau = \frac{\beta}{M}$$

Insert $\{S^z\}$ eigenstates:

$$Z = \lim_{M \to \infty} \sum_{\{S^z\}} \langle S_{(1)}^z | e^{-\Delta \tau H_1} | S_{(2)}^z \rangle \langle S_{(2)}^z | e^{-\Delta \tau H_2} | S_{(3)}^z \rangle \ldots$$

$$\tau$$

$$\tau$$

$$\tau$$

Continuous worldlines of up-spins $S^z(x, \tau) = \uparrow$

Similar representations for: fermions, bosons, higher spins
Representations of $\exp(-\beta \hat{H})$: Continuous time (1)

1D Heisenberg:

$$H = \sum_{\langle ij \rangle} \frac{J_x}{2} (S_i^+ S_j^- + S_i^- S_j^+) + J_z S_i^z S_j^z = H_0 - V, \quad (V: \text{spin flips})$$

Interaction repres.:

$$Z = \text{tr} \ e^{-\beta H} = \text{tr} \ \sum_{n=0}^{\infty} e^{-\beta H_0} \int_0^\beta d\tau_n \ldots \int_0^{\tau_2} d\tau_1 \ V(\tau_1) \ldots V(\tau_n)$$

- Leads to Worldline representation
- Worldlines are weighted with $e^{-\beta H_0} \rightarrow e^{\pm \frac{\tau}{4} J_z}$
- Get same repres. from $\lim_{\Delta \tau \rightarrow 0} \sinh \frac{\Delta \tau}{2} J_x = \frac{\Delta \tau}{2} J_x$
- Constant probability in time for spin-flip event: Poisson process  
  Beard, Wiese '96
- Store configurations by events
Continuous time (2)

Aizenman et al. ('90,'94), Farhi and Gutmann ('92)

- When $\hat{H}$ is a sum of operators with **discrete representation**

$$\hat{H} = - \sum J_b \hat{h}_b$$

then

$$e^{-\beta \hat{H}} = e^{\beta \sum J_b} \lim_{\Delta t \to 0} \left( \prod_b e^{(-J_b + J_b \hat{h}_b) \Delta t} \right)^{\beta/\Delta t}$$

$$= e^{\beta \sum J_b} \lim_{\Delta t \to 0} \left( \prod_b \left\{ (1 - J_b \Delta t) + J_b \hat{h}_b \Delta t \right\} \right)^{\beta/\Delta t}$$

$$= \text{Integral of } \left( \text{Poisson distribution of operators } \hat{h}_b, \text{ in continuous imaginary time, with rates } J_b. \right)$$

- Valid also for standard hopping representation
Representations of $\exp(-\beta \hat{H})$: SSE

Stochastic Series Expansion (A. Sandvik)

Let $V = \hat{H} = \sum_{i=1}^{N} \hat{H}_i$, i.e. $H_0 = 0$. Then the interaction representation

$$Z = \text{tr} \sum_{n=0}^{\infty} \int_{0}^{\beta} d\tau_n \ldots \int_{0}^{\tau_2} d\tau_1 \ V(\tau_1) \ldots V(\tau_n)$$

results in the SSE expansion of $e^{-\beta H}$:

$$Z = \text{tr} \ e^{-\beta \hat{H}} = \text{tr} \sum_{n=1}^{\infty} \frac{\beta^n n!}{n!} (-\hat{H})^n$$

$$= \text{tr} \sum_{n=1}^{\infty} \frac{\beta^n n!}{n!} (-\hat{H}_1 - \hat{H}_2 - \ldots (-\hat{H}_1 - \hat{H}_2 - \ldots) \ldots$$

$$= \text{Sum over sequences of operators}$$

- "Trace" produces worldlines
- Similar to continuous time, but with discrete index space.
- Diagonal operators $S_i^z S_j^z$ occur explicitly
- Dynamical correlations are very expensive to measure, since a temporal distance $\tau$ corresponds to a convolution over index distances.
Efficient measurement of dynamical correlations in SSE

Michel, HGE '07

- Go back to interaction representation: **reintroduce time**!

\[ Z = \text{tr} \sum_{n=0}^{\infty} \int_0^\beta d\tau_n \cdots \int_0^{\tau_2} d\tau_1 \ V(\tau_1) \cdots V(\tau_n) \]

- **Stochastic mapping from SSE to continuous imaginary time** \( \tau \):
  Given an SSE operator sequence, choose ordered times \( \tau_i \) uniformly between 0 and \( \beta \) for all operators

- Then measure correlations in time via FFT
- Saves factor \( O(\text{volume}) \) vs. measurement in SSE representation
Local Updates of continuous worldlines are very slow

Local Updates are like random walks:

Problems:

- Very long autocorrelation times (e.g. $\tau \sim \max (\xi, \frac{1}{\Delta})^2$)
- Not ergodic (Magnetization, Particle number, Winding number)
Loop Algorithm

- Ergodic, any dimension, almost no autocorrelations
- Can measure off-diagonal operators
- But restricted range of models

Cluster algorithm

Based on exact mapping to Worldlines + Loops

Provides loop representation: “improved estimators” as observables

Sign problem can be removed in loop representation in some cases: meron algorithm

Many generalizations
Loop representation of Heisenberg AF

\[- \vec{S}_i \vec{S}_j + \frac{1}{4} = \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \frac{1}{\sqrt{2}} \left( \langle\uparrow\downarrow| - \langle\downarrow\uparrow| \right) = \text{Singlet projection operator} \]

= \frac{1}{2} \left( + \bigcirc + \bigcirc + \bigcirc + \bigcirc \right) \text{ on bipartite lattice}

=: \frac{1}{2} \left( + \bigcirc + \bigcirc + \bigcirc + \bigcirc \right) \text{: allowed spin configurations}

\Rightarrow \text{Partition function} \quad Z = \text{tr} \ e^{-\beta \hat{H}} \sim \text{tr} \ e^{\beta \sum_{ij} \bigcirc} \text{ (in any dimension)}

- \Rightarrow \text{Poisson distribution of operators}

- \text{Trace produces Loop representation:}

- Can work purely in loop representation, e.g. Merons to solve sign problem Chandrasekharan, Wiese '99,....

- At each time \( \tau \), pairs of sites belonging to the same loop are in a singlet state: „Valence bond basis“
Loop algorithm

- Switch between operator and worldline representation

One instance of operator distribution

Loop–representation

One compatible set of arrows

Compatible Worldlines
Loop algorithm

- Switch between operator and worldline representation

\[ \tau \]

One instance of operator distribution

Loop-representation

One compatible set of arrows

Compatible Worldlines

worldlines

worldlines + loops

new worldlines

breakups

flips

- Change of configuration on large scale \((\xi, \xi_t)\)
- Note: with SSE representation: almost same, discrete index.
- Ferromagnet: similar.
Projector MC in valence bond basis

- At each time $\tau$, pairs of sites belonging to the same loop are in a singlet

- $\Rightarrow$ after many applications of $\hat{H}$, only singlets remain = Valence bond state = RVB state

- Ground state $|\psi_0\rangle = \lim_{\theta \to \infty} e^{-\theta \hat{H}} |\psi_{\text{trial}}\rangle$

- Projector Monte Carlo (→ ground state magnetization 0.30749(1)) Sandvik 2005; Sandvik,HGE 2010
Single Particle Greens function:

Brower, Chandrasekharan, Wiese ’98

contributes to \( \langle S_i^+ S_j^- \rangle, \langle c_i^\dagger c_j \rangle \)
Simulations on infinite lattices: \( L \equiv \infty \) and \( \beta \equiv \infty \)

- Two-point Greens functions get contributions only from sites on the same loop
- \( \Rightarrow \) Probability of large loops decays like correlation length
- Infinite system: Simulate single loop with fixed starting point, in an "infinite" spin system

\[ \implies \text{equilibrates region around origin. Reaches distance } r \text{ with prob. } e^{-r/\xi}. \]

Can grow without bounds \( \implies \text{Simulates directly at } L = \infty \text{ and/or } \beta = \infty \)

- Example: Heisenberg spin ladder with \( N \) chains

- Spatial correl. at \( L = \infty \):

- Temporal correlations: choose infinite size: \( \Rightarrow \text{get } \beta \equiv \infty \) (and \( L \equiv \infty \))
- Can take limits \( q \to 0 \) and \( \omega \to 0 \) directly
- Get full dynamics \( S(q, i\omega) \).
Introduce 2 sources. Allow them to move

- Local updates
- When sources meet and annihilate, a valid sourceless configuration is reached again
- Applicable to any model.
- Ergodic
- Intermediate states contribute to Greens functions
- Directed loops: efficient update designed such that for isotropic couplings the loop-algorithm is recovered
At each vertex, 2 arrows enter and 2 leave: arrow configuration has “zero divergence”

⇒ Difference between configurations also has zero divergence, i.e. it lies on loops

Solution: Each such loop follows arrows, which are then flipped

- There are 2 possible paths out of each vertex:
- Horizontal path corresponds to loop-operator
Spins and Bosons: divide and conquer
Spin - Peierls Transition

- Structural phase transition due to interaction of phonons with spins or electrons

- Example: 1D Heisenberg chain coupled to phonons

\[
\hat{H} = \sum_{i=1}^{N} \hat{S}_i \hat{S}_{i+1} \left\{ \begin{array}{cc}
1 + g & \hat{x}_i \\
1 + g & (\hat{x}_i - \hat{x}_{i+1}) \\
\end{array} \right\} f(\{\hat{x}_i\}) + \frac{1}{2} \sum_q \hat{p}_q^2 + \omega^2(q) \hat{x}_q
\]

- \( T = 0 \): Quantum Phase Transition at \( g_c \) to dimerized phase

- Issue: Does \( g_c \) depend on bare dispersion?

- Spectra: Phonon softening or central peak?
### Phonons: some difficulties

- **First quantization:** 
  \[(1 + g(x_i - x_{i+1}) S_i S_{i+1}) : \]

  Very slow phonon convergence with updates local in imaginary time; especially for acoustical phonons \((\omega(q = 0) = 0)\)

- **Second quantization:** 
  \[... (b_i^\dagger + b_i - b_{i+1}^\dagger - b_{i+1}) S_i S_{i+1} : \]

  Sign problem!
QMC method for dynamical phonons

- **Interaction representation** with $\hat{H}_{ph}$ as diagonal part:

\[
Z = \text{Tr}_s \sum_{n=0}^{\infty} \sum_{\tau_n} \int_0^\beta d\tau_n \ldots \int_0^\tau_2 d\tau_1 \int Dx \prod_{l=0}^n f(\{x(\tau)\}) S_{n}[l] \left[ \exp \left( -\int_0^\beta d\tau H_{ph}(\{x(\tau)\}) \right) \right],
\]

where $S_{n}[l]$ is the spin operator sequence.

Spin-phonon coupling $f(\{x(\tau)\})$ acts at space-time locations of spin-operators.

- **Effective action for phonon coordinates** contains $\log f(\{x\})$: not bilinear.
QMC method for dynamical phonons

- **Interaction representation** with $\hat{H}_{ph}$ as diagonal part:

$$Z = \text{Tr}_s \sum_{n=0}^{\infty} \sum_{S_n^\tau} \int_0^\beta d\tau_n \ldots \int_0^{\tau_2} d\tau_1 \int \mathcal{D}x \prod_{l=0}^{n} f(\{x(\tau)\}) S_n^\tau[l] \int \exp \left( - \int_0^\beta d\tau H_{ph}(\{x(\tau)\}) \right)$$

Spin-phonon coupling $f(\{x(\tau)\})$ acts at space-time locations of spin-operators

- **Effective action for phonon coordinates** contains $\log f(\{x_l\})$: not bilinear

- **Phonon update proposal**: Replace $f(x) = 1 + gx$ by $f^{\text{prop}} = \exp(gx) \Rightarrow$ bilinear

  $\Rightarrow$ generate new phonon configuration in $(\omega_n, k)$ space; **accept** with physical $S_{\text{eff}}$

- **Spin update**: **Directed loops** in spin operators (fast).

- Can use any bare dispersion $\omega(q)$
Optical bond phonons \((1 + g\hat{x}_i)S_iS_{i+1}\)

- Dispersion at large \(\omega_0 \gtrsim J\): Second phonon branch develops at \(g_c\) from central peak

- Dispersion at small \(\omega_0 = 0.25J\): Bare phonons soften and join central peak
Site phonons  \[ 1 + g(x_i - x_{i+1})S_i S_{i+1} : \text{QMC results} \]

- Gapless acoustic phonons:

DMRG paper (PRL) concluded that \( g_c = 0 \) !?
(measured magnetization \( M \), incorrectly assumed \( M(N) \propto \Delta_S(N) \))

QMC:
KT transition at \( g_c = 0.058(2) \)
\text{Not affected by gapless mode !}
Conclusions

- Representations of partition function (discrete, continuous, SSE)

- Common framework: Interaction representation

- Representation is different issue than update algorithm

- Loop algorithm: cluster method switching between loop and spin representations

- Infinite size lattices

- Generalization: worms and directed loops

- Efficient algorithm for coupled spins and phonons, with arbitrary phonon dispersions