(Quantum) Monte Carlo Strategies for spin liquids

Lecture 2

- QMC involves the probabilistic sampling of a d+1 dimensional (classical) configuration.

- A "zoo" of QMC methods exist (world-line, SSE, determinental QMC, path-integral MC for the continuum...)

- All are affected in some way by the "sign problem".

Similar to classical MC, our goal is to evaluate the expectation value of an observable

$$\langle \theta \rangle = \frac{1}{Z} \sum \omega_X e^{-\beta H} \omega_0 = \frac{\sum_x \omega_X \omega(x)}{\sum_x \omega(X)}$$

ie. a sum over all possible "configurations" (which are now d+1).

- Each configuration is updated according to a positive probability $P(X_{x-1} \rightarrow X_x)$

Can be determined via detailed balance:

$$W_x P(x \rightarrow y) = W_y P(y \rightarrow x)$$
QMC: must determine what are your configurations \(x\), their weights \(w_x\), and transition probabilities \(p_x\).

A 1+1 configuration is:
- a basis state \(|\lambda\rangle\) (e.g. \(S^z\) or valence-bond)
- a set of world lines (or an "operator list")

Stochastic Series Expansion (Sandvik)

Taylor expansion of the partition function:
\[ Z = Tr \sum_{\lambda} e^{-\beta \hat{H}} \]  
\[ = \sum_\lambda \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle \lambda | \hat{A} \hat{A} \hat{A} \ldots \hat{A} | \lambda \rangle \]

- associate the \(n\)-th signs with each operator \(A\)
- insert \(n-1\) resolutions of the identity \(Z_1 \ldots Z_n\)

Choose a basis \( (|\lambda\rangle = |S^z\rangle \text{ say}) \) and a local decomposition of your Hamiltonian, into "bond" operators say:
\[ \hat{H} = \sum_{b=1}^{w} \hat{H}_b \]

E.g.) Heisenberg model
\[ H = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j \]

in \(S^z\) basis separate
\[ \hat{H}_b^{\text{diagonal}} = J \sum_i \hat{S}_i^z \hat{S}_j^z \]
from
\[ \hat{H}_b^{\text{off-diagonal}} = \frac{J}{2} (\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+) \]

Diagonal \( \hat{H}_b = J \), off-diagonal \( \hat{H}_b = \) III/II
1D picture

\[ \begin{align*}
\uparrow &= \times \\
\downarrow &= 0 \\
1d_0 \times 0 \times 0 \times 1d_2 \\
1d_1 \times 0 \times 0 \\
1d_0 \times 0 \times 0 \\
\end{align*} \]

\[
\text{bond } b = 1 \times 3, 4, 5
\]

- Finite T: \( |1d_n\rangle = |d_0\rangle \) (Trace = diagonal matrix element)

- Sign problem: the ratio of weights must always be positive in order to have a transition "probability" \( 0 \leq \frac{W_{+1}}{W_{-1}} \leq 1 \) : interpret as a probability.

Standard way to do this: Make each matrix element positive: \( \langle d_{m-1} | -H_0 | d_m \rangle \geq 0 \)

1) Diagonal terms:

\[ \begin{align*}
\langle \uparrow \uparrow | -J \hat{S}^z \hat{S}^z | \uparrow \uparrow \rangle &= -\frac{3}{4} \\
\langle \uparrow \uparrow | -J \hat{S}^z \hat{S}^z | \downarrow \downarrow \rangle &= \langle \downarrow \downarrow | -J \hat{S}^z \hat{S}^z | \uparrow \uparrow \rangle = +\frac{3}{4} \\
\langle \uparrow \uparrow | -J \hat{S}^z \hat{S}^z | \uparrow \downarrow \rangle &= -\frac{3}{4}
\end{align*} \]

Could lead to positive or negative weights: the simplest "sign problem" to fix: Add a constant \( \xi \) to the Hamiltonian, e.g. \( \xi = \frac{3}{4} \)

2) Off-diagonal terms:

\[ \langle \uparrow \uparrow | -H_0 | \downarrow \uparrow \rangle = -\frac{3}{2} \]

Unaffected by \( \xi \): how do we handle this?

The occurrence is tied to the lattice geometry.
e.g.) in the SSE finite-T formulation, world-lines must be periodic.

\[
W \propto \cdots \langle \psi_{b_i b_j}^{1,2} \mid \frac{1}{3} (5^{b_5} - 5^{-b_5}) \mid \psi_{b_i b_j}^{1,2} \rangle \cdots
\]

\[
\quad \cdots \langle 1, 2 \mid -3 \mid 1, 2 \rangle \cdots
\]

These two \(-1\) signs always cancel.

2D Square lattice:
\[
\begin{align*}
\text{two paths} & \quad \begin{cases} \quad (-1) \quad \begin{cases} \quad (-1) \\ \quad (-1) \end{cases} \\
\text{or} & \quad \begin{cases} \quad (-1) \quad \begin{cases} \quad (-1) \\ \quad (-1) \end{cases} \\
\end{cases}
\end{cases}
\]

\(-1\) signs always occur in even numbers.

Triangular/Kagome lattice
\[
\begin{cases} \quad (-1) \\ \quad (-1) \end{cases}
\]

Odd numbers of \(-1\) signs can (and will) occur.

If any path can be found that takes an odd \# of "hops" to return to the original configuration, the sign problem will occur.
Marshall sign-positive:

Equivalent to saying a basis rotation can be found that makes the off-diagonal matrix elements all positive. In this case:

- Decompose into bipartite sublattices
- Apply 180° rotation of the spin space along the $S^z$ axis for one sublattice only.

Unitary rotation operator: $D(\hat{e}_y, \theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$

$\Rightarrow H_{B^B} = \frac{3}{2} (S_A^+ S_B^- + S_A^- S_B^+) $

$\Rightarrow \frac{3}{2} (-S_A^+ S_B^- - S_A^- S_B^+) = -\frac{3}{2} (S_A^+ S_B^- + S_A^- S_B^+) $

Sign of matrix element is changed in $S^z$ basis.

⇒ Not possible on triangular, Kagome.

Marshall positive Hamiltonians

- AFM Heisenberg $SU(2)$ on bipartite
- J-Q models: $H = J \sum_i \langle \vec{S}_i \cdot \vec{S}_j \rangle + \Phi \sum_i \langle \vec{S}_i \cdot \vec{S}_j \rangle \langle \vec{S}_i \cdot \vec{S}_j \rangle$  
  (sanduk)
And $SU(N)$ extensions (see R. Kaul)
- $U(1)$ Hamiltonians - bosons with unfrustrated hopping $H = t (b_i^+ b_j + b_i b_j^+)$ & ...
Q: Can Marshall sign-positive models have topological spin liquid phases?

Terhal, Bravyi: "stochastic".

Consequences for quantum complexity? (QMA-complete)

Note: other basis choices often have similar sign-structure to the standard $S^z$ basis, but not always.

E.g. Valence bond basis: $\psi_j = \frac{1}{\sqrt{2}} (|\uparrow;\downarrow\rangle - |\downarrow;\uparrow\rangle)$

Can write Heisenberg AFM in terms of projector operators $P_{ij} = \frac{1}{4} - \vec{s}_i \cdot \vec{s}_j = |S_{ij}\rangle \langle S_{ij}|$

Marshall sign rule is already built in (Sandvik).

Sign-problem free models with frustration

Balents - Fisher - Girvin (BFG) PRB 65, 224412 '02

Or "charge-cluster" models (cluster-charging?)

Kagome:

\[
H_0 = V \sum_\sigma (S_\sigma^z)^2
\]

where

\[
S_\sigma^z = \sum_i S_i^z
\]

3 spin up per kagome
The sign of $H_0$ doesn't matter for QMC.

Add a quantum term that doesn't violate the cluster-charging constraint:

$$H_K = -K \sum_{ij} (S_i^+ S_j^- + S_i^- S_j^+) + h.c.) \quad \text{"bow-tie"}$$


$\begin{align*}
\text{no sign problem:} & \quad \langle \bar{\alpha} | - H_{p}^{\text{eff}} | \bar{\alpha} \rangle \\
\Rightarrow & \quad \langle \bar{\alpha} | + K (S_i^+ S_j^- + S_i^- S_j^+) | \bar{\alpha} \rangle
\end{align*}$

$H = H_0 + H_K$

$\Rightarrow$ expect a spin liquid, with no sign problem!

BFG: Variations of this Hamiltonian have a $K$ point - exactly solvable, with a $B_2$ spin liquid.

QMC has confirmed for a host of models in this general class:

$H = H_0 + H_3 \quad (H_3 = -t_3 \sum_{ij} (S_i^+ S_j^- + S_i^- S_j^+))$

$H = H_0 + H_1 \quad (H_1 = -t \sum_{ij} (S_i^+ S_j^- + S_i^- S_j^+))$

$H = H_1 + H_K \quad (J-K \text{ model})$

Isakov, Kim, Parameswaran, Hastings, Melko, etc.

$\Rightarrow$ all of which have no sign problem.
**XXZ models**

There (should) be a similarly large number of models in the (sign-problem free) XXZ class, on the 3D pyrochlore:

\[
H_0 = J \sum_{<ij>} S_i^x S_j^x \quad \text{maps to classical spin ice.}
\]

Lowest-order ring-exchange that preserves the spin-ice state

\[
3_{\text{ring}} \quad \leftrightarrow \quad \text{Hermelle, Fisher, Balents}
\]

\( \Rightarrow \) promote 3D U(1) (deconfined) spin liquid phase

Similar to the 2D case, can study an unfrustrated hopping (3 hoppings make one ring exchange)

\[
H_1 = -t \sum_{<ij>} S_i^z S_j^z + S_i^- S_j^+
\]

QMC shows that \( H = H_0 + H_1 \) supports a U(1) spin liquid for sufficiently large \( J \).

\[ \quad \Rightarrow \quad \text{Banerjee, Isakov, Damle, Kim} \quad \text{PRB. 100 047208} \]

Other possible sign-problem-free K.E. terms exist, are experimentally motivated, and may induce interesting QSL phases.

\[ H_{xx} = -J_{xx} \left( S_i^+ S_j^- + S_i^- S_j^+ \right) \]

\[ \quad \Rightarrow \quad \text{Huang, Chen, Hermelle} \quad \text{PRL 112, 167203} \]
Ergodicity: Keep in mind, there are other difficulties besides the sign problem.

E.g.) How does one sample \( h_b \) in \( d+1 \) ?

One strategy is to choose "adjacent" diagonal operators nearby & convert:

But this type of (local) move is demonstrably non-ergodic in "winding #". \( \Rightarrow \) will not be able to measure super-fluid density \( \phi_s = T \langle W^2 \rangle \)

Loop/worm updates: (Evt'z '92, Sandvik / Syljuasen, Pule'sev)

- "trick" to speed up sampling of algorithm
- ergodically sample e.g. \( W \)-sectors
- access off-diagonal correlation functions

Open Question: Can loop updates be generalized for "larger" kinetic operators, like 6-site ring exchanges?

Multi-loop, or "membrane" updates?

Important for cluster-charging models
Monte Carlo measurements for Spin Liquids

Conventional measurements include:

- Expectation values of anything diagonal in the basis:
  
  \[ \langle \hat{S}_i^z \hat{S}_j^z \rangle = \frac{1}{N} \sum_{\{\sigma\}} e^{i (\hat{S}_i^z - \frac{1}{2}) \cdot \vec{q} \cdot \vec{r}_{ij}} \langle \hat{S}_i^z \hat{S}_j^z \rangle \]

  \[ X = \beta N \langle \left( \sum_{x=1}^{N} \hat{S}_x^z \right)^2 \rangle \]

- Expectation value of operators in d+1:
  
  e.g. Energy \( E = -T \langle N \rangle \) \( N = \# \) of operators

  Green's function (with warm algorithm)

Can go a long way in searching for an order-parameter characterizing thermal excitations, spinon correlation functions, etc.

What about entanglement (entropy)?

Imagine a modified d+1 OMC "projector" method:

\[ \mathcal{Z} = \langle 0 | 0 \rangle \]

\[ \langle 0 | = \frac{1}{2} \langle 0 | 0 | 0 \rangle \]

\[ \langle -H \rangle^n | 0 \rangle = (-H)^n \left[ \sum \frac{1}{n!} | \rangle \langle n \rangle \right] \text{(energy eigenstates) } \]
\[ (-H)^m |\alpha\rangle = c_0 |E_0|^m \left[ |\alpha\rangle + \frac{c_1}{c_0} \left( \frac{E_1}{E_0} \right)^m |\beta\rangle + \ldots \right] \]

\[ \rightarrow c_0 |E_0|^m |\alpha\rangle \quad \text{as} \quad m \rightarrow \infty \]

Assume that we can access the g.s. wavefunction \( |\alpha\rangle \rightarrow \rightarrow \) a vector in TN notation

\[ \text{sub-divide indices} \]

\[ \text{Tr}_B (\rho) = \rho_A \]

\[ = \text{Tr}_A (\rho_A^2) = \]

\[ = \langle 000 | \text{SWAP}_A | 1000 \rangle \]

\[ S_2 = - \log(\text{Tr} \rho_A^2) = - \log \left( \langle \text{SWAP}_A \rangle \right) \]

- Projector QMC
- Variational MC
- Path integral (PIGS)
- Aux field/DQMC

To translate to finite-\( T \) QMC, need to use PBC in imaginary time.

\[ Z = \sum_\alpha \langle \alpha | e^{-\beta H} | \alpha \rangle \]
multi-sheeted Riemann surface.

\[ 2\beta = 2'(A_{j2,7}) \]

\[ S_n(A) = \frac{1}{1-n} \log \left( \frac{2'(A_{j,n,7})}{2^n} \right), \text{ } n\text{-sheets.} \]