(Quantum) Monte Carlo Strategies for spin Liquids

Lecture 2

R. Melko

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

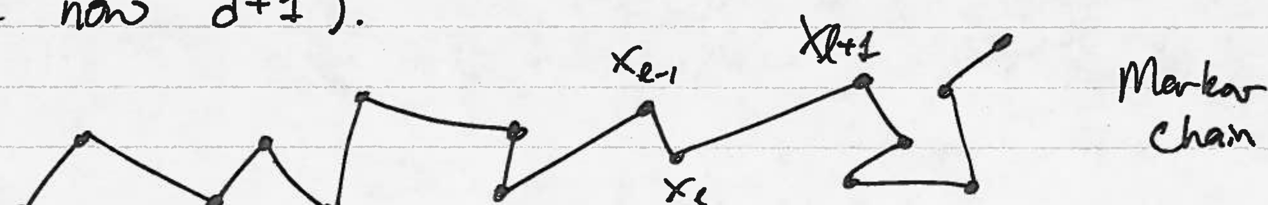
- A "zoo" of QMC methods exist (World-line, SSE, determinental QMC, path-integral MC for the continuum...)

- 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

$$\langle O \rangle = \frac{1}{Z} \mathrm{Tr}\left\{ e^{-\beta H} O \right\} = \frac{\sum_x O(x)\, W_x}{\sum_x W_x}$$

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



- Each configuration is updated according to a positive probability $P(x_{l-1} \to x_l)$

Can be determined via detailed balance:

$$W_x P(x \to y) = W_y P(y \to x)$$

QMC: must determine what are your configurations x, their weights W_x, & transition probabilities P.

A d+1 configuration is:
- a basis state $|\alpha\rangle$ (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:

$$Z = Tr\{e^{-\beta \hat{H}}\} = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle \alpha | \overbrace{\hat{H} \cdot \hat{H} \cdot \hat{H} \cdots \hat{H}}^{n \text{ times}} | \alpha \rangle$$

- associate the n -ve signs with each operator H
- insert n-1 resolutions of the identity $\sum_{\alpha} |\alpha\rangle\langle\alpha|$

$$Z = \sum_{\{\alpha\}} \sum_{n} \frac{\beta^n}{n!} \langle \alpha_0 | -\hat{H} | \alpha_1 \rangle \langle \alpha_1 | -\hat{H} | \alpha_2 \rangle \cdots \langle \alpha_{n-1} | -\hat{H} | \alpha_n \rangle$$

Choose a basis ($|\alpha\rangle = |S^z\rangle$ say) and a local decomposition of your Hamiltonian, into "bond" operators say:

$$\hat{H} = \sum_{b=1}^{N_b} \hat{H}_b$$

e.g.) Heisenberg model $\quad H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = J \sum_b \vec{S}_{b_i} \cdot \vec{S}_{b_j}$

in S^z basis separate $\quad H_b^{\text{diagonal}} = J S_i^z S_j^z$

from $\quad H_b^{\text{off-d}} = \frac{J}{2}(S_i^+ S_j^- + S_i^- S_j^+)$

diagonal $H_b =$  , off-diagonal $H_b =$ 

1D picture

$\uparrow = \times$

$\downarrow = 0$

$\times \quad 0 \quad \times \quad \times \quad 0 \quad \times \qquad |\alpha_3\rangle = |\alpha_0\rangle$

$\times \quad 0 \quad \times \quad 0 \quad \times \quad \times \qquad |\alpha_2\rangle$

$\times \quad 0 \quad \times \quad \times \quad 0 \quad \times \qquad |\alpha_1\rangle$

$\times \quad 0 \quad \times \quad \times \quad 0 \quad \times \qquad |\alpha_0\rangle$

bond b 1 2 3 4 5

- Finite T: $|\alpha_n\rangle = |\alpha_0\rangle$ (Trace = diagonal matrix elem

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

Standard way to do this: Make each matrix element positive: $\langle \alpha_{m-1} | -H_b | \alpha_m \rangle \geq 0$

1) Diagonal terms: $\langle \uparrow\uparrow | -J S^z S^z | \uparrow\uparrow \rangle = -J/4$

$\langle \uparrow\downarrow | -J S^z S^z | \uparrow\downarrow \rangle = \langle \downarrow\uparrow | -J S^z S^z | \downarrow\uparrow \rangle = +J/4$

$\langle \downarrow\downarrow | -J S^z S^z | \downarrow\downarrow \rangle = -J/4$

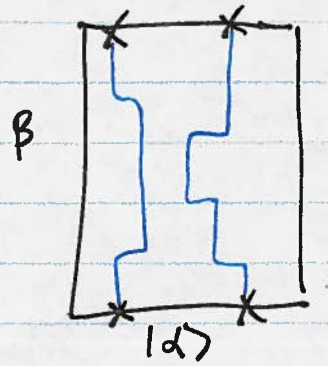
Could lead to positive or negative weights: the simplest "sign problem" to fix: Add a constant $C_1 N_b$ to the Hamiltonian, e.g. $C_1 = J/4$

2) Off-diagonal terms: $\langle \uparrow\downarrow | -H_b^{od} | \downarrow\uparrow \rangle = -J/2$

Unaffected by C_1: how do we handle this?

The occurrance is tied to the lattice geometry.

e.g.) in the SSE finite-T formulation,
world-lines must be periodic.



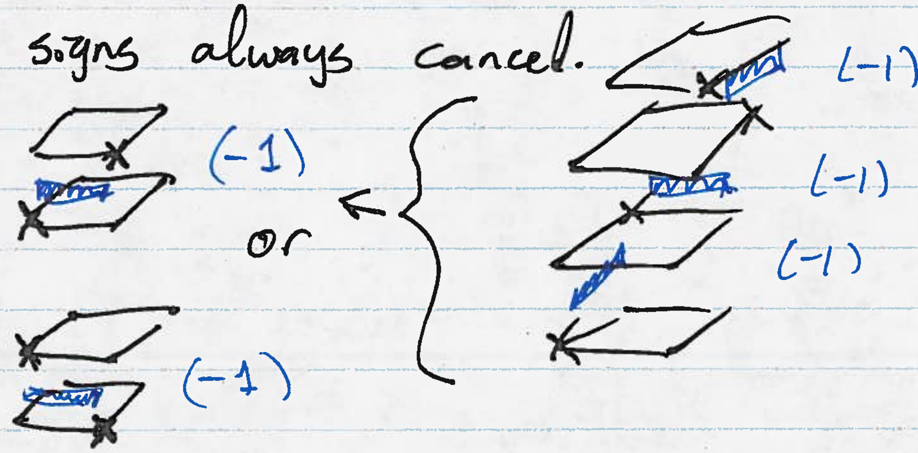
1D

operators must always occur in pairs.

$$W \propto \cdots \langle \downarrow_{b_i} \uparrow_{b_j} | -\tfrac{J}{2}(S^+S^- + S^-S^+) | \uparrow_{b_i} \downarrow_{b_j} \rangle \cdots$$
$$\cdots \langle \uparrow_{b_i} \downarrow_{b_j} | -J(\quad) | \downarrow_{b_i} \uparrow_{b_j} \rangle \cdots$$

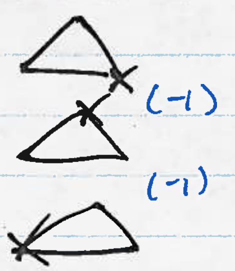
These two -ve signs always cancel.

2D Square lattice:
two paths



-ve signs always occur in even numbers.

Triangular/Kagome lattice

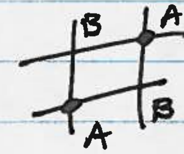


odd numbers of -ve sigs can (and will) occur.

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 <u>all</u> positive. In this case:



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

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

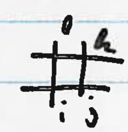
$$\Rightarrow \quad H_b^{\text{off-d}} = \frac{J}{2}\left(S_A^+ S_B^- + S_A^- S_B^+\right)$$

$$\Rightarrow \frac{J}{2}\left(-S_A^+ S_B^- - S_A^- S_B^+\right) = -\frac{J}{2}\left(S_A^+ S_B^- + S_A^- S_B^+\right)$$

sign of matrix element is changed in S^z basis.

$\Rightarrow$ <u>Not</u> possible on triangular, Kagome.

Marshall positive Hamiltonians



- AFM Heisenberg SU(2) on bipartite
- J-Q models: (sandvik) $\quad H = J \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) + Q \sum_{\langle ijkl \rangle} (\vec{S}_i \cdot \vec{S}_j)(\vec{S}_k \cdot \vec{S}_l)$

  And SU(N) extensions (see R. Kaul)

- U(1) Hamiltonians – bosons with unfrustrated hopping $\quad H = t\left(b_i^\dagger b_j + b_i b_j^\dagger\right) + \ldots$

Q: Can ~~Ma~~ Marshall sign-positive models have topological spin liquid phases?

Terhal, Bravyi: "stoquastic".

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: $|S_{ij}\rangle$ $\underset{i\quad j}{\frown} = \frac{1}{\sqrt{2}}\left(|\uparrow_i \downarrow_j\rangle - |\downarrow_i \uparrow_j\rangle\right)$

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

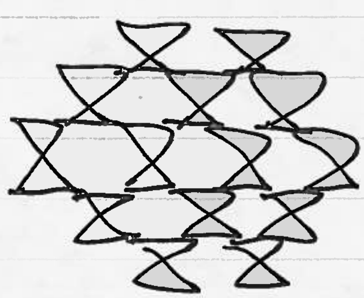
Marshal sign rule is already built in (Sandvik).

Sign-problem free models with frustration

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

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

Kagome:



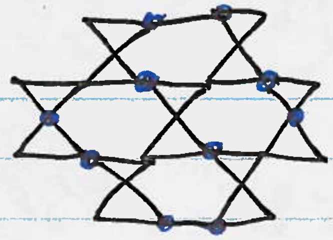
$$H_0 = V \sum_{\hexagon} (S^z_{\hexagon})^2$$

where $S^z_{\hexagon} = \sum_{\hexagon} S_i^z$

3 spin up per hexagon

$\uparrow = \bullet$

$\downarrow = $



(classical) H_0 promotes a highly degenerate manifold of states.

The sign of H_0 doesn't matter for QMC.

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

$\bowtie \leftrightarrow \bowtie$ "bow-tie"

$$H_K = -K \sum_{\bowtie} \left(S_i^+ S_j^- S_k^+ S_\ell^- + h.c. \right)$$

no sign problem: $\langle \bowtie | -H_p^{\text{off-d}} | \bowtie \rangle$

$$= \langle \bowtie | +K \left(S^+ S^- S^+ S^- + \dots \right) | \bowtie \rangle$$

$$\boxed{H = H_0 + H_K}$$

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

BFG: Variations of this Hamiltonian have a RK point - exactly solvable, with a Z_2 spin liquid.

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

$$H = H_0 + H_3 \quad \left(H_3 = -t_3 \sum_{\langle ij \rangle_3} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) \right)$$

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

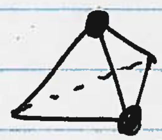
$$H = H_1 + H_K \quad \text{(J-K model)}$$

Isakov, Kim, Paramekanti, Hastings, Melko, etc.

$\Rightarrow$ all of which have no sign problem.

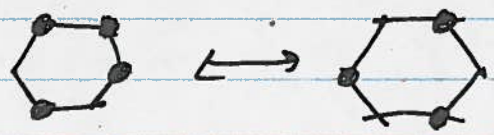
XXZ models

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



$$H_0 = J \sum_{\langle ij \rangle} S_i^z S_j^z$$ maps to classical spin ice.

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

J_{ring}  Hermele, 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)

$$H_1 = -t \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_i^- S_j^+)$$

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

$\rightarrow$ Banerjee, Isakov, Damle, Kim PRB 100 047208 '0

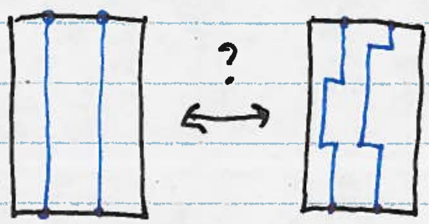
Other possible sign-problem free K.E. terms exist, are experimentally motivated, & may induce interesting QSL phases.

e.g. $H_{\pm\pm} = -J_{\pm\pm} (S_i^+ S_j^+ + S_i^- S_j^-)$

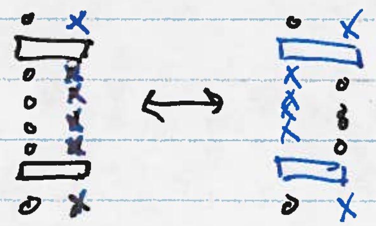
Huang, Chen, Hermele
PRL 112, 167203 '1

Ergodicity: Keep in mind, there are other difficulties besides the sign problem.

e.g.) How does one sample $H_b^{\text{off-d}} = -\frac{J}{2}(S_i^+ S_j^- + S_i^- S_j^+)$ in $d+1$?



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



But this type of (local) move is demonstratably non-ergodic in "winding #".

$\Rightarrow$ will not be able to measure superfluid density $\rho_s = T\langle W^2 \rangle$

Loop/worm updates: (Evertz '92, Sandvik/Syljuasen 2003, Prokof'ev)

- "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:

e.g. $$S(\vec{q}) = \frac{1}{N} \sum_{k,l} e^{i(\vec{r}_k - \vec{r}_l)\cdot\vec{q}} \langle S_k^z S_l^z \rangle$$

$$\chi = \beta/N \left\langle \left(\sum_{k=1}^{N} S_k^z \right)^2 \right\rangle$$

- expectation value of operators in d+1

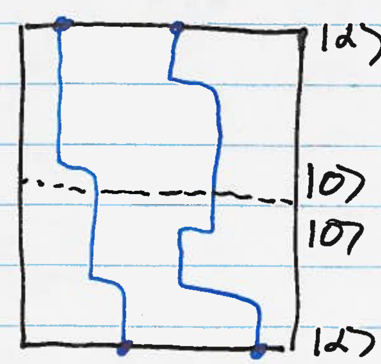
e.g. energy $E = -T\langle N \rangle$ $N = \#$ of operators

Green's function (with worm 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 QMC "projector" method:



$$Z = \langle 0|0\rangle$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \langle 0|\mathcal{O}|0\rangle$$

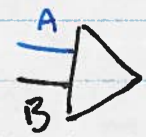
$$(-H)^m|\alpha\rangle = (-H)^m\left[\sum_n c_n |n\rangle\right]$$ (energy eigenstates)

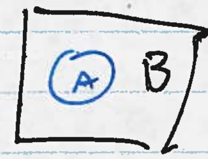
$$(-H)^m|\alpha\rangle = c_0|E_0|^m\left[|0\rangle + \frac{c_1}{c_0}\left(\frac{E_1}{E_0}\right)^m|1\rangle + \dots\right]$$

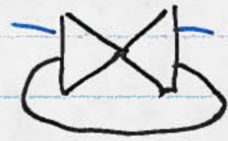
$$\to c_0|E_0|^m|0\rangle \quad \text{as} \quad \underline{m\to\infty}$$

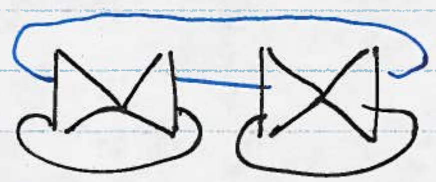
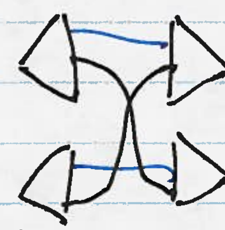
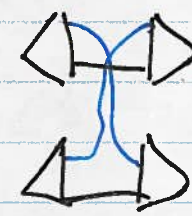
Assume that we can access the g.s. wavefunction

$|0\rangle \longrightarrow$  a vector in TN notation



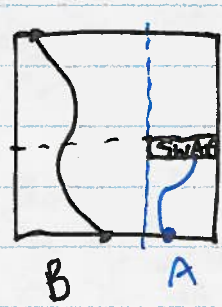
sub-divide indizes 

 $Tr_B(\rho) = \rho_A$

 $= Tr_A(\rho_A^2) =$  $=$ 

$= \langle 0\otimes 0|SWAP_A|0\otimes 0\rangle$

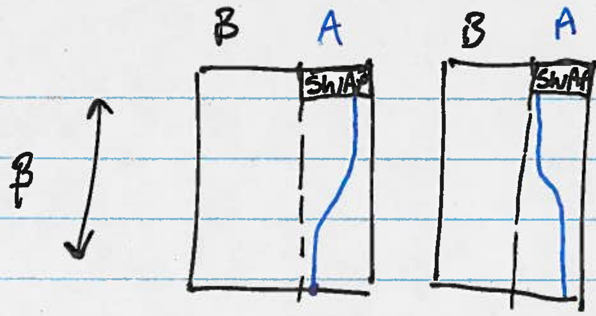
$$S_2 = -\log(Tr\,\rho_A^2) = -\log\left[\langle SWAP_A\rangle\right]$$



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

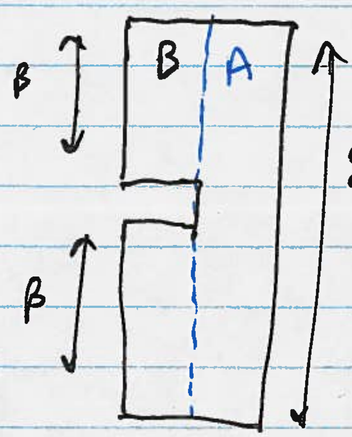
To translate to finite-T QMC, need to use PBC in imaginary time.

$$Z = \sum_\alpha \langle\alpha|e^{-\beta H}|\alpha\rangle$$



multi-sheeted
Riemann surface.

$=$



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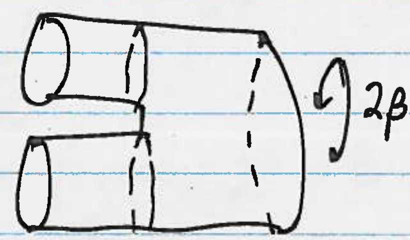

$= Z'[A,2,T]$

c.f. classical definition (Friday's lecture).

$$S_n(A) = \frac{1}{1-n}\log\left(\frac{Z'[A,n,T]}{Z^n}\right), \quad n\text{-sheets}.$$