Stochastic Series Expansion

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Reading: "Quantum Monte Carlo with Directed Loops"
Syljuåsen and Sandvik, PRE 66, 046701

Goal of QMC: to evaluate the expectation value of an operator $\hat{O}$:

$$\langle O \rangle = \frac{1}{Z} Tr\{ e^{-\beta \hat{H}} O \}$$

alternately, in Monte Carlo, we are used to writing this as a sum over all possible system "configurations", X, with weights W_X

$$\langle O \rangle = \frac{\sum_X O(x) W_X}{\sum_X W_X}, \quad \text{where } \sum_X = \text{sum over all "configurations"}$$

E.g. classically, the weight $W_X \propto e^{-\beta E(x)}$.
In quantum mechanics, not so simple...

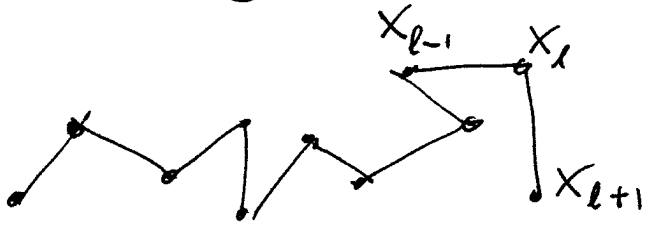
Our task is to construct weights for a quantum configuration, and a method to sample configurations. If we sample a list of configurations $l = 1 \cdots L$ according to their respective weights, then

$$\langle O \rangle = \langle O(x) \rangle_W = \frac{1}{L} \sum_{l=1}^{L} O(x_l)$$

when $L \to \infty$

the list of configurations is a "Markov Chain"
- each configuration X_ℓ depends only on $X_{\ell-1}$, and is chosen by a (positive) probability: $P(X_{\ell-1} \to X_\ell)$

- any two states must be connected by a finite sequence (a finite chain length)
  ⇒ "ergodicity"



configuration space

- "detailed balance" $W_x(P(x \to y) = W_y P(y \to x)$

<u>Constructing a QMC</u>: determine what are your configurations x, their respective weights W_x, and the transition probabilities $P(x \to y)$.

A configuration is
- a basis state $|\alpha\rangle$ (say S^z or valence-bond)
- a set of world lines or an operator list (in "d+1" dimensions...)

Finite-T QMC: W and P derived from

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

SSE (Handscomb, Sandvik) an approximation-free method using

$$e^{-\beta\hat{H}} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \hat{H}^n$$

($\hat{H}^n$: n times)

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

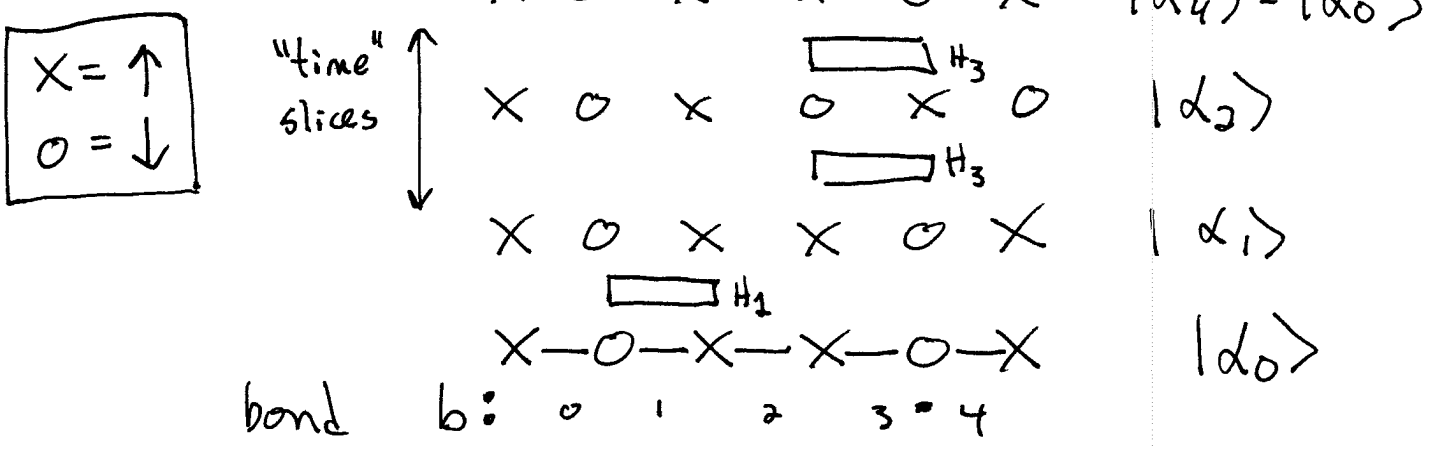
insert a resolution of the identity

$$= \sum_{\{\alpha\}} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \langle\alpha_0|\hat{H}|\alpha_1\rangle\langle\alpha_1|\hat{H}|\alpha_2\rangle\cdots\langle\alpha_{n-1}|\hat{H}|\alpha_n\rangle$$

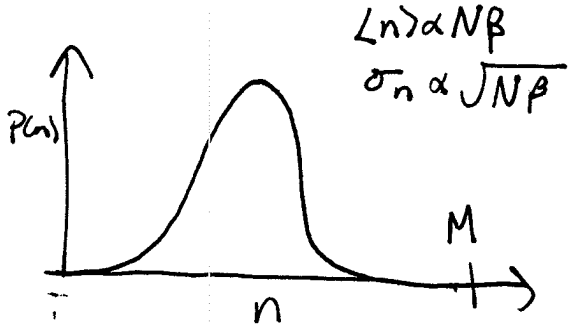
Time to define a "configuration" to sample: choose a product basis (S^z spins, boson density), and "Local" (bond) operators:

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

Then the picture is (1d spin system)



Sample the expansion order n with the bond operators & basis states



Simplest scheme: cut off the number of "slices" needed to some fixed value $M > n_{max}$.

Pad the remaining $M-n$ "time" slices with null (or zero) operators. There are

$$\binom{M}{n} = \frac{M!}{n!(M-n)!}$$ ways to do this.

The partition function of the fixed-length simulation cell must be divided by this #:

$$Z = \sum_{\{\alpha\}} \sum_{\{H_b\}} \frac{(-\beta)^n (M-n)!}{M!} \langle \alpha_0 | H_{b1} | \alpha_1 \rangle \cdots \langle \alpha_{n-1} | H_{bn} | \alpha_n \rangle$$

↑ sampling includes $H = \Pi$, allowing n to fluctuate.

Now we are ready to devise different weights & updates schemes.

1) Diagonal update:
   - insert and remove operators
   -

To construct this update we need to split the Hamiltonian into diagonal and off-diag parts:

$$H = \sum_{b=1}^{N_b} H_b \quad (b \text{ labels "bonds" on a lattice})$$

$$H_b = H_{1,b} + H_{2,b} \quad (1 = \text{diagonal}, \; 2 = \text{off-diagonal})$$

for concreteness: XXZ model

$$H = \sum_{\langle i,j \rangle} \left[\Delta S_i^z S_j^z - \tfrac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \right]$$

diagonal part: $H_{1b} = \Delta S_{b_i}^z S_{b_j}^z$

Weights are proportional to the matrix elements:

$$\langle \uparrow\uparrow | H_{1b} | \uparrow\uparrow \rangle = \Delta/4$$
$$\langle \uparrow\downarrow | H_{1b} | \uparrow\downarrow \rangle = -\Delta/4$$
$$\langle \downarrow\uparrow | H_{1b} | \downarrow\uparrow \rangle = -\Delta/4$$
$$\langle \downarrow\downarrow | H_{1b} | \downarrow\downarrow \rangle = \Delta/4$$

The probability to insert or remove one diagonal operator in the simulation cell, size M: contains the ratio of weights before and after:

$$\circledast \quad W(\alpha, \{H_b\}) = \frac{(-\beta)^n (M-n)!}{M!} \prod_{p=0}^{M-1} W(p), \quad W_p = \langle \alpha_p | H_b | \alpha_{p+1} \rangle$$

To insert an operator on a blank timeslice has N_b ways to do it, but removing only has 1:

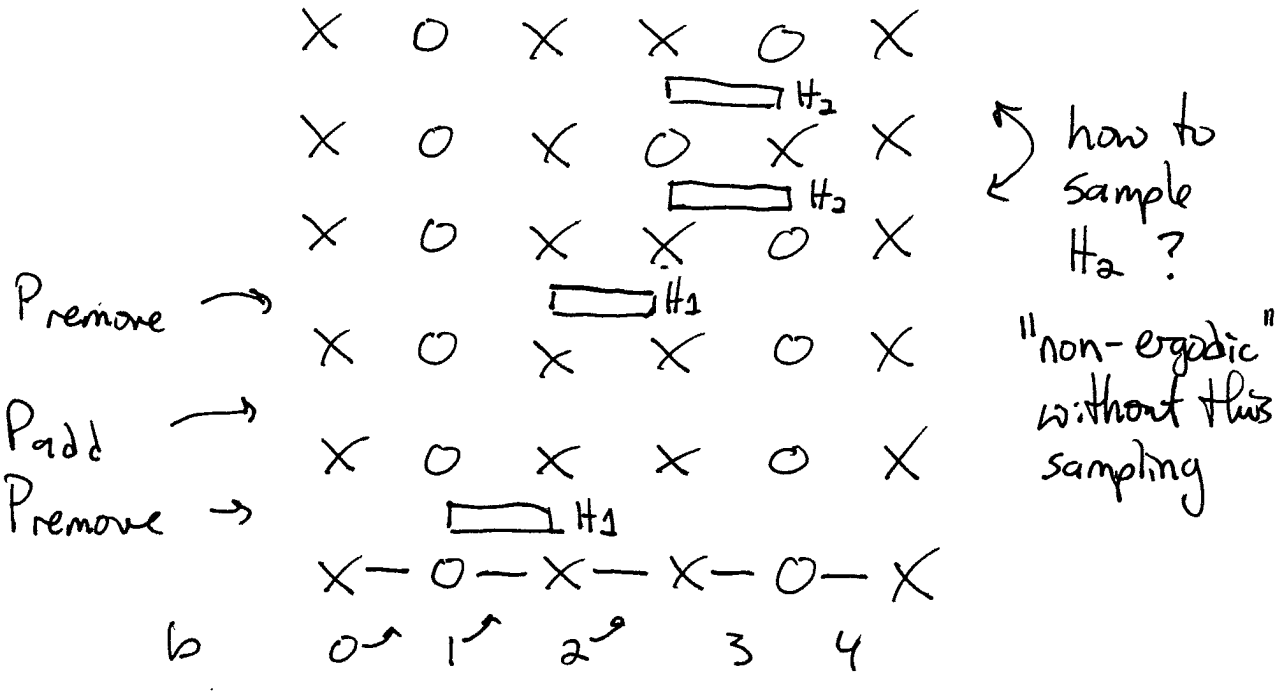
$$P_{add}(n \to n+1) = \frac{(-\beta)^{n+1}}{(-\beta)^n} \frac{(M-(n+1))!}{(M-n)!} \langle \alpha_p | H_b | \alpha_{p+1} \rangle N_b$$

$$= N_b \frac{(-\beta)}{(M-n)} \langle \alpha_p | H_b | \alpha_{p+1} \rangle$$

$$P_{remove}(n \to n-1) = \frac{(M-n+1)}{N_b (-\beta) \langle \alpha_p | H_b | \alpha_{p+1} \rangle}$$

These are the transition probabilities: but they can be negative! - the simplest "sign problem" to fix: add or subtract a constant CN_b from the Hamiltonian to make $P > 0$.

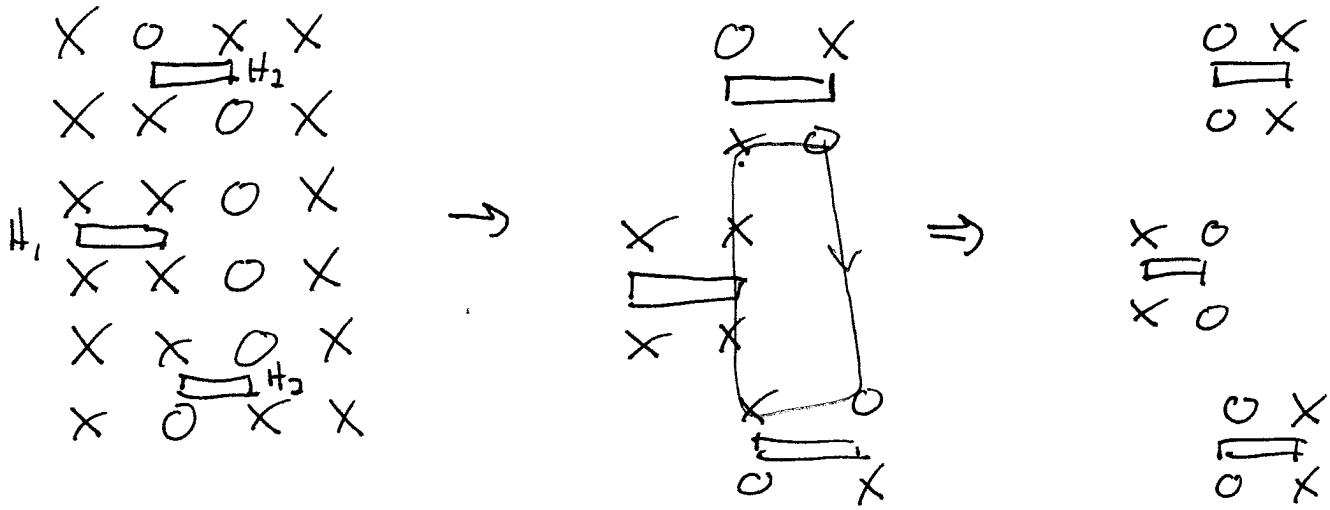
e.g. $H_{1b} \to H_{1b} - \Delta/4$ will do it.



2) Off diagonal updates

- Local (change 2 "neighboring" operators): very inefficient, cannot sample winding numbers.
- Operator-loop, "Worm", (Evertz, Sandvik, Syljv.)

Imagine abstracting several operators:



- efficiently samples both H_1 and H_2 type operators.
- samples different magnetization states (when loops wind "temporally") and winding numbers (winding over PBCs).

An transition probability table need to be constructed for each loop-building step:

$$\frac{\circ\ \circ}{\circ\ \circ} \Rightarrow \frac{\circ\ \circ}{\circ\ \circ} \text{ or } \frac{\times\ \circ}{\circ\ \times} \text{ or } \frac{\circ\ \times}{\times\ \circ}$$

incoming ↑ (4^{th} case not allowed in $\vec{H}$)

ie: transition probabilities depend on incoming "leg", outgoing "leg" and "vertex" type.

Simplest: Probability of selecting an exit $\propto$ to matrix element

One more to calculate: $\langle\uparrow\downarrow|H_{2b}|\downarrow\uparrow\rangle = -\frac{1}{2}$

nob: Let's take the full weight ⊛ and absorb the $(-1)^n$ into the matrix element of each operator (each of which is negative).

with $G = -\Delta/4$

$$\langle\uparrow\uparrow|H_1|\uparrow\uparrow\rangle = \langle\downarrow\downarrow|H_1|\downarrow\downarrow\rangle = 0 = W_1$$
$$\langle\uparrow\downarrow|H_1|\uparrow\downarrow\rangle = \langle\downarrow\uparrow|H_1|\downarrow\uparrow\rangle = \Delta/2 = W_2$$
$$\langle\uparrow\downarrow|H_2|\downarrow\uparrow\rangle = \langle\downarrow\uparrow|H_2|\uparrow\downarrow\rangle = \tfrac{1}{2} = W_3$$

Then (e.g.)

$$P\left(\begin{array}{cc} \circ & \circ \\ \uparrow & \circ \end{array} \to \begin{array}{cc} \circ & \times \\ \times & \circ \end{array}\right) = \frac{\langle\updownarrow|H_2|\downarrow\uparrow\rangle}{\langle\uparrow\downarrow|H_1|\uparrow\downarrow\rangle + \langle\downarrow\downarrow|H_1|\downarrow\downarrow\rangle + \langle\uparrow\downarrow|H_2|\downarrow\uparrow\rangle}$$

is a "heat bath" solution to an update transition probability.

Main efficiency drawback: large "bounce" probabilities. Can be eliminated with generalizations:

- directed loops (Syljuasen and Sandvik)
- generalized d.l. (Alet, Wessel, Troyer)

3) Other updates (used less frequently)
- "Wolff" type (multi-branch) cluster updates: long range / ring exchange models
- high-temperature spin-flip updates.

Questions: A) What can we measure?
B) What models can we do?
C) What models are impossible?

A) - anything diagonal in the basis $|\alpha\rangle$:

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

Static susceptibility: $\chi_s(\vec{q}) = \frac{1}{N}\sum_{k,l} e^{i(\vec{r}_k - \vec{r}_l)\cdot\vec{q}} \int_0^\beta d\tau \langle S_k^z(\tau) S_l^z(0)\rangle$

e.g. compressibility: $\chi_s(0,0) = \frac{\beta}{N}\left\langle \left(\sum_{k=1}^{N} S_k^z\right)^2 \right\rangle$

- expectation values of operators:

most important $\langle H_t \rangle = \frac{\langle N[t]\rangle}{\beta}$ (N = number of operators type t)

gives the energy $E = \frac{-\langle n\rangle}{\beta}$

- Correlation functions of operators that occur in the Hamiltonian

e.g.) $\langle B_a B_b \rangle = \frac{1}{\beta^2} \langle (n-1) N[a,b] \rangle$

where $B_a = \frac{1}{2}(S^+_{a_i} S^-_{a_j} + S^-_{a_i} S^+_{a_j})$ and

$N[a,b]$ = the number of occurrences of B_a and B_b next to each other in the operator list (including the temporal PBC).

- superfluid density $\rho_s = \frac{\partial^2 E(\phi)}{\partial \phi^2}$

from the winding number $\rho_s^x = \frac{\langle W_x^2 \rangle}{\beta}$

B) A wide variety fo model types can be done:

- Hard- and soft-core bosons ($B_a = b^+_i b_j + b_i b^+_j$)
- SU(2) (Heisenberg) and SU(N)
- long range models ($J_1 - J_2$, dipolar interactions)
- symmetry breaking fields (uniform, staggered)
- multi-particle "ring" exchange

$\sum_{ijkl} (\vec{S}_i \vec{S}_j)(\vec{S}_k \vec{S}_l)$ or $\sum_{ijkl} (S^+_i S^-_j S^+_k S^-_l + h.c.)$

4) The most important restriction on models is the "sign problem": (see lecture by M. Troyer).

In the SSE, we see that the diagonal operators can *always* be made to give positive probabilities (transition) by adding CN_b to the Hamiltonian.

The difficult sign problem lies with off-diagonal terms: in our e.g.

$$H_{2b} = -\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$$

and the weight $W(\alpha, \{H_b\}) \propto (-\beta)^n \prod_{p=0}^{M-1} \langle \alpha_p | H_b | \alpha_{p+1} \rangle$

since the $(-1)^n$ cancelled each -ve sign from the matrix elements, $\langle H_b \rangle$, each weight is positive.

What about $H_{2b} = \oplus\frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)$?

case 1) Bipartite lattice (or lattice with even # of spins per "plaquette").

$|\alpha_3\rangle = |\alpha_0\rangle$ × × ○ ○ (□ H_2)

$|\alpha_2\rangle$ × ○ × ○

$|\alpha_1\rangle$ × ○ × ○ (□ H_2)

$|\alpha_0\rangle$ × × ○ ○

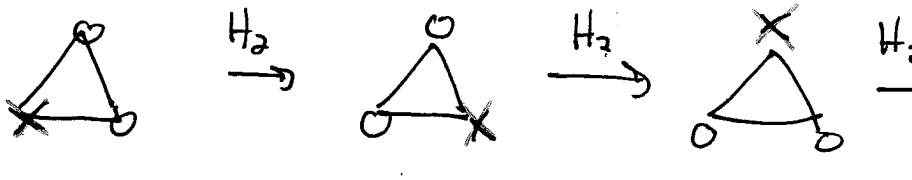
off-diagonal operators must occur in pairs. Since the un-cancelled part of the $(-1)^n$ is $(-1)^{n_2}$

n_2 = even $\Rightarrow W(\alpha, \{H_b\}) > 0$ always!

Case 2) Lattice with odd # of sites per plaquette:
eg triangular

2 "hops" 

$\Rightarrow (-1)^2 = 1$

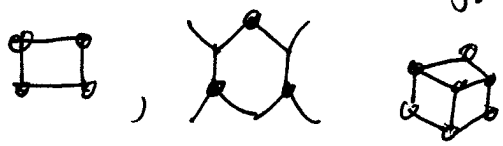
3 "hops" 

$\Rightarrow (-1)^3 = -1$

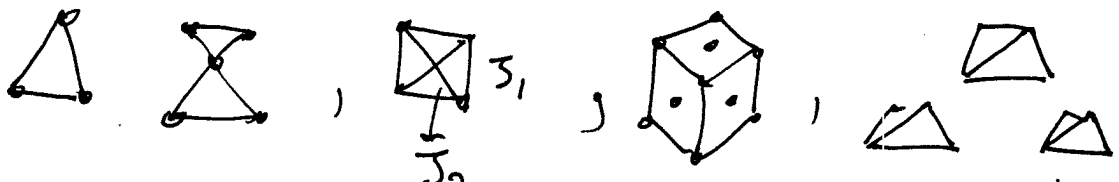
so n_2 can be odd, and you get the possibility of negative weights.

Theorem: If a path can be found through the lattice that takes an odd number of "hops" (ie off-diagonal operations of any length), then the sign problem can occur.
(Sometimes a clever basis rotation can get rid of this).

e.g.) No sign problem: $H = \sum_{\langle ij \rangle} \left(S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \right)$

on  , etc.

However this has an uncorrectable sign problem on



pyrochlore.