

Stochastic Series Expansion quantum Monte Carlo

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Ref.

Quantum Spin Systems, A. W. Sandvik, AIP Conf. Proc. **1297**, 135 (2010)

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Classical analogue

Thermal expectation value from classical statistical mechanics

$$\langle f \rangle = \frac{1}{Z} \sum_{\{\sigma\}} f(\sigma) e^{-\beta E(\sigma)}, \quad Z = \sum_{\{\sigma\}} e^{-\beta E(\sigma)}$$
$$\sigma \equiv (\sigma_1, \sigma_2, \dots, \sigma_N)$$

Can be evaluated using standard Monte Carlo method – importance sampling of the configurations according to the Boltzmann probability distribution (Metropolis algorithm)

$$P(\sigma) = \frac{1}{Z} W(\sigma), \quad W(\sigma) = e^{-\beta E(\sigma)}$$

The exponential can be expanded in a Taylor series

$$\langle f \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sum_{n=0}^{\infty} f(\sigma) \frac{(-\beta E(\sigma))^n}{n!}, \quad Z = \sum_{\{\sigma\}} \sum_{n=0}^{\infty} \frac{(-\beta E(\sigma))^n}{n!}$$

Expanded configuration / sampling space – Monte Carlo sampling possible if all terms are positive – can be ensured by subtracting a constant from the energy – does not change the physics. Weight for sampling extended configuration space is

$$W(\sigma, n) = \frac{\beta^n [\epsilon - E(\sigma)]^n}{n!}$$

Let us now look at the calculation of a couple of observables:

Energy: $H = \epsilon - E$

$$\langle H \rangle = \frac{1}{Z} \sum_{\{\sigma\}, n} H(\sigma) W(\sigma, n), \quad Z = \sum_{\{\sigma\}, n} W(\sigma, n), \quad W(\sigma, n) = \frac{\beta^n H(\sigma)^n}{n!}$$

Shifting the summation index $n \rightarrow n + 1$

$$\sum_{\{\sigma\}, n} H(\sigma) W(\sigma, n) = \sum_{\{\sigma\}, n} \frac{n}{\beta} W(\sigma, n)$$

The expectation value simplifies to

$$\langle H \rangle = \frac{1}{\beta} \langle n \rangle_W \quad \Rightarrow \quad E = \epsilon - \frac{1}{\beta} \langle n \rangle_W$$

SSE: basic principles

Thermal expectation value of an operator A for a system described by a Hamiltonian H

$$\langle A \rangle = \frac{1}{Z} \text{Tr} \{ A e^{-\beta H} \}, \quad Z = \text{Tr} \{ e^{-\beta H} \}$$

Problem: evaluate exponential of the Hamiltonian – non-commuting terms.


Expand the density matrix in a Taylor series and express the trace as a sum over all states in a suitably chosen basis

$$Z = \sum_{\{\alpha\}} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha | (-H)^n | \alpha \rangle$$

The S=1/2 Heisenberg model:

For concreteness, let us consider the S=1/2 Heisenberg model

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad |\alpha\rangle \equiv |S_1^z, S_2^z, \dots, S_N^z\rangle, \quad S_i^z = \pm \frac{1}{2}$$


Basis

Separate the Hamiltonian into Ising and exchange terms and express as a sum over bonds

$$H = J \sum_{b=1}^{N_b} \left[S_{i(b)}^z S_{j(b)}^z + \frac{1}{2} \left(S_{i(b)}^+ S_{j(b)}^- + S_{i(b)}^- S_{j(b)}^+ \right) \right]$$

Introduce the bond operators

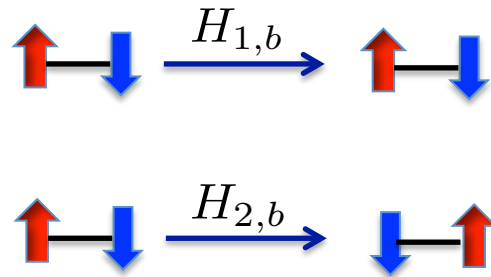
$$H_{1,b} = \frac{1}{4} - S_{i(b)}^z S_{j(b)}^z, \quad H_{2,b} = \frac{1}{2} \left(S_{i(b)}^+ S_{j(b)}^- + S_{i(b)}^- S_{j(b)}^+ \right)$$

where we have introduced an additive constant to the Ising term – this will help ensure positivity of the Boltzmann weights

The Hamiltonian takes the form

$$H = -J \sum_{b=1}^{N_b} [H_{1,b} - H_{2,b}] + \frac{JN_b}{4}$$

In the chosen basis, the Ising and the exchange terms act as diagonal and off-diagonal operators respectively



Indeed, with the particular choice of ε , there are only 4 non-zero matrix elements on any bond

$${}_b \langle \uparrow \downarrow | H_{1,b} | \uparrow \downarrow \rangle_b = \frac{1}{2}$$

$${}_b \langle \uparrow \downarrow | H_{2,b} | \downarrow \uparrow \rangle_b = \frac{1}{2}$$

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$${}_b \langle \downarrow \uparrow | H_{2,b} | \uparrow \downarrow \rangle_b = \frac{1}{2}$$

The powers of the Hamiltonian operator can now be expressed as a sum over all possible strings of bond operators

$$(-H)^n = \sum_{\{H_{a,b}\}} (-1)^{n_2} \prod_{p=1}^n H_{a[p],b[p]}$$

n_2 is the number of off-diagonal operators in the string. The bond operators do not commute – hence the order of the operators in the sequence is important

The Taylor series expanded partition function can now be written as

$$Z = \sum_{\{\alpha\}} \sum_{n=0}^{\infty} (-1)^{n_2} \frac{\beta^n}{n!} \sum_{S_n} \left\langle \alpha \left| \prod_{p=1}^n H_{a[p],b[p]} \right| \alpha \right\rangle$$

where S_n denotes the collection of all possible strings of bond operators of length n

$$S_n = \{a[1], b[1]\}, \{a[2], b[2]\}, \dots, \{a[n], b[n]\},$$

Computationally, it is much more convenient to work with operator strings of fixed length, rather than of variable lengths. We convert all operator strings to length L by padding with unit operators

$$H_{0,0} = \mathbb{1}$$

The value of L is determined dynamically during the equilibration stages such that the truncation results in an exponentially small, completely negligible error. Since the unit operators can be introduced at any position in the operator string,

$$Z = \sum_{\{\alpha\}} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L - n)!}{L!} \left\langle \alpha \left| \prod_{p=1}^L H_{a[p],b[p]} \right| \alpha \right\rangle$$

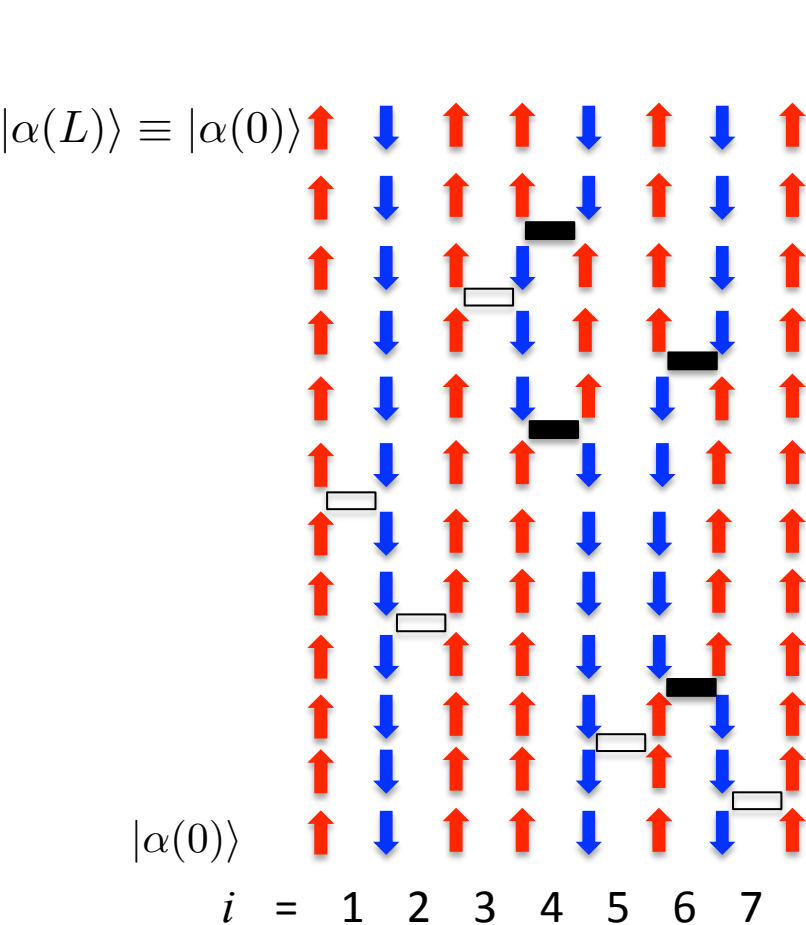
For non-zero contribution to the trace, the off-diagonal operators must occur in pairs. Hence n_2 is necessarily even for relevant operator strings. Alternatively, for *bipartite* lattices, one can apply a sublattice rotation that maps the AFM exchange to FM exchange without altering the energy spectrum.

For future convenience, let us introduce the state of the system after propagation through the first p terms in the operator string as

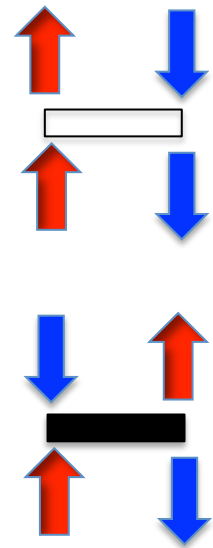
$$|\alpha[p]\rangle \propto \prod_{i=1}^p H_{a[i],b[i]} |\alpha[0]\rangle$$

Graphical representation

Represent the combined configuration space of operator strings + spin states graphically for an intuitive explanation of the SSE algorithm



p	$a(p)$	$b(p)$
11	0	0
10	2	4
9	1	3
8	2	6
7	2	4
6	1	1
5	0	0
4	1	2
3	2	6
2	1	5
1	1	7



Vertex

Monte Carlo scheme

Goal is to sample all configurations (α, S_L) according to their weights

$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

Attempt updates $(\alpha, S_L) \rightarrow (\alpha', S'_L)$

(1) Diagonal update

Go through the operator sequence and attempt to replace every unit operator by a diagonal operator (at a randomly chosen bond) and vice-versa – changes the expansion power $n \leftrightarrow n + 1$

$$[0, 0]_p \leftrightarrow [1, b]_p$$

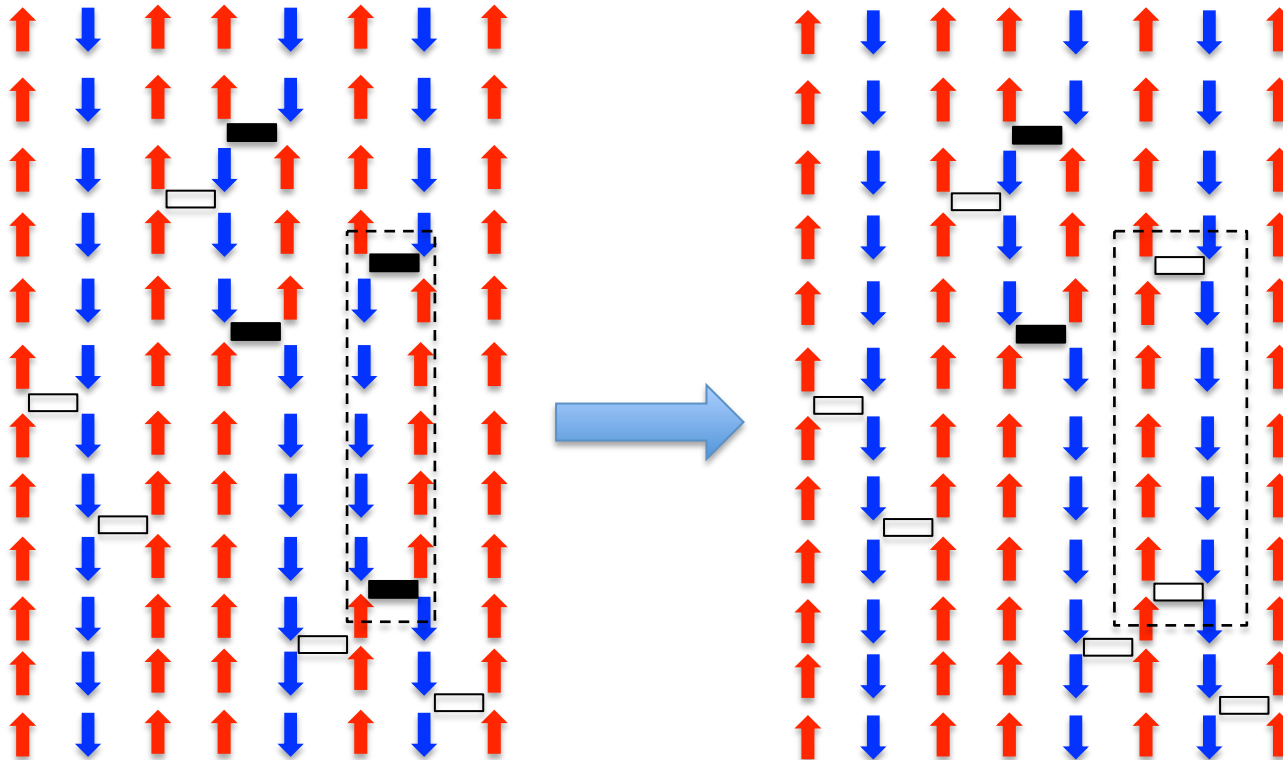
Acceptance probabilities

$$P_{\text{accept}}([0, 0]_p \rightarrow [1, b]_p) = \min \left[\frac{\beta N_b}{2(L-n)}, 1 \right]$$

$$P_{\text{accept}}([1, 0]_p \rightarrow [0, 0]_p) = \min \left[\frac{2(L-n+1)}{\beta N_b}, 1 \right]$$

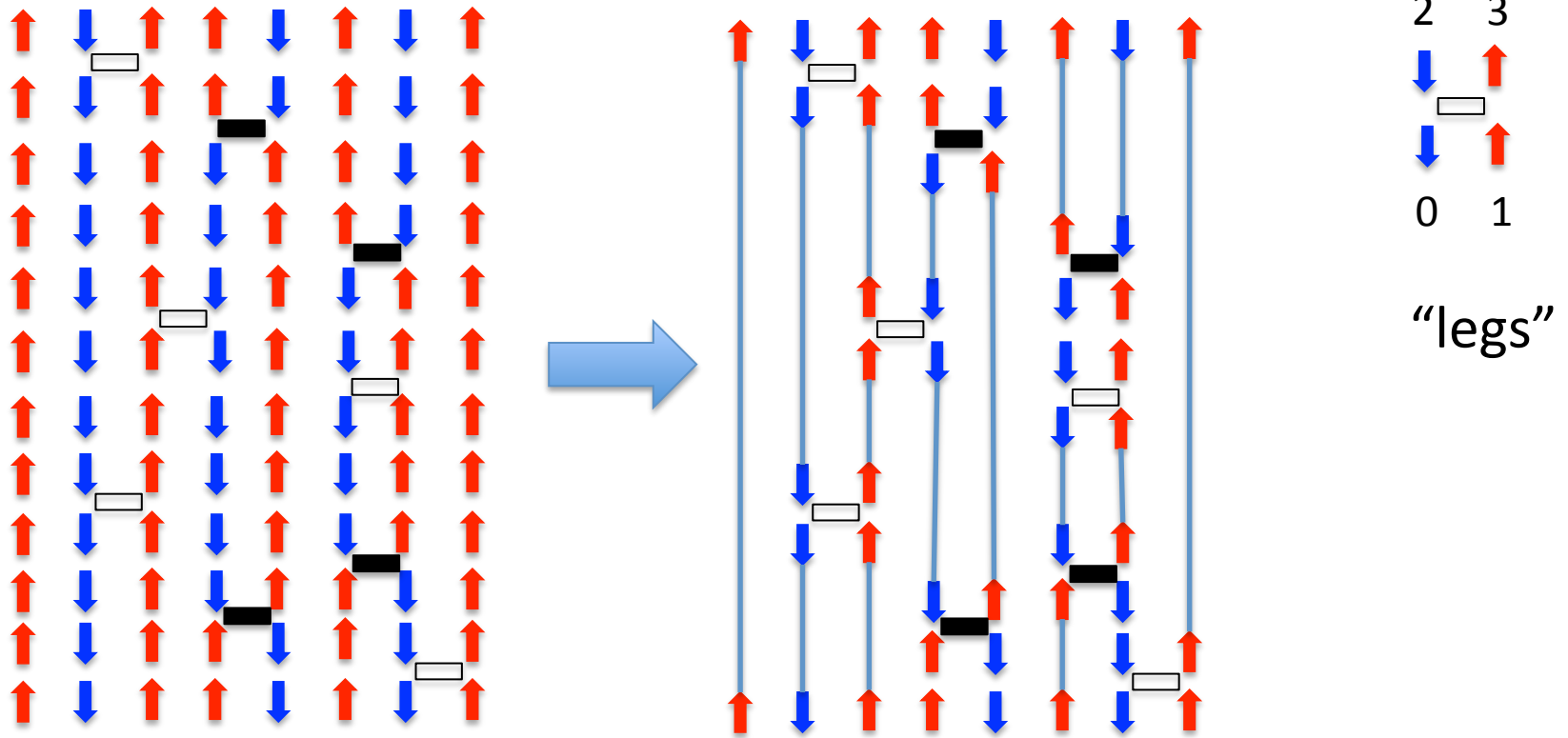
(2) Off-diagonal update

Pair flip: Identify pairs of diagonal (off-diagonal) operators on the same bond with no other intervening operators on the relevant spins and change them to off-diagonal (diagonal) ops.



Not very efficient

Linked vertex list



Construct a linked list that stores the vertices and connections of each leg of the linked vertex-leg combination

Probabilistic loop update

- Choose a vertex at random
- Choose an “entry leg” at random
- Make an update of the state at the entry leg
- Choose an “exit leg” according to probabilities calculated based on the weights of the resulting vertex – make the appropriate update of the state at the exit leg
- Follow the linked list to the next vertex/leg connected to the exit leg
- Continue till loop closes.

Measurements

(1) Total energy: $E = \varepsilon - \frac{\langle n \rangle}{N\beta}$

(2) Static longitudinal spin-spin correlation: $C(i, j) = \langle S_i^z S_j^z \rangle$

In terms of the propagated state through the operator string,

$$C(i, j) = \left\langle \frac{1}{n+1} \sum_{p=0}^n S_i^z[p] S_j^z[p] \right\rangle, \quad S_i^z[p] = \langle \alpha[p] | S_i^z | \alpha[p] \rangle$$