# SSE formalism and program implementation for S=1/2 Heisenberg models (and a bit about TFIMs)

arXiv:1101.3281 [pdf, ps, other] cond-mat.str-el hep-lat doi

**Computational Studies of Quantum Spin Systems**

arXiv:1909.10591 [pdf, other] cond-mat.str-el

**Stochastic Series Expansion Methods**

# Series expansion representation

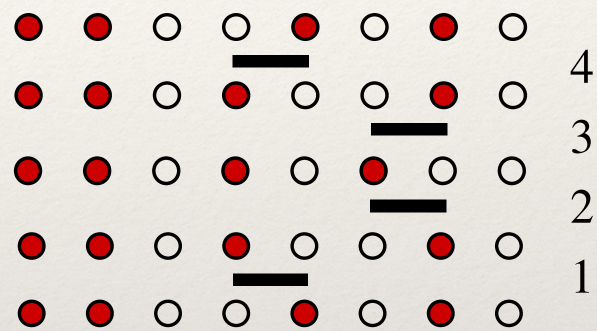
Start from the **Taylor expansion** (no approximation)

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\alpha_0} \langle \alpha_0 | H^n | \alpha_0 \rangle$$

**Index sequence** (string) referring to terms of H

$$H = \sum_{i=1}^{m} H_i \qquad S_n = (a_1, a_2, \ldots, a_n)$$

$$a_i \in \{1, \ldots, m\}$$




**Break up $\mathbf{H^n}$** into strings:

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\alpha_0} \sum_{S_n} \langle \alpha_0 | H_{a_n} \cdots H_{a_2} H_{a_1} | \alpha_0 \rangle$$

We should have (always possible): $H_i |\alpha_j\rangle \propto |\alpha_k\rangle$

- **no branching** during propagation with operator string
- some strings not allowed (illegal operations)

For hard-core bosons the (allowed) path weight is: $W(S_n, \alpha_0) = \dfrac{\beta^n}{n!}$

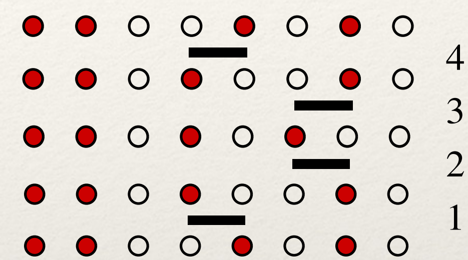
We can make this look more similar to a path integral by introducing partially propagated states: $|\alpha_p\rangle = H_{a_p} \cdots H_{a_2} H_{a_1} |\alpha_0\rangle$

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\alpha_0} \sum_{S_n} \langle \alpha_0 | H_{\alpha_n} | \alpha_{n-1} \rangle \langle \alpha_{n-1} | \cdots | \alpha_1 \rangle \langle \alpha_1 | H_{a_1} | \alpha_0 \rangle$$

$$|\alpha_n\rangle = |\alpha_0\rangle$$

Same looking paths, different weights

- we can relate to continuous time (**arXiv:1909.10591**)




**Energy:** $$\langle H \rangle = \frac{1}{Z} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\alpha_0} \langle \alpha_0 | H^n H | \alpha_0 \rangle$$

Relabel terms of n-sum: replace n+1 by n

$$\langle H \rangle = -\frac{1}{Z} \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{n}{\beta} \sum_{\alpha_0} \langle \alpha_0 | H^n | \alpha_0 \rangle$$

we can extend the sum to include n=0, because that term vanishes

Therefore the energy is: $E = -\langle n \rangle / \beta$

Can also derive specific heat: $C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle$

Follows: $\langle n \rangle \propto \beta N, \quad \sigma_n \propto \sqrt{\beta N}$

## Fixed string-length scheme

- n fluctuating → varying size of the sampled configurations
- the expansion can be truncated at some $n_{max}=L$
  (exponentially small error if large enough)
- cutt-off at n=L, fill in operator string with unit operators **$H_0=I$**

| n=10 | $H_4$ | $H_7$ | $H_1$ | $H_6$ | $H_2$ | $H_1$ | $H_8$ | $H_3$ | $H_3$ | $H_5$ | $\Longrightarrow$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

| L=14 | $H_4$ | I | $H_7$ | I | $H_1$ | $H_6$ | I | $H_2$ | $H_1$ | $H_8$ | $H_3$ | $H_3$ | I | $H_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

- conisider all possible locations in the sequence
- overcounting of original strings, correct by

$$\binom{L}{n}^{-1} = \frac{n!(L-n)!}{L!}$$

$$Z = \sum_{\alpha_0} \sum_{S_L} \frac{(-\beta)^n (L-n)!}{L!} \langle \alpha_0 | H_{a_m} \cdots H_{a_2} H_{a_1} | \alpha_0 \rangle$$

Here n is the number of $H_i$, i>0 instances in the sequence of L ops
- the summation over n is now implicit

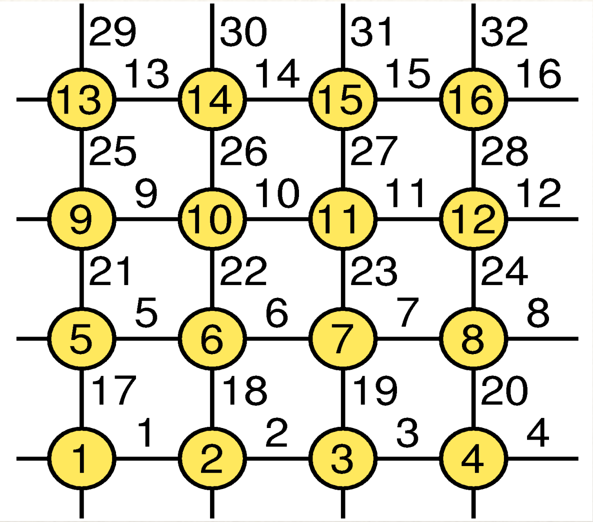
**L can be chosen automatically by the simulation** (shown later)

# Stochastic Series expansion (SSE): S=1/2 Heisenberg model

Write H as a bond sum for arbitrary lattice

$$H = J \sum_{b=1}^{N_b} \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)},$$

2D square lattice
bond and site labels




Diagonal (1) and off-diagonal (2) bond operators

$$H_{1,b} = \frac{1}{4} - S^z_{i(b)} S^z_{j(b)},$$

$$H_{2,b} = \frac{1}{2}(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}).$$

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

Four non-zero matrix elements

$$\langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{1,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \frac{1}{2} \qquad \langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{2,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \frac{1}{2}$$

$$\langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{1,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \frac{1}{2} \qquad \langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{2,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \frac{1}{2}$$

Partition function

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

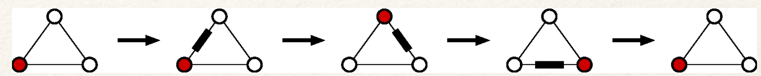
$n_2$ = number of a(i)=2 (off-diagonal operators) in the sequence

Index sequence: $S_n = [a(0), b(0)], [a(1), b(1)], \ldots, [a(n-1), b(n-1)]$

For fixed-length scheme

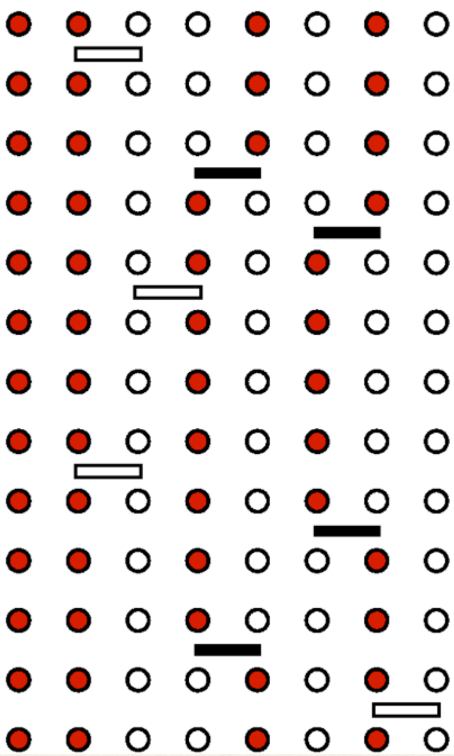
$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

W>0 ($n_2$ even) for bipartite lattice
Frustration leads to **sign problem**



Propagated states: $|\alpha(p)\rangle \propto \prod_{i=0}^{p-1} H_{a(i),b(i)} |\alpha\rangle$

| $i$ | = | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|---|---|---|---|---|---|---|---|---|---|
| $\sigma(i)$ | = | -1 | +1 | -1 | -1 | +1 | -1 | +1 | +1 |



| $p$ | $a(p)$ | $b(p)$ | $s(p)$ |
|---|---|---|---|
| 11 | 1 | 2 | 4 |
| 10 | 0 | 0 | 0 |
| 9 | 2 | 4 | 9 |
| 8 | 2 | 6 | 13 |
| 7 | 1 | 3 | 6 |
| 6 | 0 | 0 | 0 |
| 5 | 0 | 0 | 0 |
| 4 | 1 | 2 | 4 |
| 3 | 2 | 6 | 13 |
| 2 | 0 | 0 | 0 |
| 1 | 2 | 4 | 9 |
| 0 | 1 | 7 | 14 |

**In a program:**

s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

σ(i) = spin state, i=1,...,N
- only one has to be stored

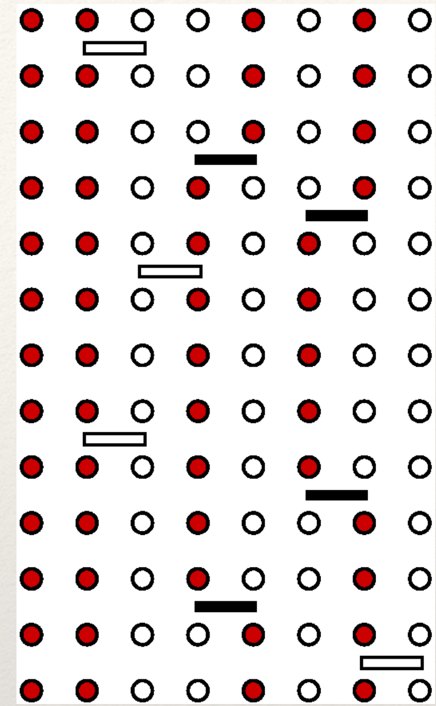
**SSE effectively provides a discrete representation of the time continuum!**
- computational advantage; only integer operations in sampling

## Monte Carlo sampling scheme

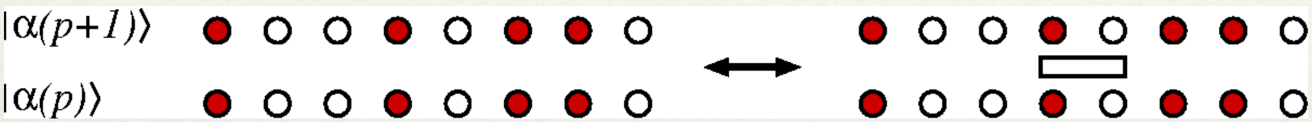
Change the configuration; $(\alpha, S_L) \to (\alpha', S'_L)$

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

$$P_{\rm accept} = \min\left[\frac{W(\alpha', S_L)}{W(\alpha, S_L)} \frac{P_{\rm select}(\alpha', S'_L \to \alpha, S_L)}{P_{\rm select}(\alpha, S_L \to \alpha', S'_L)}, 1\right]$$



**Diagonal update:** $[0,0]_p \leftrightarrow [1,b]_p$




Attempt at p=0,...,L-1. Need to know |α(p)>

- generate by flipping spins when off-diagonal operator

$$P_{\rm select}(a=0 \to a=1) = 1/N_b, \quad (b \in \{1,\ldots,N_b\})$$

$$P_{\rm select}(a=1 \to a=0) = 1$$

$$\frac{W(a=1)}{W(a=0)} = \frac{\beta/2}{L-n} \qquad \frac{W(a=0)}{W(a=1)} = \frac{L-n+1}{\beta/2}$$

n is the current power

- n → n+1 (a=0 → a=1)
- n → n-1 (a=1 → a=0)

**Acceptance probabilities**

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

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

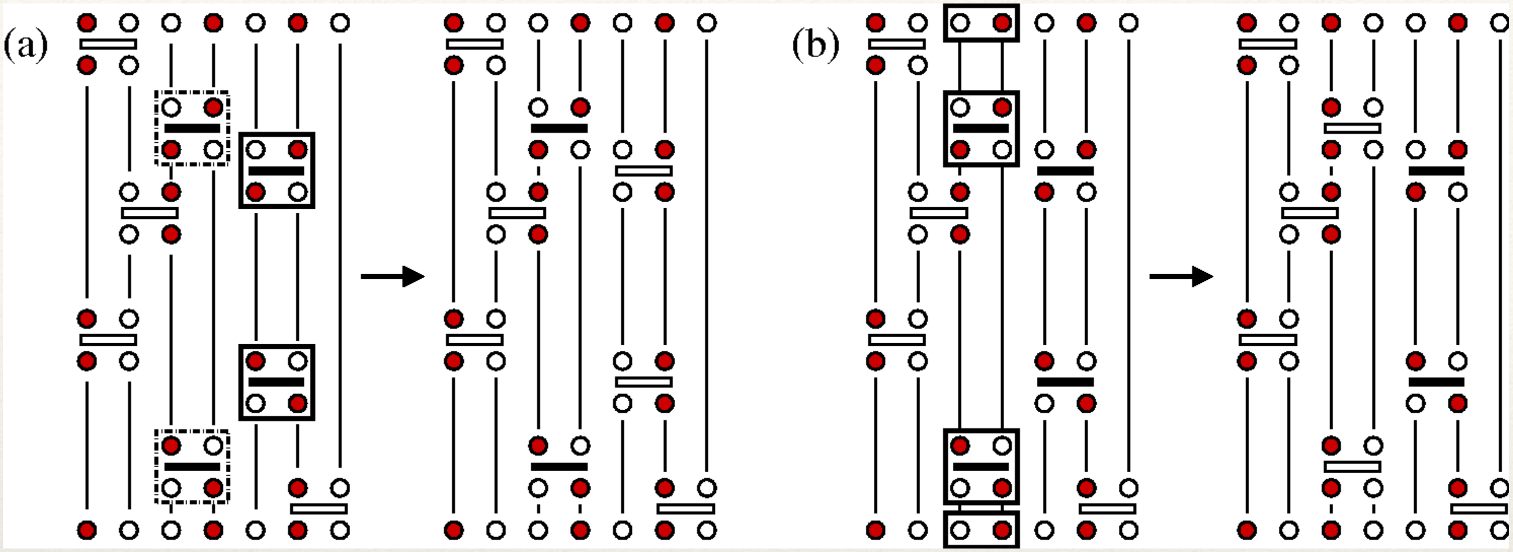
## Pseudocode: Sweep of diagonal updates

```
do p = 0 to L − 1
    if (s(p) = 0) then
        b = random[1, . . . , N_b]
        if  σ(i(b)) = σ(j(b)) cycle
        if (random[0 − 1] < P_insert(n)) then s(p) = 2b; n = n + 1 endif
    elseif (mod[s(p), 2] = 0) then
        if (random[0 − 1] < P_remove(n)) then s(p) = 0; n = n − 1 endif
    else
        b = s(p)/2; σ(i(b)) = −σ(i(b)); σ(j(b)) = −σ(j(b))
    endif
enddo
```

**Code explanation:**

- To insert operator, bond b generated at random among 1,...,$N_b$
  - can be done only if connected spins i(b),j(b) are anti-parallel
  - if so, do it with probability $P_{insert}(n)$
- Existing diagonal operator can always be removed
  - do it with probability $P_{remove}(n)$
- If off-diagonal operator, advance the state
  - extract bond b, flip spins at i(b),j(b)

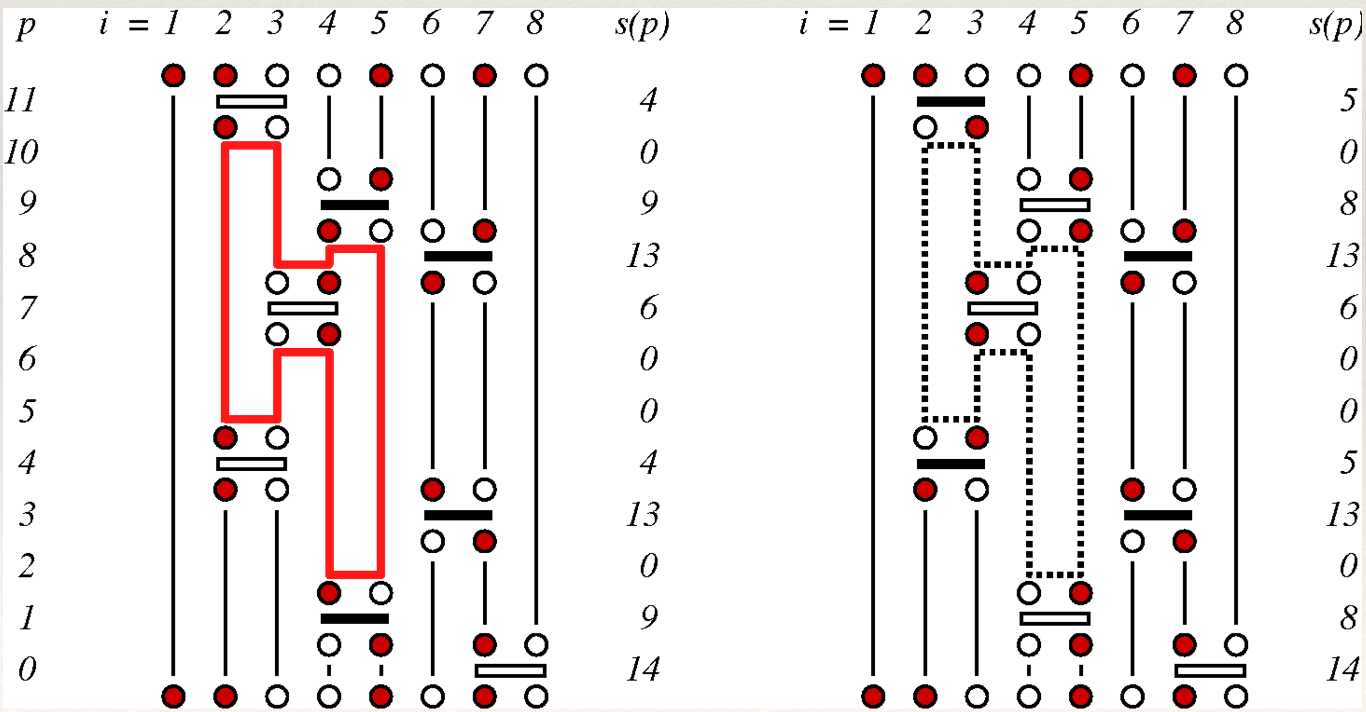
# Off-diagonal updates




**Local update**

Change the type of two operators

- constraints
- inefficient
- cannot change winding numbers




**Operator-loop update**

- Many spins and operators can be changed simultaneously
- can change winding numbers