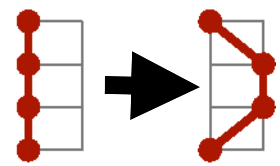
Including interactions

For any diagonal interaction V (Trotter, or split-operator, approximation)

$$e^{-\Delta_\tau H} = e^{-\Delta_\tau K} e^{-\Delta_\tau V} + \mathcal{O}(\Delta_\tau^2) \to \langle \alpha_{l+1} | e^{-\Delta_\tau H} | \alpha_l \rangle \approx e^{-\Delta_\tau V_l} \langle \alpha_{l+1} | e^{-\Delta_\tau K} | \alpha_l \rangle$$

Product over all times slices →

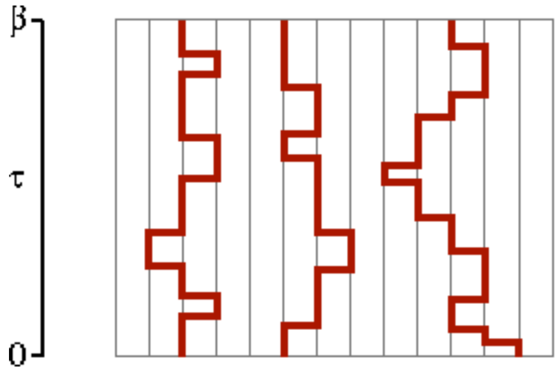
$$W(\{\alpha\}) = \Delta_\tau^{n_K} \exp\left(-\Delta_\tau \sum_{l=0}^{L-1} V_l \right)$$

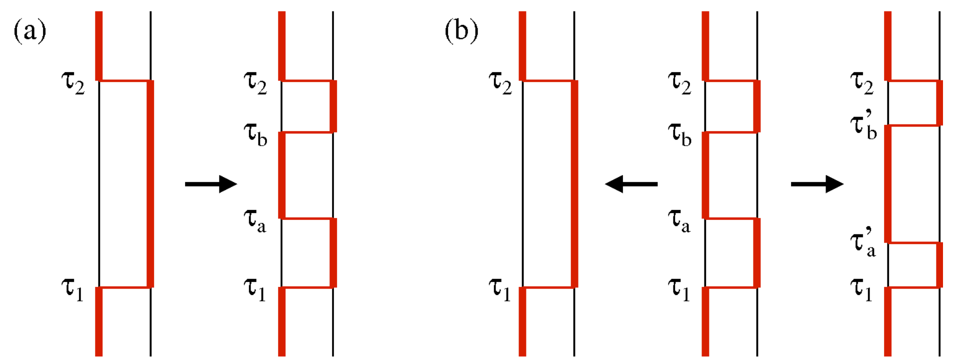


$$P_{\mathrm{acc}} = \min\left[\Delta_\tau^2 \frac{V_{\mathrm{new}}}{V_{\mathrm{old}}}, 1 \right]$$

The continuous time limit

Limit $\Delta_\tau \to 0$: number of kinetic jumps remains finite, store events only





Special methods (**loop and worm updates**) developed for efficient sampling of the paths in the continuum

local updates (problem when $\Delta_\tau \to 0$?)

- consider probability of inserting/removing events within a time window

⇐ Evertz, Lana, Marcu (1993), Prokofev et al (1996) Beard & Wiese (1996)

Series expansion representation

Start from the Taylor expansion $\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$ (approximation-free method from the outset)

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

Similar to the path integral; $1 - \Delta\tau H \to H$ and weight factor outside

For hard-core bosons the (allowed) path weight is $W(\{\alpha\}_n) = \beta^n / n!$

For any model, the energy is

this is the operator we "measure"

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

one more "slice" to sum over here

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

relabel terms to "get rid of" extra slice

$$C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle$$

From this follows: narrow n-distribution with $\langle n \rangle \propto N\beta, \quad \sigma_n \propto \sqrt{N\beta}$

Fixed-length scheme: cut-off at N=L, fill in with unit operators $H_0=1$

$$Z = \sum_{\{\alpha\}_L} \sum_{\{H_i\}} \frac{(-\beta)^n (L-n)!}{L!} \langle \alpha_0 | H_{i(L)} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | H_{i(2)} | \alpha_1 \rangle \langle \alpha_1 | H_{i(1)} | \alpha_0 \rangle$$

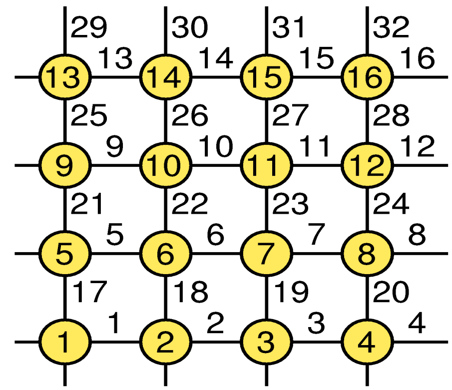
Here n is the number of H_i, i>0 instances in the sequence of L operators

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

$$\begin{aligned} H_{1,b} &= \tfrac{1}{4} - S^z_{i(b)} S^z_{j(b)}, \\ H_{2,b} &= \tfrac{1}{2}(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}). \end{aligned}$$

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

Four non-zero matrix elements

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

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

Partition function

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

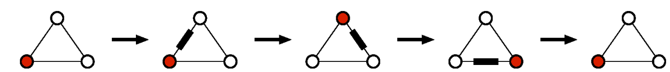
n_2 = number of a(i)=2 (off-diagonal operators) in the sequence

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

For fixed-length scheme

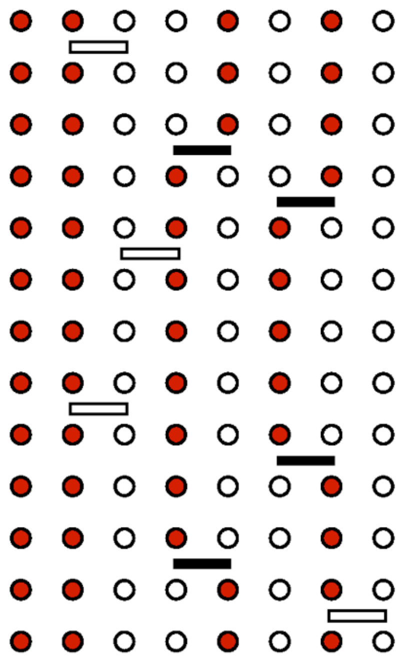
$$Z = \sum_{\alpha}\sum_{S_L}(-1)^{n_2}\frac{\beta^n (L-n)!}{L!}\left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

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:

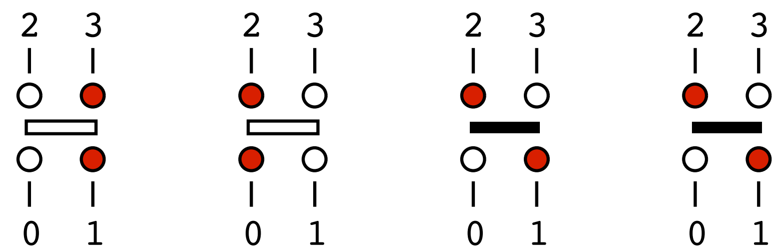
s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

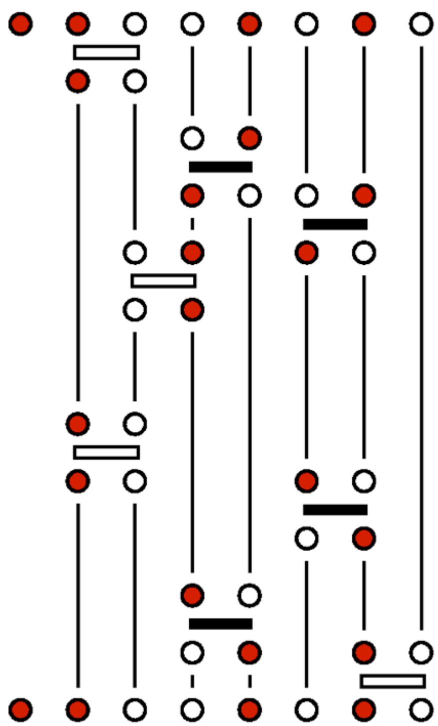
σ(i) = spin state, i=1,...,N
- only one has to be stored

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

Linked vertex storage

The "legs" of a vertex represents the spin states before (below) and after (above) an operator has acted





p	v	X(v)	v	X(v)	v	X(v)	v	X(v)
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	31	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
1	4	38	5	39	6	29	7	37
0	0	35	1	3	2	13	3	1
	$l=0$		$l=1$		$l=2$		$l=3$	

X( ) = vertex list

- operator at p→X(v)
  v=4p+l, l=0,1,2,3
- links to next and previous leg

Spin states between operations are redundant; represented by links

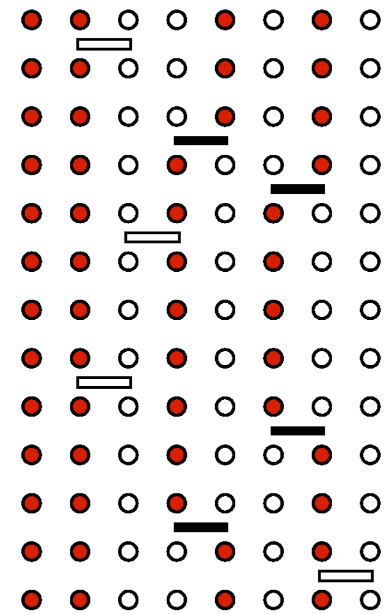
- network of linked vertices will be used for loop updates of vertices/operators

Monte Carlo sampling scheme

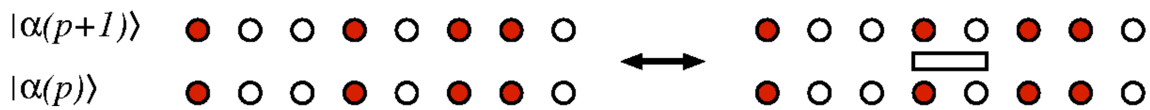
Change the configuration; $(\alpha, S_L) \to (\alpha', S'_L)$

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

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



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

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

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

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

n is the current power

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

Acceptance probabilities

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

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