Quantum Monte Carlo for spin systems

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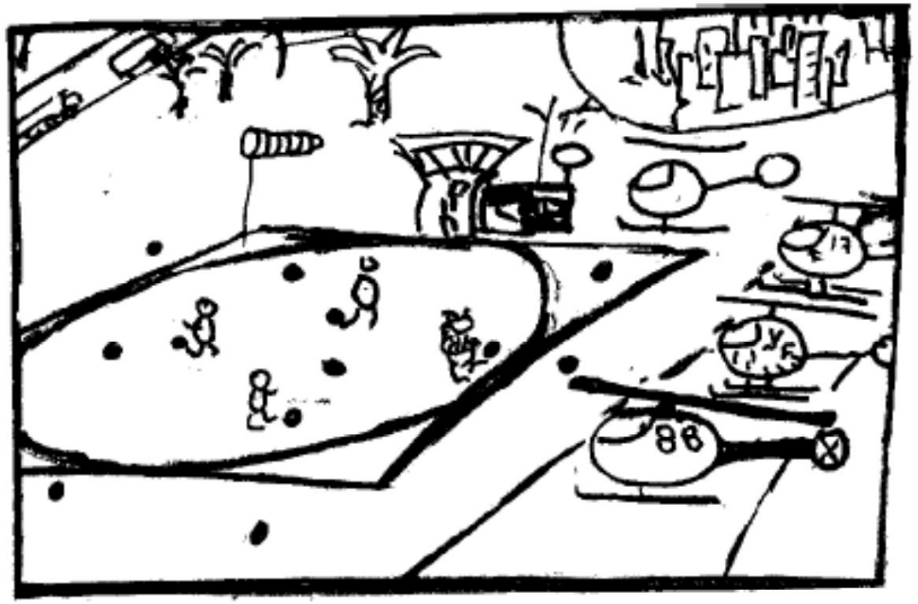
Nov.4, 2019

HKU-UCAS Study Group

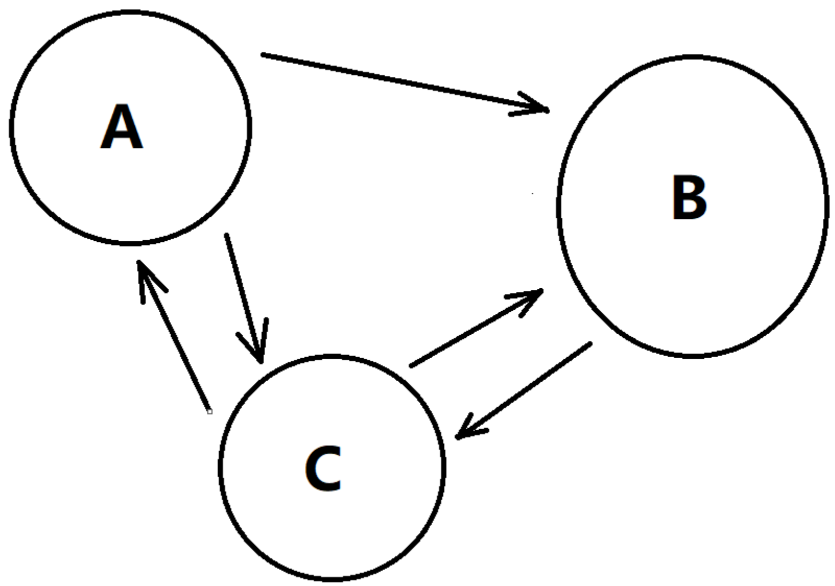
Sampling method

- Direct sampling



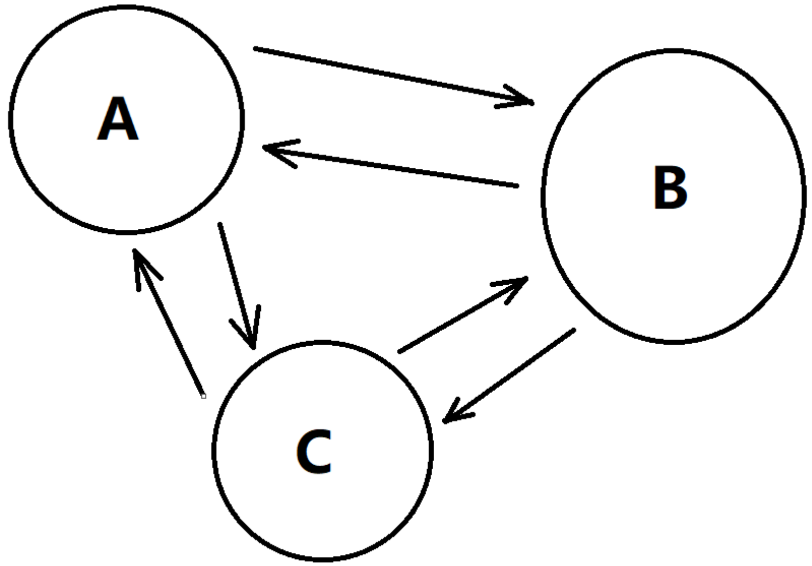
- Markov chain sampling

Balance and probability



- Balance: $P(A_{out})=P(A_{in})$

- Detail Balance: P(A to B)=P(B to A)

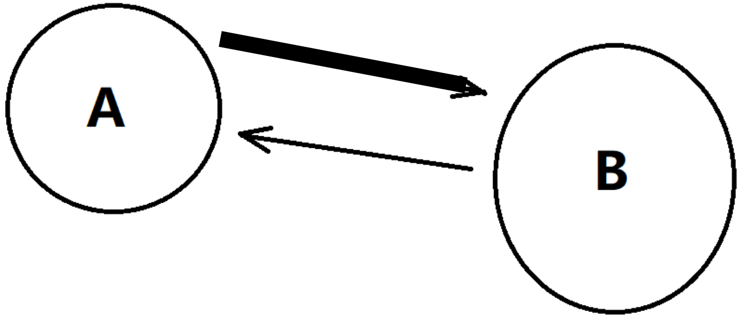


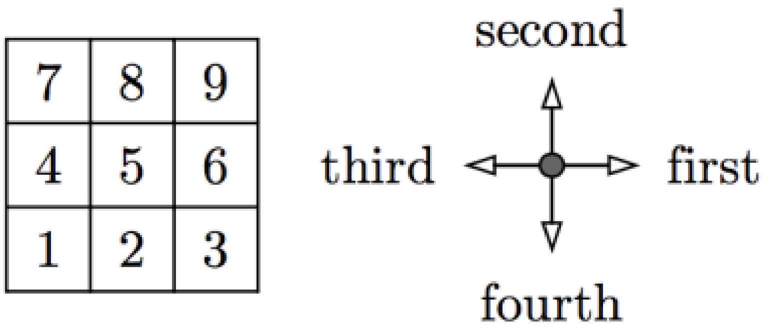
- Ergodicity!

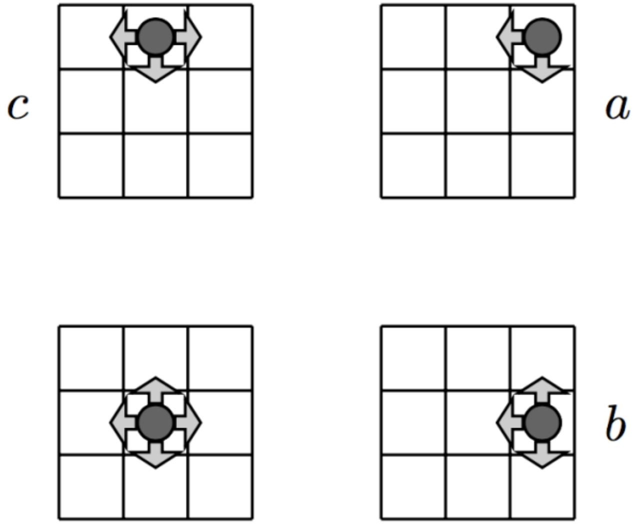
Metroplis Probability

$$P(A\ to\ B) = \min[1, \frac{W_B}{W_A}]$$

$$P(A\ to\ B) = \min[1, \frac{W_B\ P_{select}(B\ to\ A)}{W_A\ P_{select}(A\ to\ B)}]$$







Sampling in statistic mechanics: sampling for partition function

$$Z=\sum_{\mathcal{C}} e^{-\beta H[\mathcal{C}]}=\sum_{\mathcal{C}} W(\mathcal{C})$$

Sign problem?!

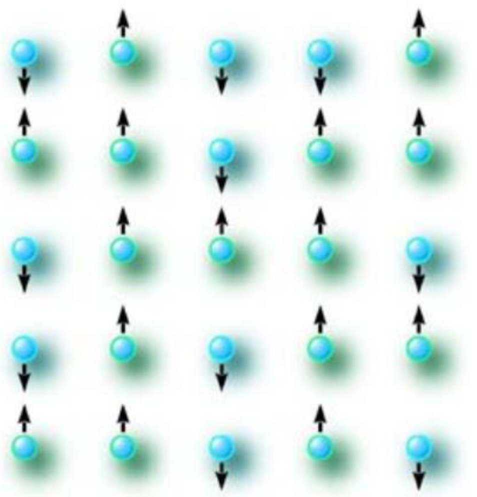
$$1=\frac{z}{z}=\frac{\sum_c w_c}{z}=\sum_c P_c$$

$$\langle A\rangle=\frac{\sum_C A_C P_C}{\sum P_C},$$

- **The Ising model: Introduction**

Hamiltonian: $H=-J\sum_{<i,j>}\sigma_i\sigma_j$

Spin: σ=±1
<i,j>: Sum over nearest neighbor pairs.
|J|=1: Coupling strength
J>0—ferromagnetic
J<0—antiferromagnetic



Quantum spin systems

Stochastic Series Expansion (SSE) picture

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\}$$

$$H = -\sum_{a,b} H_{a,b} \quad \begin{cases} H = \sum_{b=1}^{B} \left[S^z_{i(b)} S^z_{j(b)} + \frac{1}{2} \left(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)} \right) \right] \\ H_{1,b} = \frac{1}{4} - S^z_{i(b)} S^z_{j(b)}, \qquad H_{2,b} = \frac{1}{2} \left(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)} \right) \end{cases}$$

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha | (-H)^n | \alpha \rangle \qquad (-H)^n = \sum_{\{H_{ab}\}} \frac{(M-n)!n!}{M!} \prod_{p=1}^{M} H_{a(p),b(p)}$$

$$Z = \sum_{\alpha} \sum_{\{H_{ab}\}} \frac{\beta^n (M-n)!}{M!} \left\langle \alpha \left| \prod_{i=1}^{M} H_{a(i),b(i)} \right| \alpha \right\rangle$$

http://physics.bu.edu/~sandvik/programs/ssebasic/ssebasic.html

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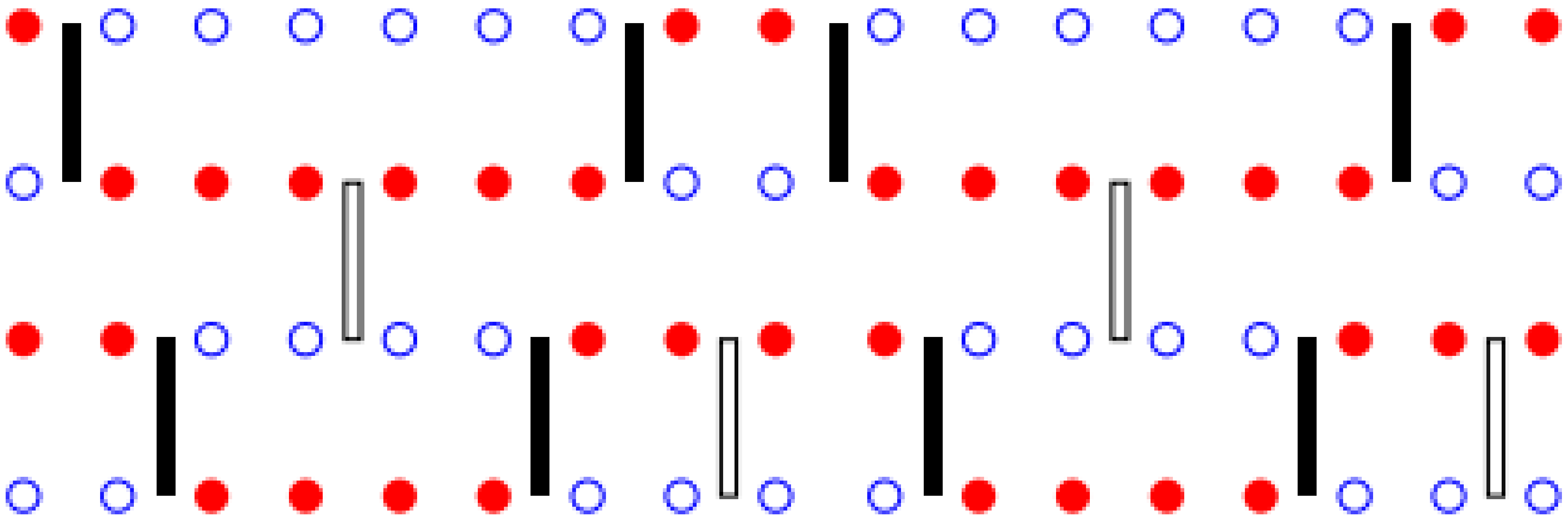
Stochastic Series Expansion (SSE) picture

$$Z_{\mathrm{SSE}} = \sum_{\{\alpha\}} \sum_{S_M} \frac{\beta^n (M-n)!}{M!} \langle \alpha_0 | H_{b_M} | \alpha_{M-1} \rangle \cdots \langle \alpha_2 | H_{b_2} | \alpha_1 \rangle \langle \alpha_1 | H_{b_1} | \alpha_0 \rangle,$$



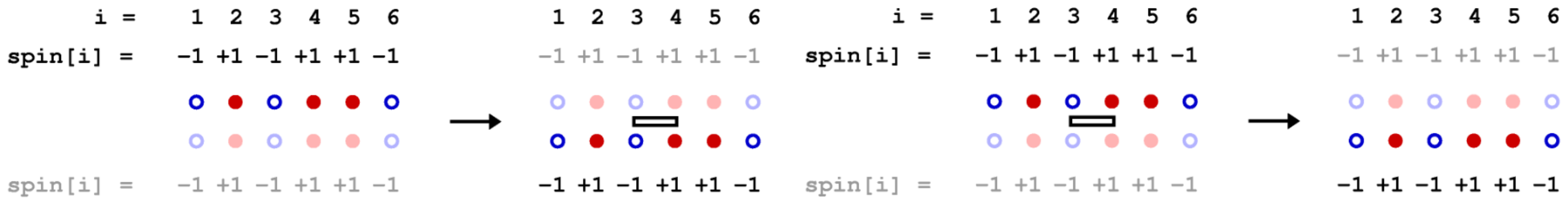
Diagonal update（e.g. Heisenberg model）

$$H_{1,b} = \frac{1}{4} - S^z_{i(b)} S^z_{j(b)}, \qquad H_{2,b} = \frac{1}{2}\left(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}\right)$$

$$Z = \sum_{\alpha} \sum_{\{H_{ab}\}} \frac{\beta^n (M-n)!}{M!} \left\langle \alpha \left| \prod_{i=1}^{M} H_{a(i),b(i)} \right| \alpha \right\rangle$$

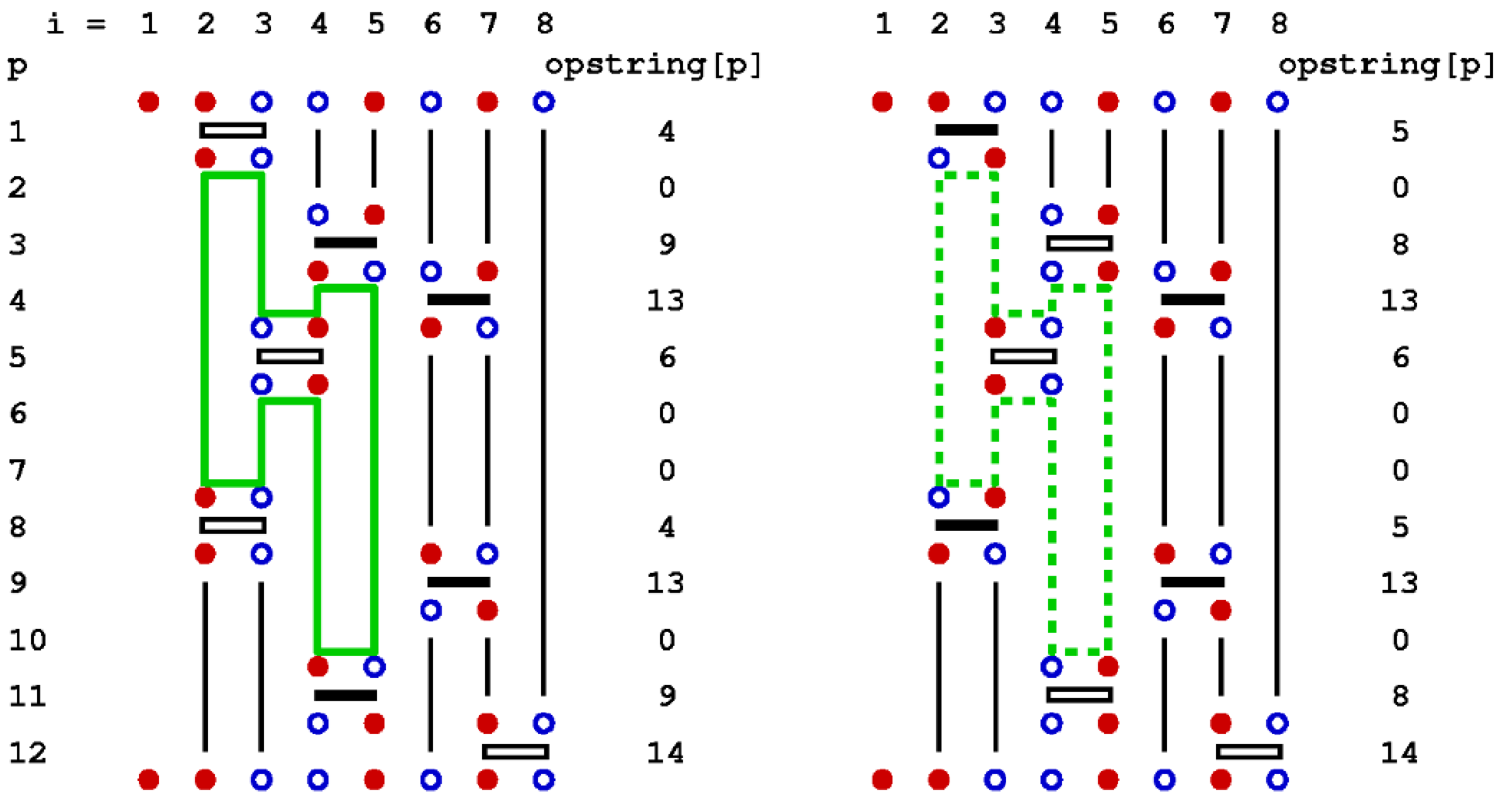
$$P_{\text{accept}}(A \to B) = \min\left(\frac{W(B) P_{\text{select}}(B \to A)}{W(A) P_{\text{select}}(A \to B)}, 1\right)$$

$$P_{\text{accept}}(n \to n+1) = \min\left(\frac{B\beta/2}{M-n}, 1\right) \qquad P_{\text{accept}}(n \to n-1) = \min\left(\frac{M-n+1}{B\beta/2}, 1\right)$$



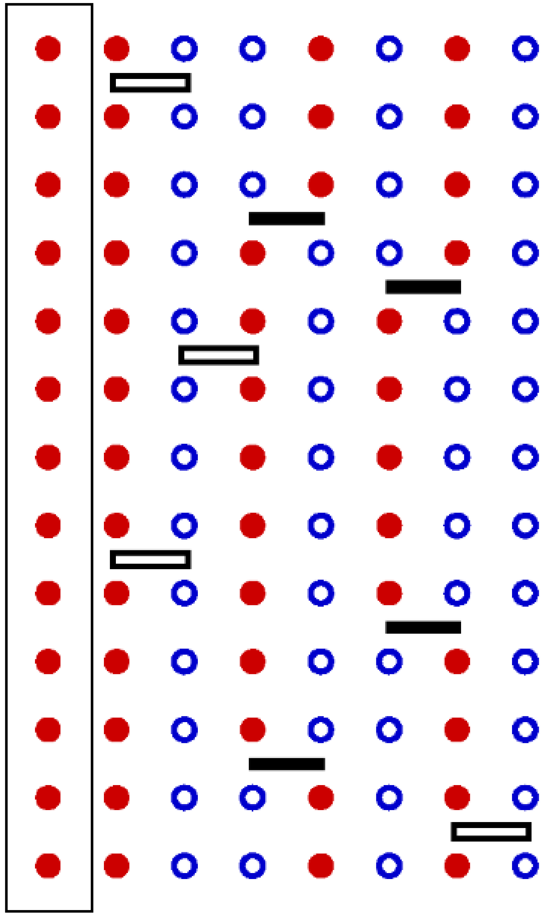
Off-diagonal update（e.g. Heisenberg model）

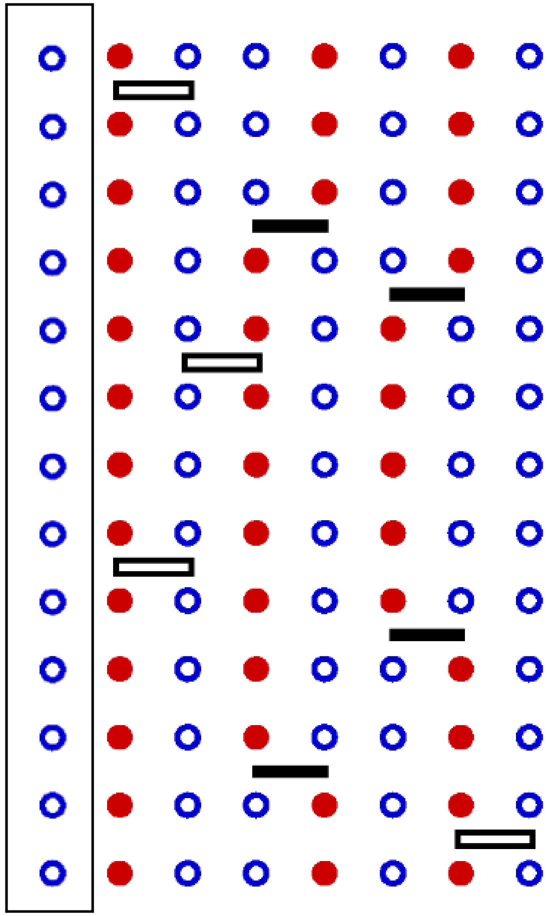
Another choice: P=W2/(W1+W2)



Free spin update to change total S^z

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





Code: http://physics.bu.edu/~sandvik/programs/ssebasic/ssebasic.f90

Measurement

- Energy：

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

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

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

$$E = -\frac{\langle n \rangle}{\beta}.$$

- Specific heat： since C = (<E^2> - <E>^{2})/T^2 we have $C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle.$

Diagonal operators. Expectation values of operators diagonal in the z-component basis are also easy to evaluate, using averages over the propagated states;

$$\langle O_z \rangle = \frac{1}{L} \sum_{p=0}^{L-1} \langle \alpha(p) | O_z | \alpha(p) \rangle = \frac{1}{L} \sum_{p=0}^{L-1} O_z(p).$$

Imaginary time: from path integral to SSE

$$e^{-\tau\mathcal{H}_0}U(\tau) = e^{-\tau(\mathcal{H}_0+V)}. \quad V(\tau) = e^{\tau\mathcal{H}_0}Ve^{-\tau\mathcal{H}_0}$$

$$\frac{dU(\tau)}{d\tau} = -V(\tau)U(\tau) \qquad U(\tau) = 1 - \int_0^\tau d\tau'\, V(\tau')U(\tau').$$

$$\begin{aligned}
Z &= \mathrm{Tr}\,[e^{-\beta\mathcal{H}_0}U(\beta)] \\
&= \mathrm{Tr}\left[e^{-\beta\mathcal{H}_0}\left(1 - \int_0^\beta d\tau_1\, V(\tau_1) + \int_0^\beta d\tau_2 \int_0^{\tau_2} d\tau_1\, V(\tau_2)V(\tau_1) - \cdots\right)\right] \\
&= \mathrm{Tr}\Big[\sum_{n=0}^{\infty}(-1)^n \int_0^\beta d\tau_n \int_0^{\tau_n} d\tau_{n-1} \cdots \int_0^{\tau_2} d\tau_1\, e^{-(\beta-\tau_n)\mathcal{H}_0} V e^{-(\tau_n-\tau_{n-1})\mathcal{H}_0} \\
&\qquad \times V \cdots V e^{-\tau_1\mathcal{H}_0}\Big] \\
&= \sum_{n=0}^{\infty}(-1)^n \sum_{\phi_n,\cdots,\phi_1} \int_0^\beta d\tau_n \int_0^{\tau_n} d\tau_{n-1} \cdots \int_0^{\tau_2} d\tau_1\, \langle\phi_1|e^{-(\beta-\tau_n)\mathcal{H}_0}|\phi_1\rangle\langle\phi_1|V|\phi_n\rangle \\
&\qquad \times \langle\phi_n|e^{-(\tau_n-\tau_{n-1})\mathcal{H}_0}|\phi_n\rangle\langle\phi_n|V|\phi_{n-1}\rangle \cdots \langle\phi_2|V|\phi_1\rangle\langle\phi_1|e^{-\tau_1\mathcal{H}_0}|\phi_1\rangle.
\end{aligned}$$

$$\begin{aligned}
&w(c)\, d\tau_n \cdots d\tau_1 \\
&\quad = \left(\frac{\Gamma}{2}\right)^n e^{-(\beta-\tau_n)E_0(\phi_1)} e^{-(\tau_n-\tau_{n-1})E_0(\phi_n)} \cdots e^{-\tau_1 E_0(\phi_1)} d\tau_n \cdots d\tau_1,
\end{aligned}$$

Another useful continuous time path integral representation can be obtained by splitting the Hamiltonian into $\mathcal{H}_0 = 0$ and $V = \mathcal{H}$. The weight of configuration c is then written as

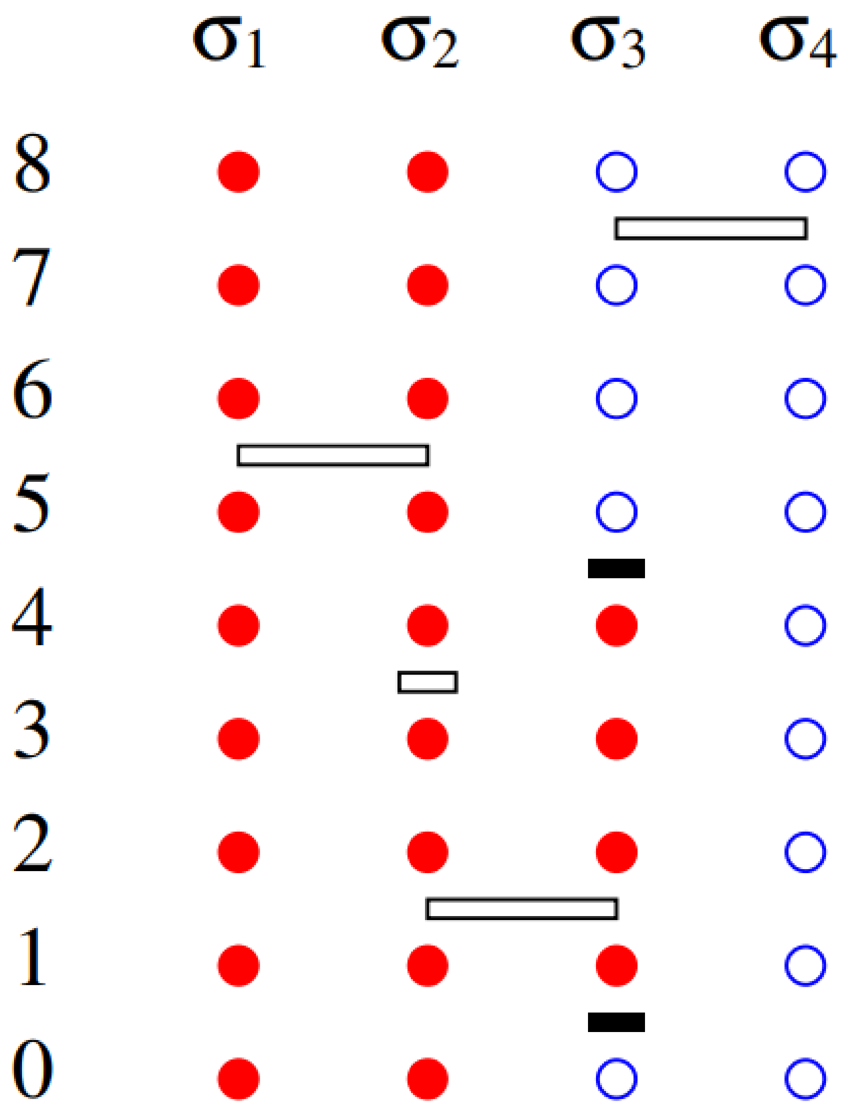
$$\begin{aligned}
&w(c)\, d\tau_m \cdots d\tau_1 \\
&\quad = (-1)^m \langle\phi_1|\mathcal{H}|\phi_m\rangle\langle\phi_m|\mathcal{H}|\phi_{m-1}\rangle \cdots \langle\phi_2|\mathcal{H}|\phi_1\rangle\, d\tau_m \cdots d\tau_1.
\end{aligned}$$

$$\Downarrow$$

$$Z = \sum_{m=0}^{\infty} \frac{(-\beta)^m}{m!} \sum_{\phi_m,\cdots,\phi_1} \langle\phi_1|\mathcal{H}|\phi_m\rangle\langle\phi_m|\mathcal{H}|\phi_{m-1}\rangle \cdots \langle\phi_2|\mathcal{H}|\phi_1\rangle.$$

Sign the imaginary time on every piece!

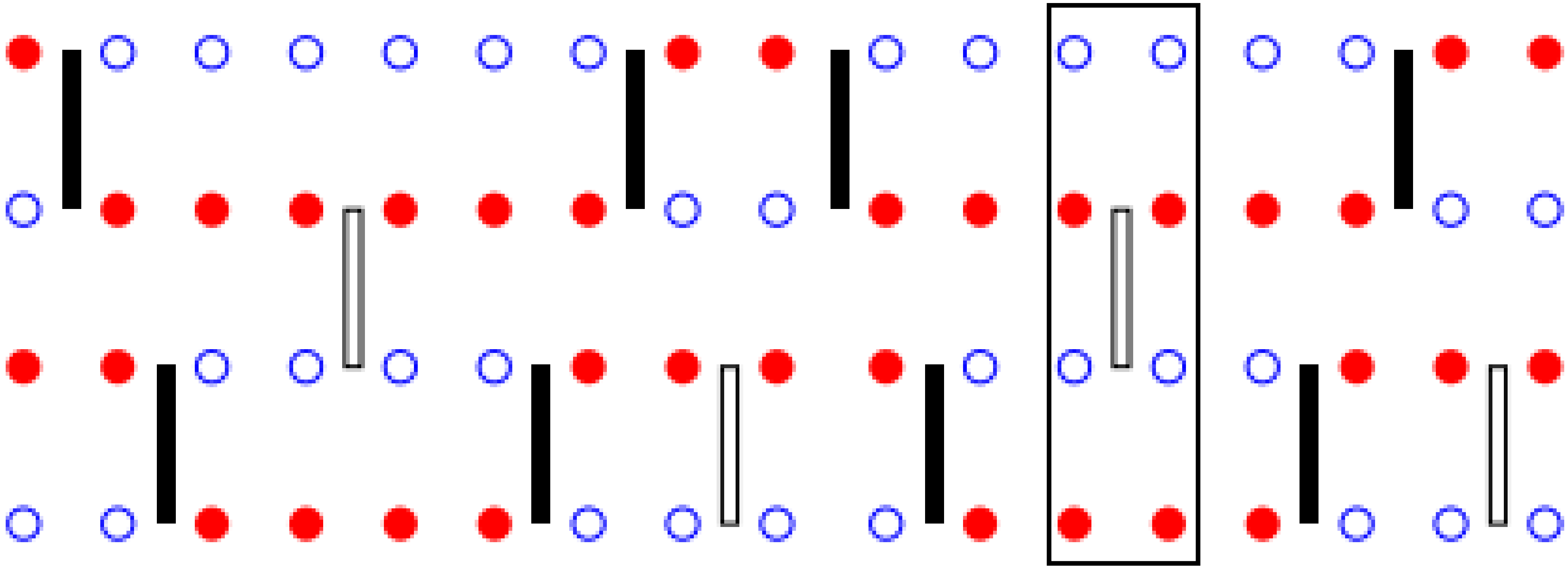
Note: get random numbers from 0 to beta with equal probability!



http://physics.bu.edu/~sandvik/programs/ssebasic/ssebasic.html

Stochastic Series Expansion (SSE) picture

$$Z_{\mathrm{SSE}} = \sum_{\{\alpha\}} \sum_{S_M} \frac{\beta^n (M-n)!}{M!} \langle \alpha_0 | H_{b_M} | \alpha_{M-1} \rangle \cdots \boxed{\langle \alpha_2 | H_{b_2} | \alpha_1 \rangle} \langle \alpha_1 | H_{b_1} | \alpha_0 \rangle,$$



A. W. Sandvik, Phys. Rev. E **68**, 056701 (2003)

Diagonal update for TFIM

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x,$$

$$\begin{aligned} H_{0,0} &= I, \\ H_{-1,a} &= h(\sigma_a^+ + \sigma_a^-), \\ H_{0,a} &= h, \\ H_{1,a} &= J(\sigma_i^z \sigma_j^z + 1). \end{aligned}$$

$$\langle \bullet \; |H_{-1,a}| \; \circ \rangle = \langle \circ \; |H_{-1,a}| \; \bullet \rangle = h,$$
$$\langle \bullet \; |H_{0,a}| \; \bullet \rangle = \langle \circ \; |H_{0,a}| \; \circ \rangle = h.$$

$$\langle \bullet \; \bullet \; |H_{1,a}| \; \bullet \; \bullet \rangle = \langle \circ \; \circ \; |H_{1,a}| \; \circ \; \circ \rangle = 2J.$$

Choose a kind of operators to be inset.

$$P(h) = \frac{hN}{hN + (2J)N_b},$$

$$P(J) = \frac{(2J)N_b}{hN + (2J)N_b}.$$

Probability of inset.

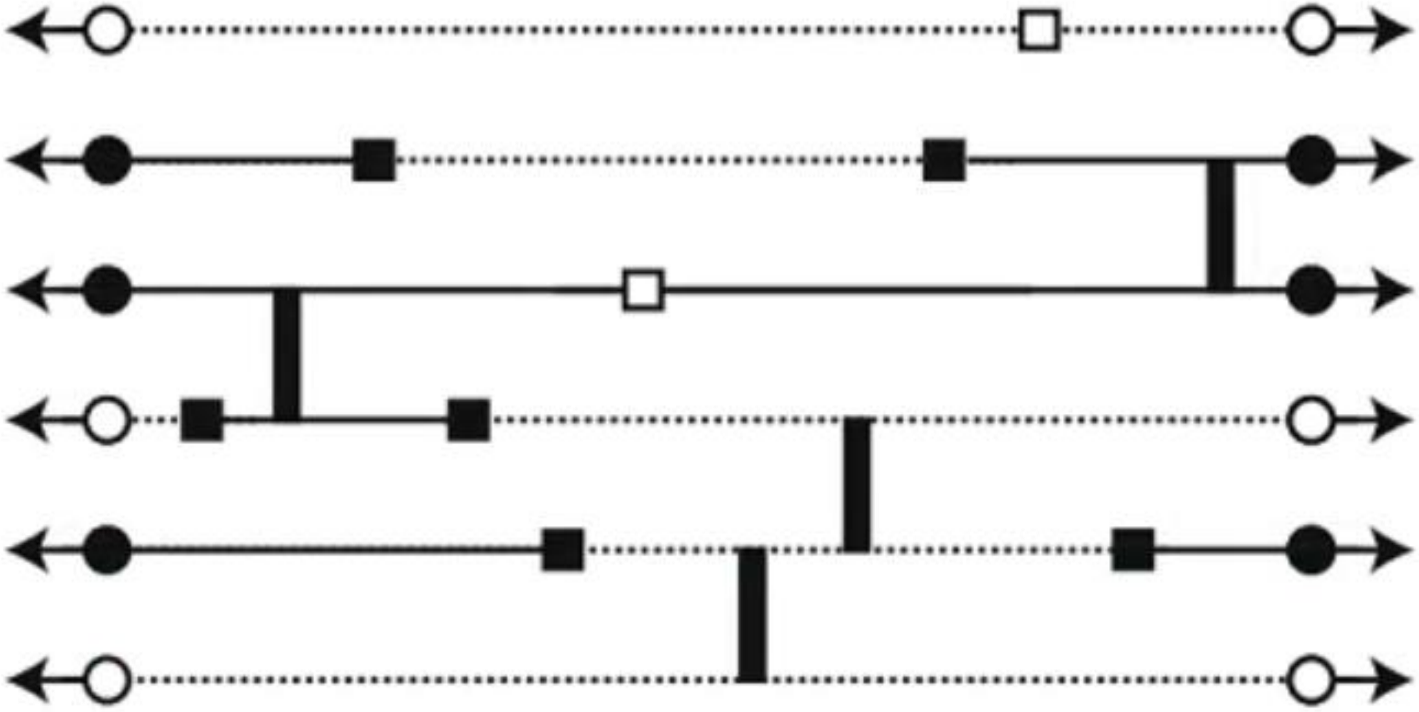
$$P = \min\left(\frac{\beta(hN + (2J)N_b)}{M - n}, 1\right),$$

Another choice?

Probability of remove

$$P = \min\left(\frac{M - n + 1}{\beta[hN + (2J)N_b]}, 1\right),$$

What's the probability here? ——0.5

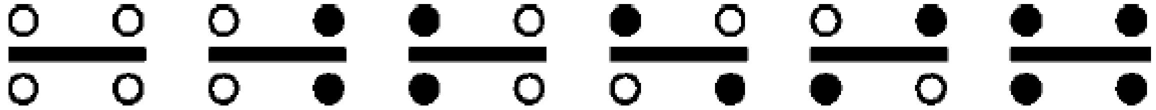


O. F. Syljuasen, A. W. Sandvik. Phys. Rev. E **66**, 046701 (2002)

Directed loop update

$$H = J\sum_{\langle i,j\rangle}[S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z] - h\sum_i S_i^z \;\Longrightarrow\; \begin{aligned} H_{1,b} &= C - \Delta S^z_{i(b)}S^z_{j(b)} + h_b[S^z_{i(b)} + S^z_{j(b)}] \\ H_{2,b} &= \frac{1}{2}[S^+_{i(b)}S^-_{j(b)} + S^-_{i(b)}S^+_{j(b)}] \end{aligned}$$

Only 6 configurations:



$$\langle\downarrow\downarrow|H_b|\downarrow\downarrow\rangle = \epsilon, \quad C = C_0 + \epsilon, \quad C_0 = \Delta/4 + h_b,$$

$$\langle\downarrow\uparrow|H_b|\downarrow\uparrow\rangle = \langle\uparrow\downarrow|H_b|\uparrow\downarrow\rangle = \Delta/2 + h_b + \epsilon,$$

$$\langle\uparrow\downarrow|H_b|\downarrow\uparrow\rangle = \langle\downarrow\uparrow|H_b|\uparrow\downarrow\rangle = 1/2,$$

$$\langle\uparrow\uparrow|H_b|\uparrow\uparrow\rangle = \epsilon + 2h_b.$$

Probability:

$$P([0,0]_p \to [1,b]_p) = \frac{N_b\beta\langle\alpha(p)|H_{1,b}|\alpha(p)\rangle}{M-n}$$

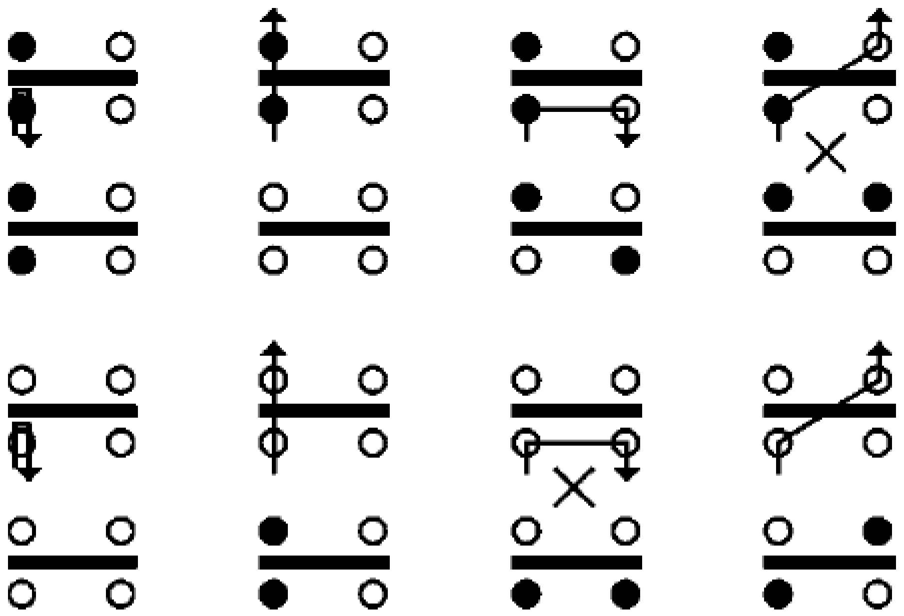
$$P([1,b]_p \to [0,0]_p) = \frac{M-n+1}{N_b\beta\langle\alpha(p)|H_{1,b}|\alpha(p)\rangle}$$

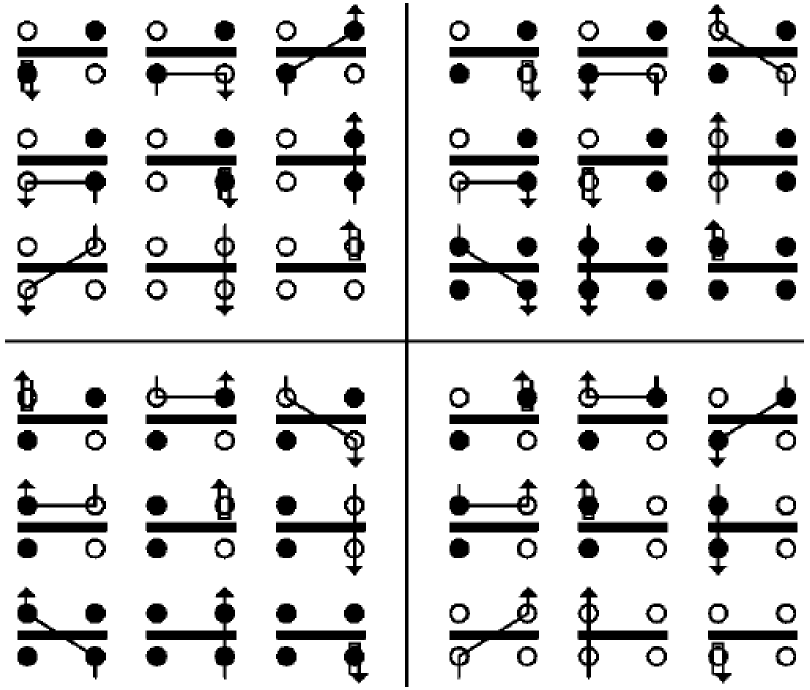
Question: if flip-symmetry doesn’t work, how to do it??

Directed loop update

$$\langle\downarrow\downarrow|H_b|\downarrow\downarrow\rangle=\epsilon,$$
$$\langle\downarrow\uparrow|H_b|\downarrow\uparrow\rangle=\langle\uparrow\downarrow|H_b|\uparrow\downarrow\rangle=\Delta/2+h_b+\epsilon,$$
$$\langle\uparrow\downarrow|H_b|\downarrow\uparrow\rangle=\langle\downarrow\uparrow|H_b|\uparrow\downarrow\rangle=1/2,$$
$$\langle\uparrow\uparrow|H_b|\uparrow\uparrow\rangle=\epsilon+2h_b\,.$$

Which types are acceptant??





$$a=W_1W_2/(W_1+W_2+W_3),$$
$$b=W_1W_3/(W_1+W_2+W_3),$$
$$c=W_2W_3/(W_1+W_2+W_3),$$
$$b_i=W_i^2/(W_1+W_2+W_3).$$

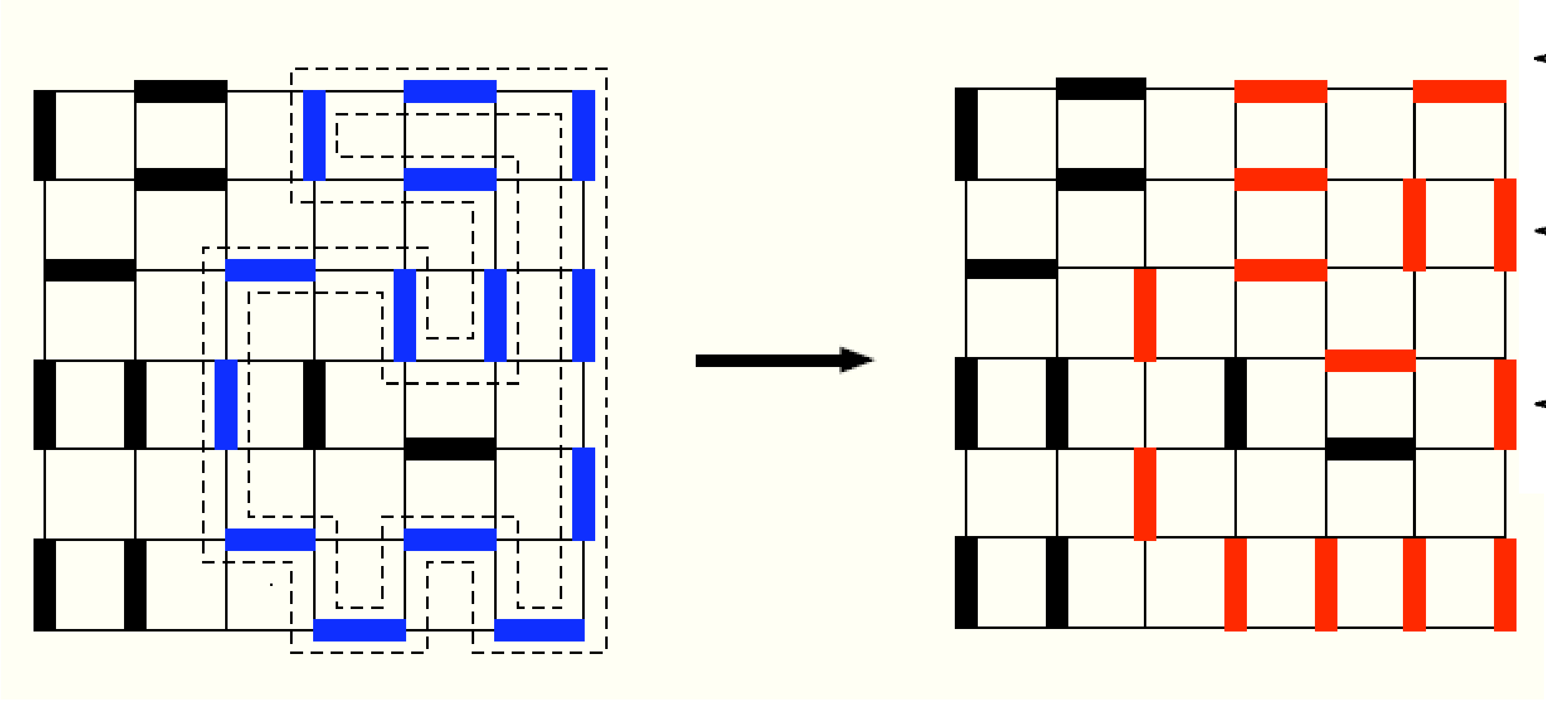
Because of symmetry reasons,
there are only two different types of sets

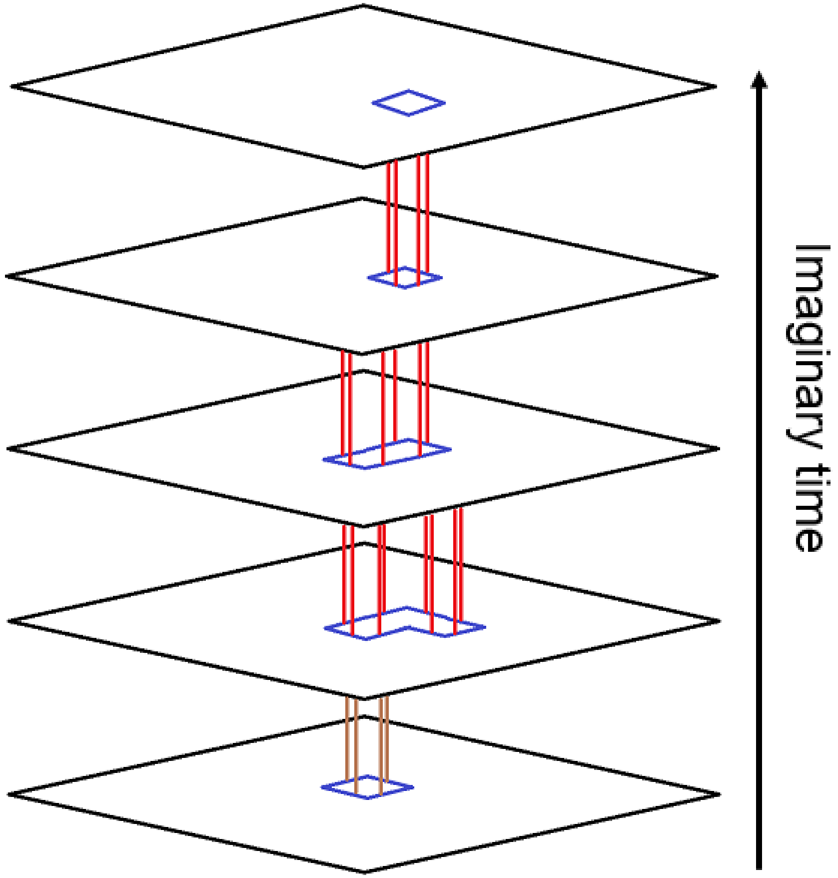
$$W_1=b_1+a+b, \qquad W_1=b_1'+a'+b',$$
$$W_2=a+b_2+c, \qquad W_2=a'+b_2'+c',$$
$$W_3=b+c+b_3, \qquad W_4=b'+c'+b_3'.$$

Zheng Yan, et al. Phys. Rev. B **99**, 165135 (2019)

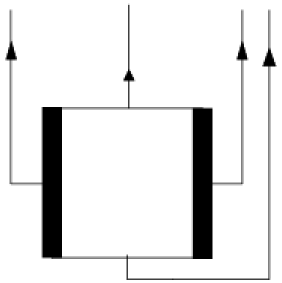
Sweeping cluster algorithm

$$H = -J \sum_{\mathrm{plaq}} \left(|\,\|\,\rangle\langle = | + \mathrm{H.c.} \right) + V \sum_{\mathrm{plaq}} \left(|\,\|\,\rangle\langle\,\|\,| + |=\rangle\langle = | \right)$$

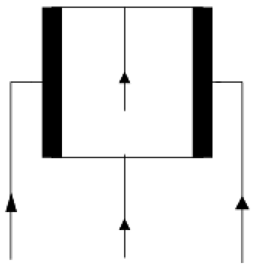




Along imaginary time-Sweeping cluster

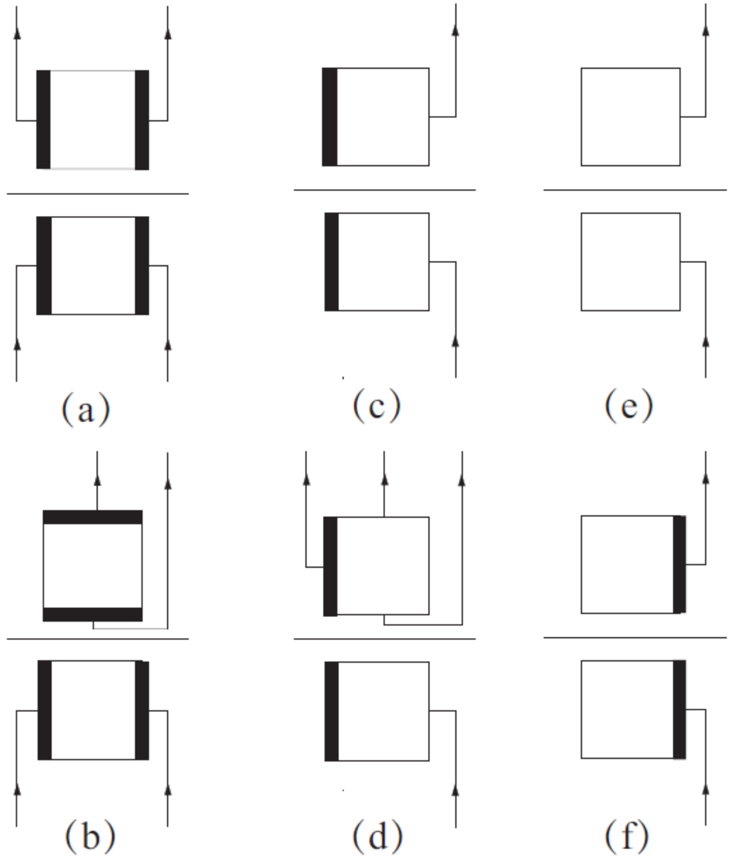


Select a flippable block to start the update, and generate/destroy a dimer where the update line passes.

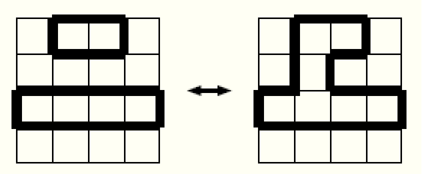


Cluster completion until only 4 update lines remain and terminate in a flippable plaquette.

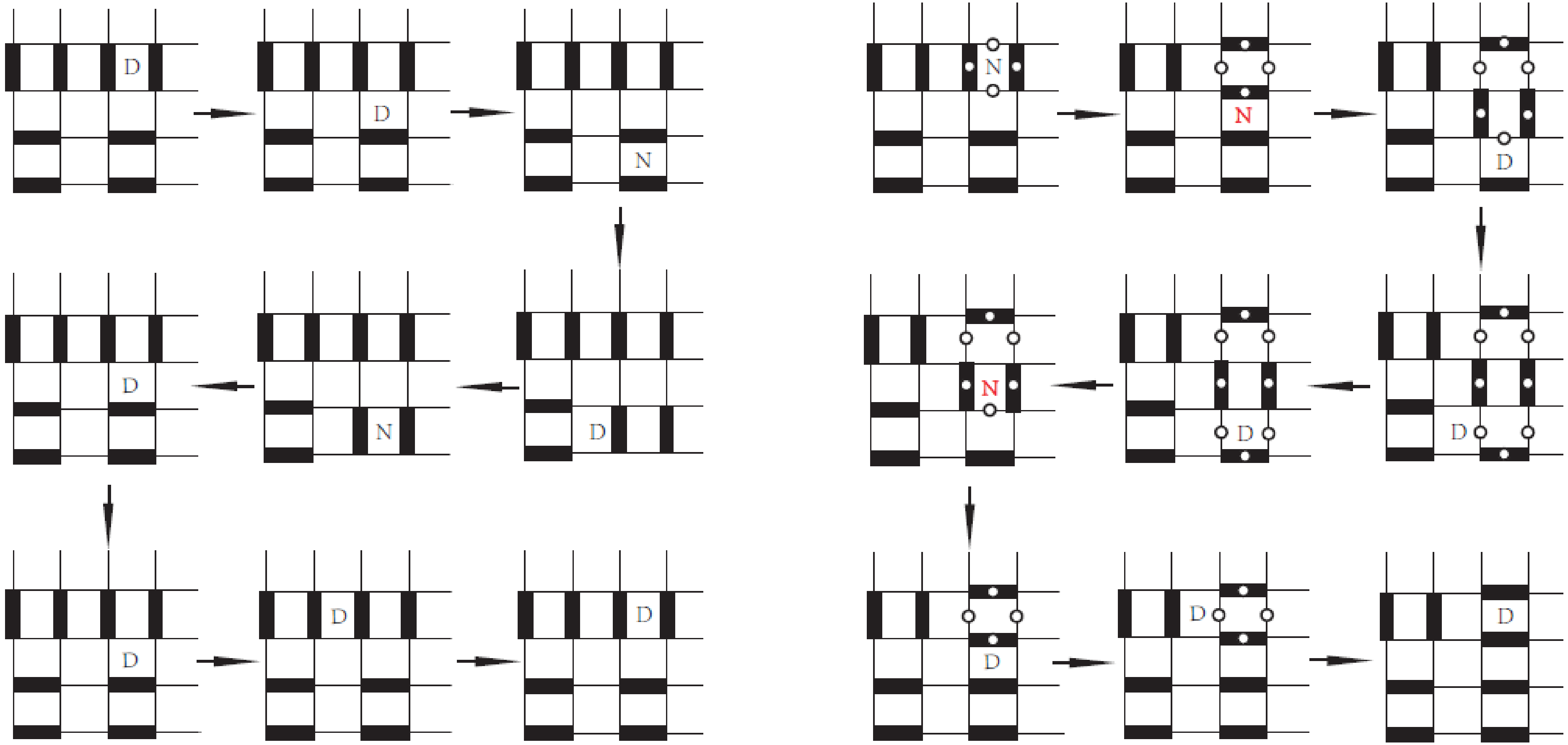
$$H = -J\sum_{\text{plaq}}\left(|\Vert\rangle\langle=| + \text{H.c.}\right) + V\sum_{\text{plaq}}\left(|\Vert\rangle\langle\Vert| + |=\rangle\langle=|\right)$$



Details show



There are cases of split/synthesis of loops!



(a) (b)

Thanks for your attentions!