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Quantum Monte Carlo

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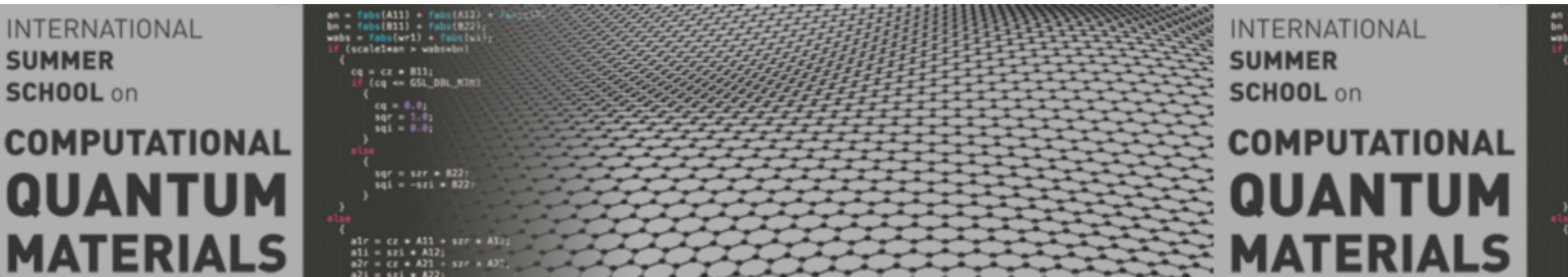


The need for Quantum Monte Carlo

Many-Body Quantum Mechanics:

Schrödinger equation $$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

Time Evolution operator $$\hat{U}(t) = e^{-\frac{it}{\hbar}\hat{H}}$$

Thermal Expectation value $$\langle\mathcal{O}\rangle = \frac{\mathrm{Tr}\ \ e^{-\beta\hat{H}}\mathcal{O}}{\mathrm{Tr}\ \ e^{-\beta\hat{H}}}$$

T=0 Expectation Value $$\langle\mathcal{O}\rangle = \langle\Psi|\mathcal{O}|\Psi\rangle$$

Would like to solve the dynamic, thermodynamic, and groundstate properties of a system

Consider the Time Independent Schrödinger Equation

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

matrix $M \times M$ M vector

Then for example the thermal expectation value:

$$\langle \mathcal{O} \rangle = \frac{\sum_{i=1}^{M} e^{-\beta E_i} \langle \Psi_i | \mathcal{O} | \Psi_i \rangle}{\sum_{i=1}^{M} e^{-\beta E_i}}$$

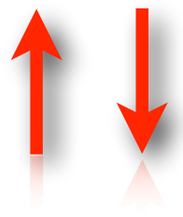
ie. we can solve the model thermodynamic properties if we can solve the eigenvalue problem (i.e. diagonalize the Hamiltonian)

Many efficient eigenvalue libraries exist (LAPACK, ARPACK...)

Difficulty: Hilbert space is exponential

Consider a spin 1/2 system (e.g. electron spin)

$$S^z = \pm\frac{1}{2}$$



two states

For an N-spin system, the Hilbert space is $M = 2^N$

If each vector element is an integer (4 bytes), the memory needed to store it can be calculated:

$N = 9$ 2048 bytes

$N = 40$ $\sim 10^{12}$ bytes

$N = 256$ $\sim 10^{77}$ bytes

Can we diagonalize “parts” of the Hamiltonian?

For example, assume: $\hat{H} = \hat{T} + \hat{V}$

$$e^{-\beta \hat{H}} \not\equiv e^{-\beta \hat{T}} e^{-\beta \hat{V}}$$ no

since $[\hat{T}, \hat{V}] \neq 0$

to see this: compare Taylor expansions of

$\mathrm{e}^{\lambda(\hat{A}+\hat{B})}$ and $\mathrm{e}^{\lambda \hat{A}} \mathrm{e}^{\lambda \hat{B}}$

only agree up to order $O(\lambda^2)$

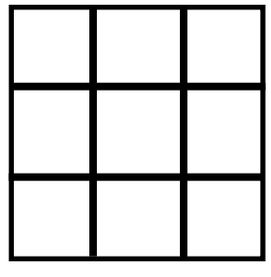
Numerical Methods for Quantum Systems

- Exact diagonalization

  obtain full spectrum

$$\langle \mathcal{O} \rangle = \frac{\sum_{i=1}^{M} e^{-\beta E_i} \langle \Psi_i | \mathcal{O} | \Psi_i \rangle}{\sum_{i=1}^{M} e^{-\beta E_i}}$$

$$N \approx 16 - 20$$



If you are interested in dynamics, full-spectrum diagonalization is often all you can do

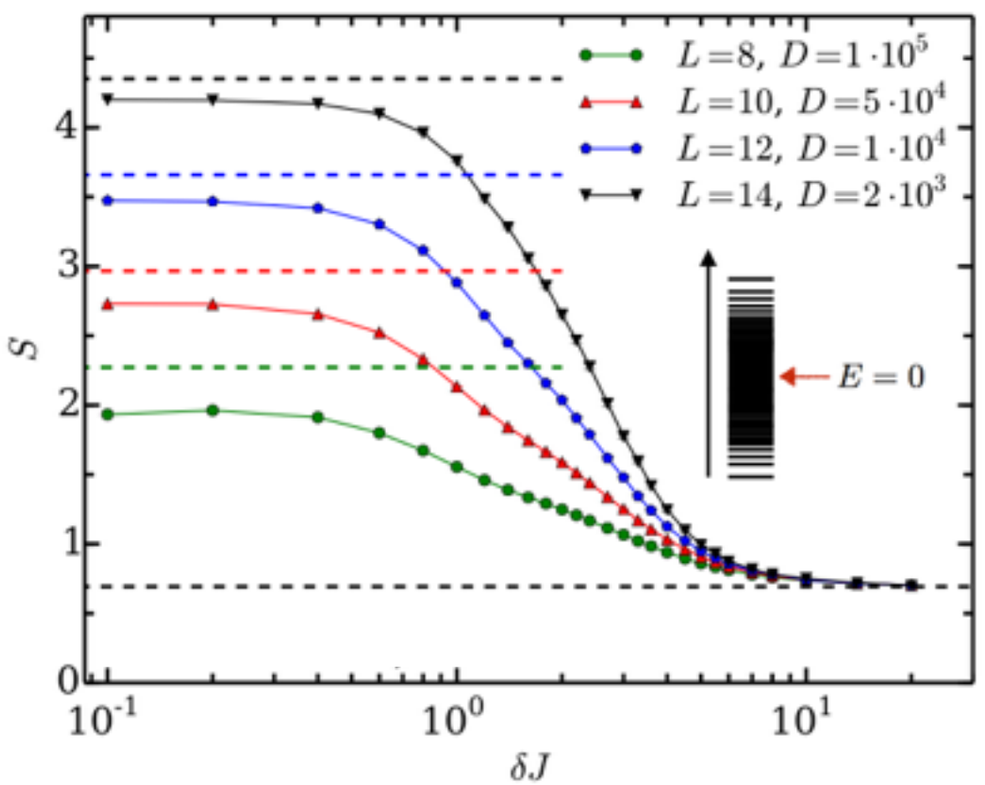
- Spectral weight, structure factor

$$A(\mathbf{k}, \omega) \qquad S(\mathbf{q}, \omega)$$

- Properties of excited states
  – e.g. Many-body localization

volume law / area law

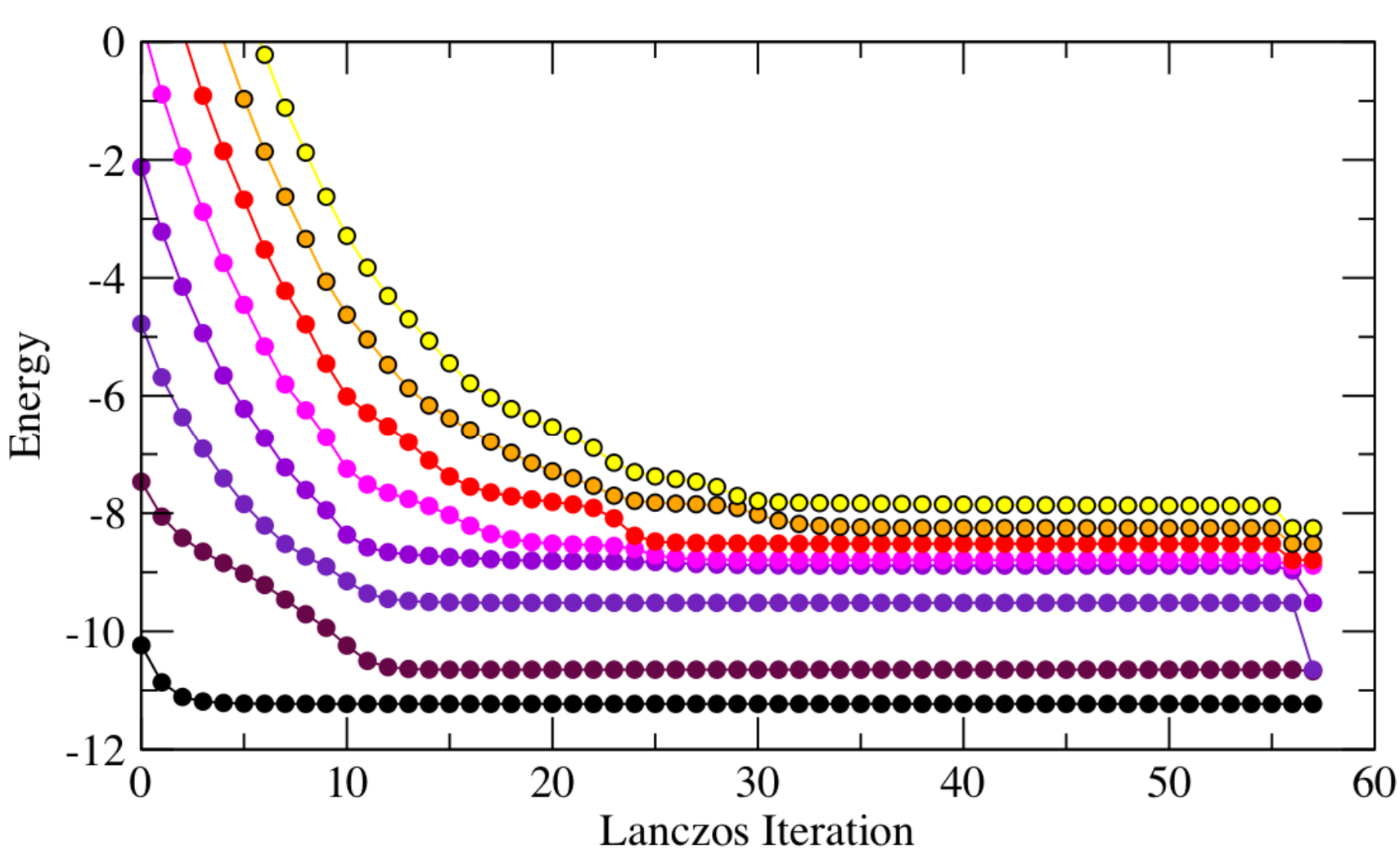
Bauer and Nayak (2013)
Page (1993)



Numerical Methods for Quantum Systems

- Lanczos diagonalization

  Iterative: project out the groundstate (and some low-lying excited states) only



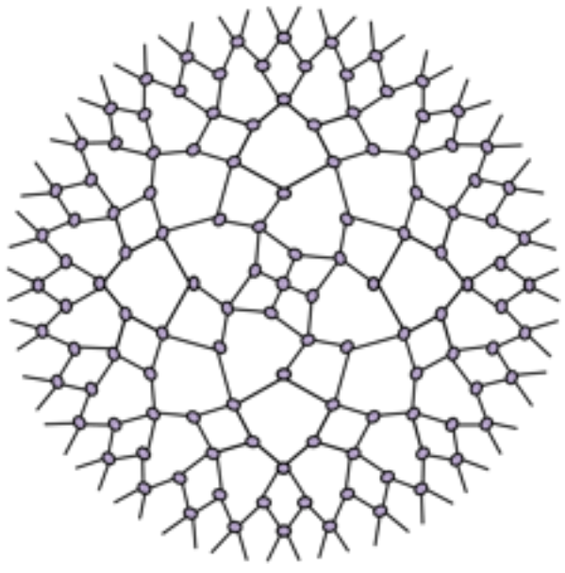
$N \approx 40$

Numerical Methods for Quantum Systems

- Density Matrix Renormalization Group
  - Reduce the size of the Hilbert space through some clever decimation procedure
  - Keep only the “important” information (entanglement)
  - Perform a Lanczos diagonalization using the remaining Hilbert space

Steve White

- Tensor Networks



ITensor

Schollwoeck, Stoudenmire

Quantum Monte Carlo

Suzuki, 1993

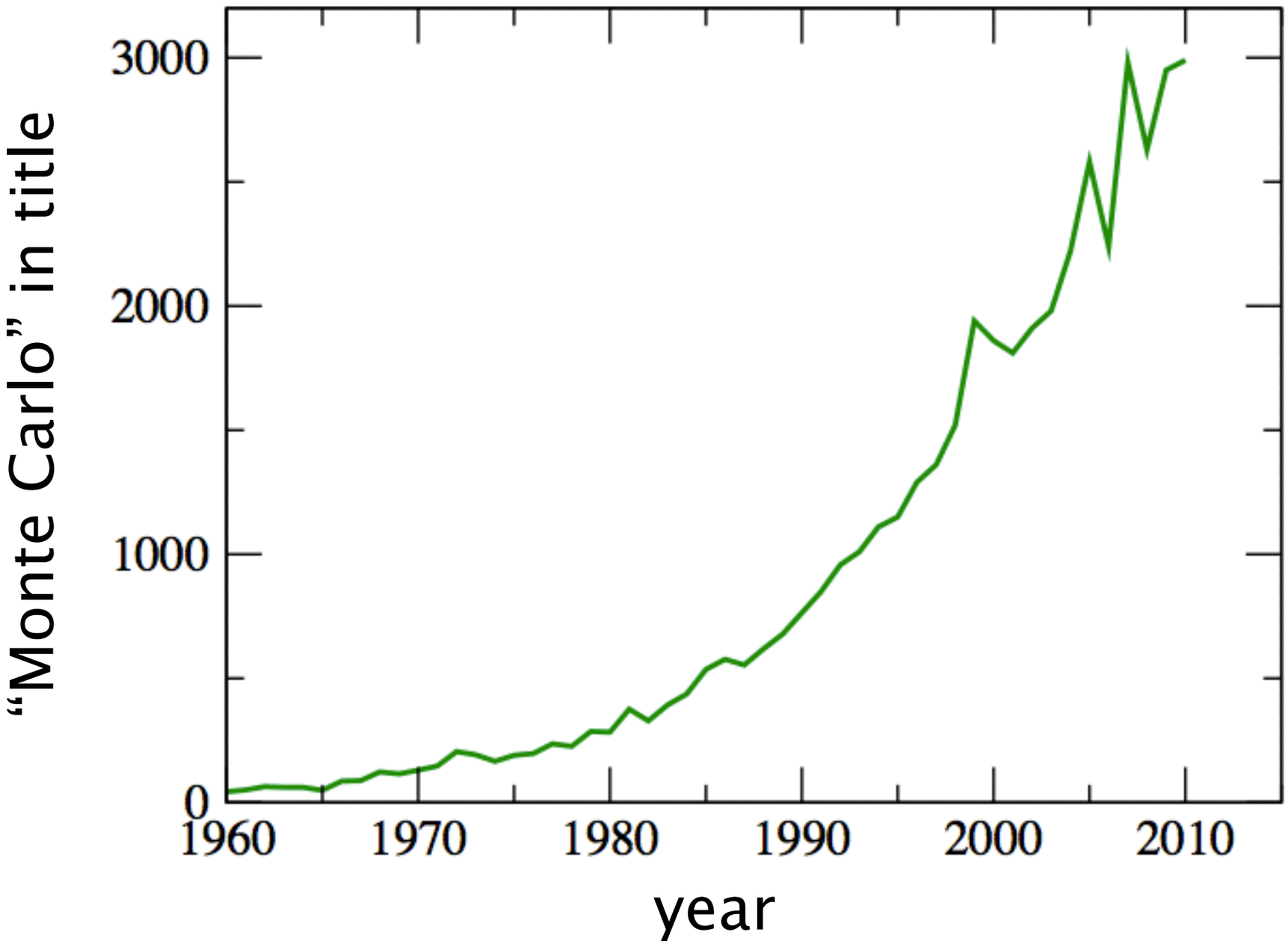
Performs **importance sampling** of state space

Goal: simulate quantum many-body models, particularly those with strong interactions, D>1

- lattice or continuum
- free of systematic errors or bias
- equilibrium properties only
- often done on as large sizes as possible:

Can characterize phases (and phase transitions) $\xi \to \infty$

Condensed matter, materials, atomic systems, quantum information systems, lattice gauge theory, nuclear and particle physics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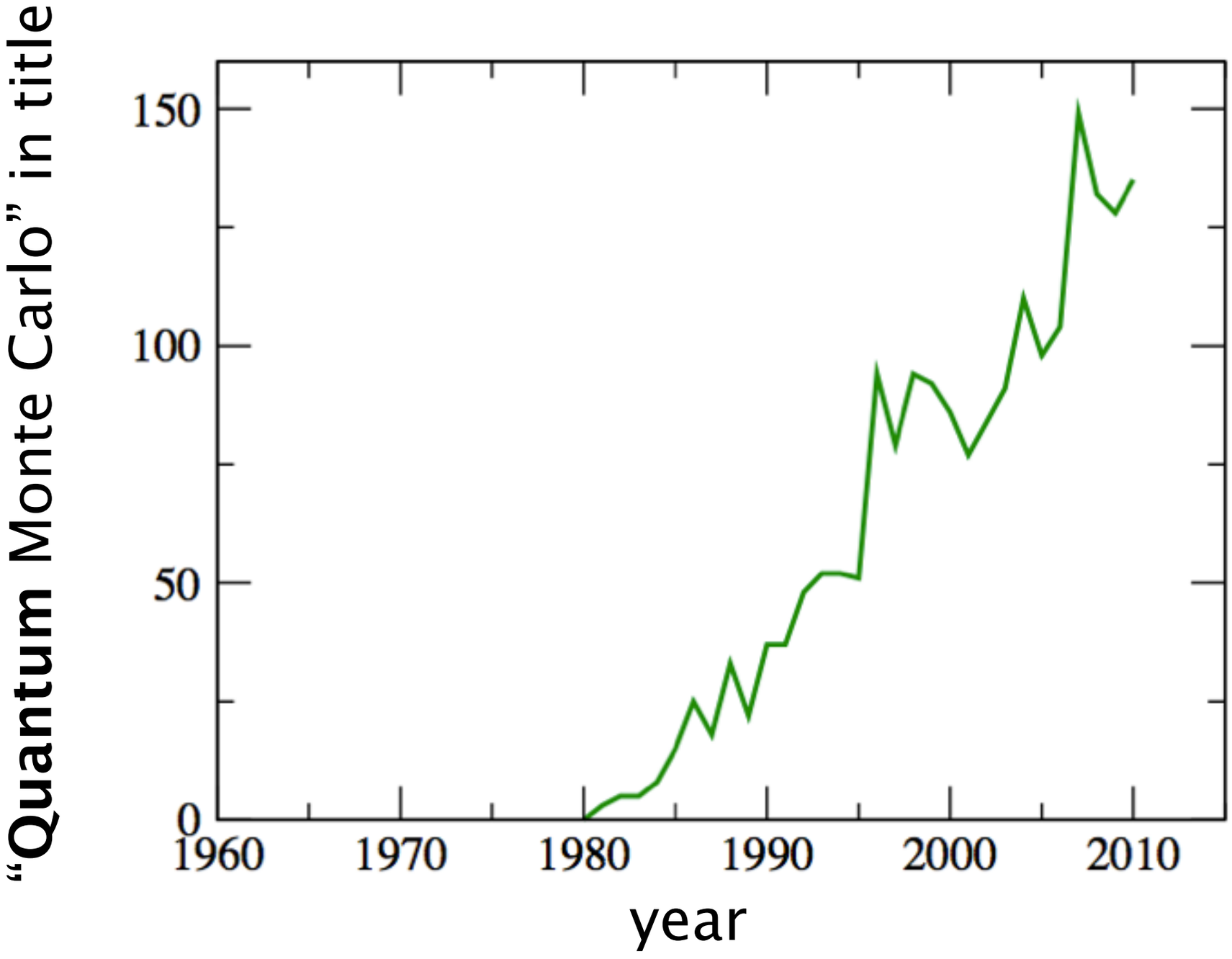
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year

A “zoo” of QMC methods, depending on which system you want to study

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \hat{\nabla}_i^2 + \sum_i \hat{V}_{\rm ext}(\vec{r}_i) + \sum_{i<j} \hat{V}_{\rm int}(|\vec{r}_i - \vec{r}_j|)$$

Path Integral Monte Carlo — Ceperly, Del Maestro

$$H = -J\sum\left(|\uparrow\uparrow\rangle\langle\downarrow\downarrow| + \text{H.c.}\right) + V\sum\left(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|\right)$$

Diffusion Monte Carlo — Syljuåsen

$$\hat{H} = J\sum_{\langle ij\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \qquad \hat{H} = J\sum_{\langle ij\rangle}\left(b_i^\dagger b_j + b_i b_j^\dagger\right)$$

Continuous world-line, Stochastic Series Expansion — Prokof’ev, Sandvik

$$\hat{H} = -t\sum_{\langle ij\rangle,\sigma}\left(c_{i,\sigma}^\dagger c_{j,\sigma} + h.c.\right) + U\sum_{i=1}^{N} n_{i,\uparrow}n_{i,\downarrow}$$

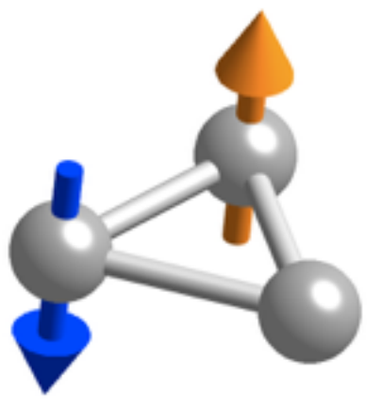
Auxiliary field Monte Carlo — AMT, Assaad, Evertz

What unifies these methods as “Quantum” Monte Carlo?

- A D-dimensional quantum model has a $D+1$ dimensional representation on the computer

- The presence of some form of **sign problem:**

Not all quantum models are amenable to efficient simulation by QMC. Something very **fundamental** precludes certain (very interesting) models.



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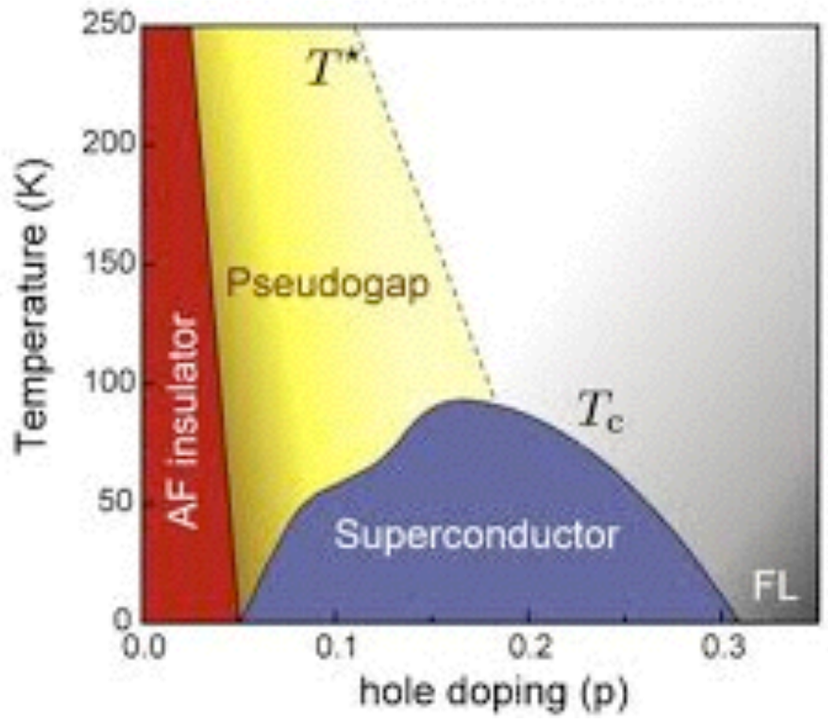


Quantum Monte Carlo consists of three ingredients

- A $D+1$ dimensional "representation" on the computer

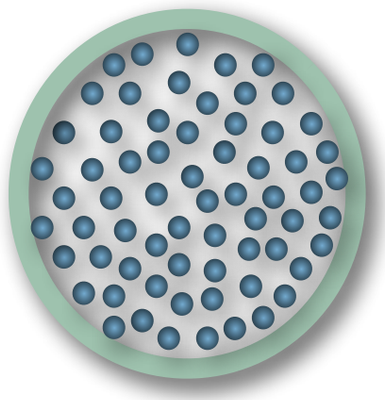
- A procedure for updating configurations of the representation

- A way of devising measurements

The first thing you need is a choice of basis:

$S^z = \pm\frac{1}{2}$ 

 $= \frac{1}{\sqrt{2}}$ (|  ⟩ - |  ⟩)



$$|R\rangle = |\vec{r}_1, \ldots \vec{r}_N\rangle$$

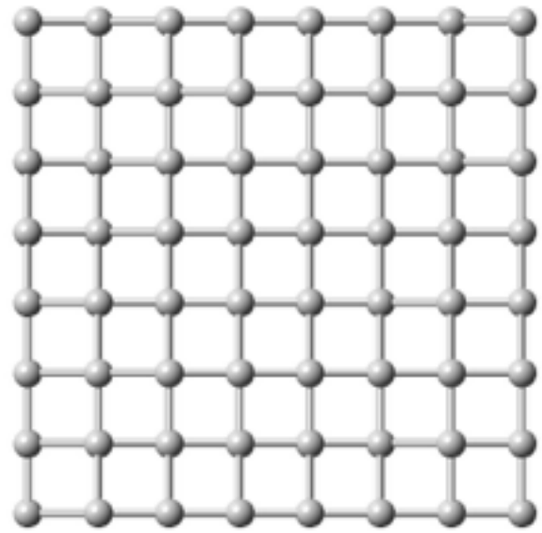
Stochastic Series Expansion QMC

Anders Sandvik

A simple to implement, powerful QMC method for lattice models

$$\hat{H} = J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \qquad \hat{H} = J \sum_{\langle ij \rangle} \left(b_i^\dagger b_j + b_i b_j^\dagger \right)$$

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



- Scales linearly in system size (and inverse temperature)
- Free of systematic Trotter error
- Finite and Zero-temperature representations available

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\{ \mathcal{O} e^{-\beta H} \} \qquad \langle \mathcal{O} \rangle = \frac{1}{Z} \langle \Psi | \mathcal{O} | \Psi \rangle$$

SSE Finite-T representation

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

$$\langle \mathcal{O} \rangle = \frac{\sum_x \mathcal{O}_x W(x)}{\sum_x W(x)}$$

partition function $Z = \sum_x W(x) = \mathrm{Tr}\{e^{-\beta H}\}$

Taylor expand the exponential:

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

Insert *n-1* resolutions of the identity

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

$\alpha_0 = \alpha_n$ to keep the trace nonzero

i.e. periodic in "imaginary time" (the propagation direction)

The weight $W(x)$ is derived from this;

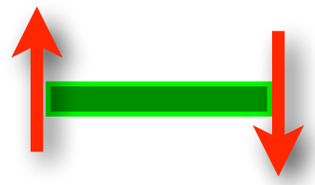
- proportional to the product of n matrix elements
- each $\langle \alpha_i | -H | \alpha_{i+1} \rangle$ is a real number
- must be positive to be interpreted as a probability for use in a Metropolis condition: otherwise get the "sign problem"

The Hamiltonian is broken into elementary lattice operators

$$H = -\sum_t \sum_a H_{t,a}$$

"type"

lattice unit (e.g. bond)



$$Z = \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \sum_{S_n} \frac{\beta^n}{n!} \prod_{i=1}^{n} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle$$

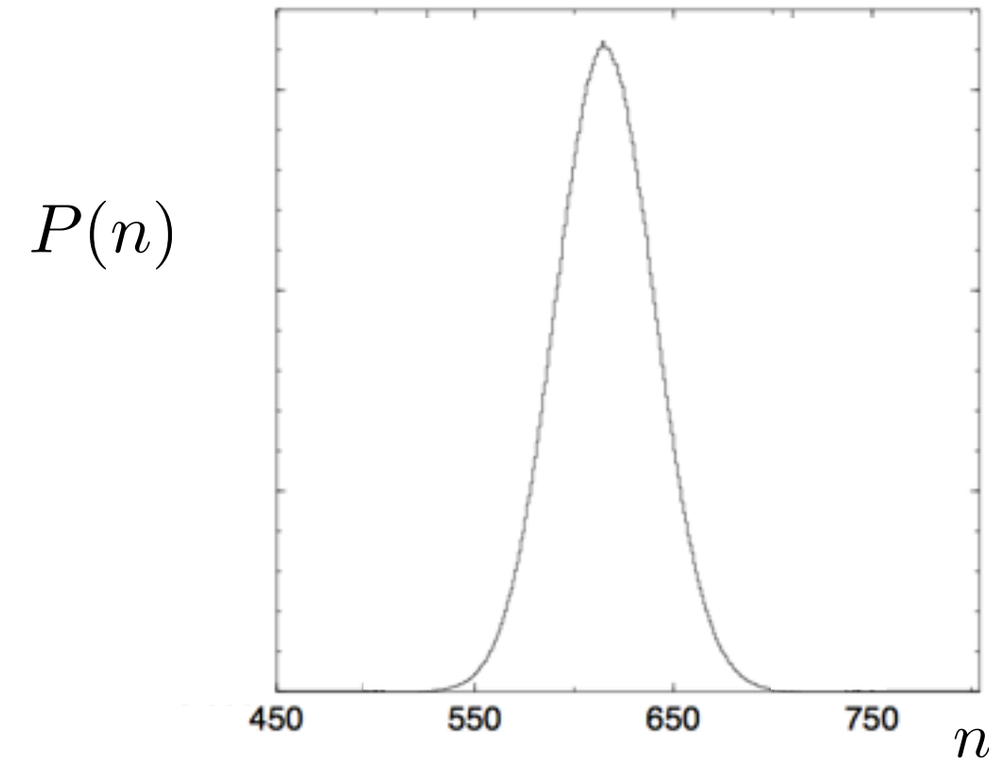
sequence of operator indices

$$S_n = [t_1, a_1], [t_2, a_2], \ldots, [t_n, a_n]$$

We sample (using Monte Carlo) the operator sequence, basis state, and expansion power n

A final (practical) step: truncate the length of the operator list

$$M > n_{\max}$$



Keeping M fixed but sampling different n: need to introduce M-n null operators $H_{0,0} \equiv \mathbb{I}$

Statistically, the number of different way of picking the placement of the null operators in the expansion list is given by the binomial coefficient

$$\binom{M}{n} = \frac{M!}{(M-n)!n!}$$

$$Z = \sum_{\alpha} \sum_{S_M} \frac{(\beta)^n (M-n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle$$

SSE Zero-T representation (projector)

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \langle \Psi | \mathcal{O} | \Psi \rangle \qquad\qquad Z = \langle \Psi | \Psi \rangle$$

$$\langle \mathcal{O} \rangle = \frac{\sum_x \mathcal{O}_x W(x)}{\sum_x W(x)}$$

The ground state wavefunction is estimated by a procedure where a large power of the Hamiltonian is applied to a “trial” state $|\alpha\rangle$

First, write in terms of energy eigenstates: $|\alpha\rangle = \sum_n c_n |n\rangle$

$$\begin{aligned} (-H)^m |\alpha\rangle &= c_0 |E_0|^m \left[|0\rangle + \frac{c_1}{c_0} \left(\frac{E_1}{E_0} \right)^m |1\rangle \cdots \right], \\ &\rightarrow c_0 |E_0|^m |0\rangle \ \text{ as } \ m \rightarrow \infty \end{aligned}$$

$Z = \langle 0|0\rangle$ is then $Z = \langle\alpha|(-H)^m(-H)^m|\alpha\rangle$

using a Hamiltonian breakup: $H = -\sum_t \sum_a H_{t,a}$

insert a resolution of the identity between each operator

$$Z = \sum_{\{\alpha\}} \sum_{S_m} \prod_{j=1}^{2m} \langle \alpha_\ell \left| H_{t_j,a_j} \right| \alpha_r \rangle$$

essentially identical to the finite-T representation, except:

- a fixed value of m is always used
- the simulation cell is not periodic: $|\alpha_\ell\rangle \neq |\alpha_r\rangle$

SSE QMC: Representations

- Finite-T and zero-T representations available
- Both result in very similar practical implementations
- Both can have very similar updating schemes

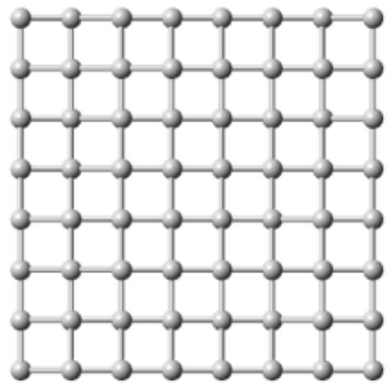
Thermal Expectation value $$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\ \ e^{-\beta H}\mathcal{O}}{\mathrm{Tr}\ \ e^{-\beta \hat{H}}}$$

T=0 Expectation Value $$\langle \mathcal{O} \rangle = \langle \Psi | \mathcal{O} | \Psi \rangle$$

To understand in more detail, we should examine a specific example

SSE QMC: Spin-1/2 Heisenberg Model

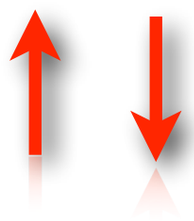
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

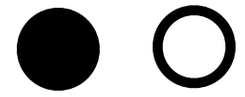


Let's examine the finite-T representation:

$$Z = \sum_{\alpha} \sum_{S_M} \frac{(\beta)^n (M-n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle$$

First: choose a basis $|\alpha\rangle$ $S^z = \pm \frac{1}{2}$





Next: specify a specific lattice decomposition: $H = -\sum_t \sum_a H_{t,a}$

Choose a “bond” decomposition

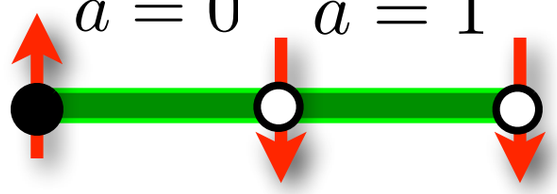
$$H = -\sum_t \sum_a H_{t,a}$$

null $\quad H_{0,0} = \mathbb{I},$

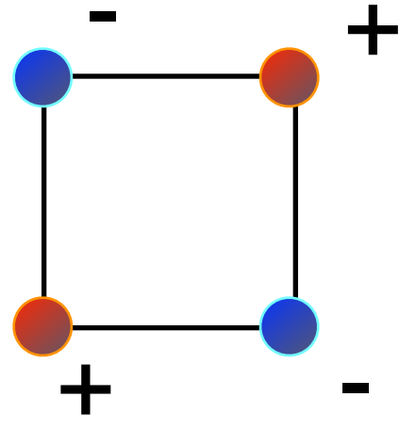
diagonal $\quad H_{1,a} = \frac{1}{4} - S_i^z S_j^z,$

off-diagonal $\quad H_{2,a} = \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$

“type” bond label



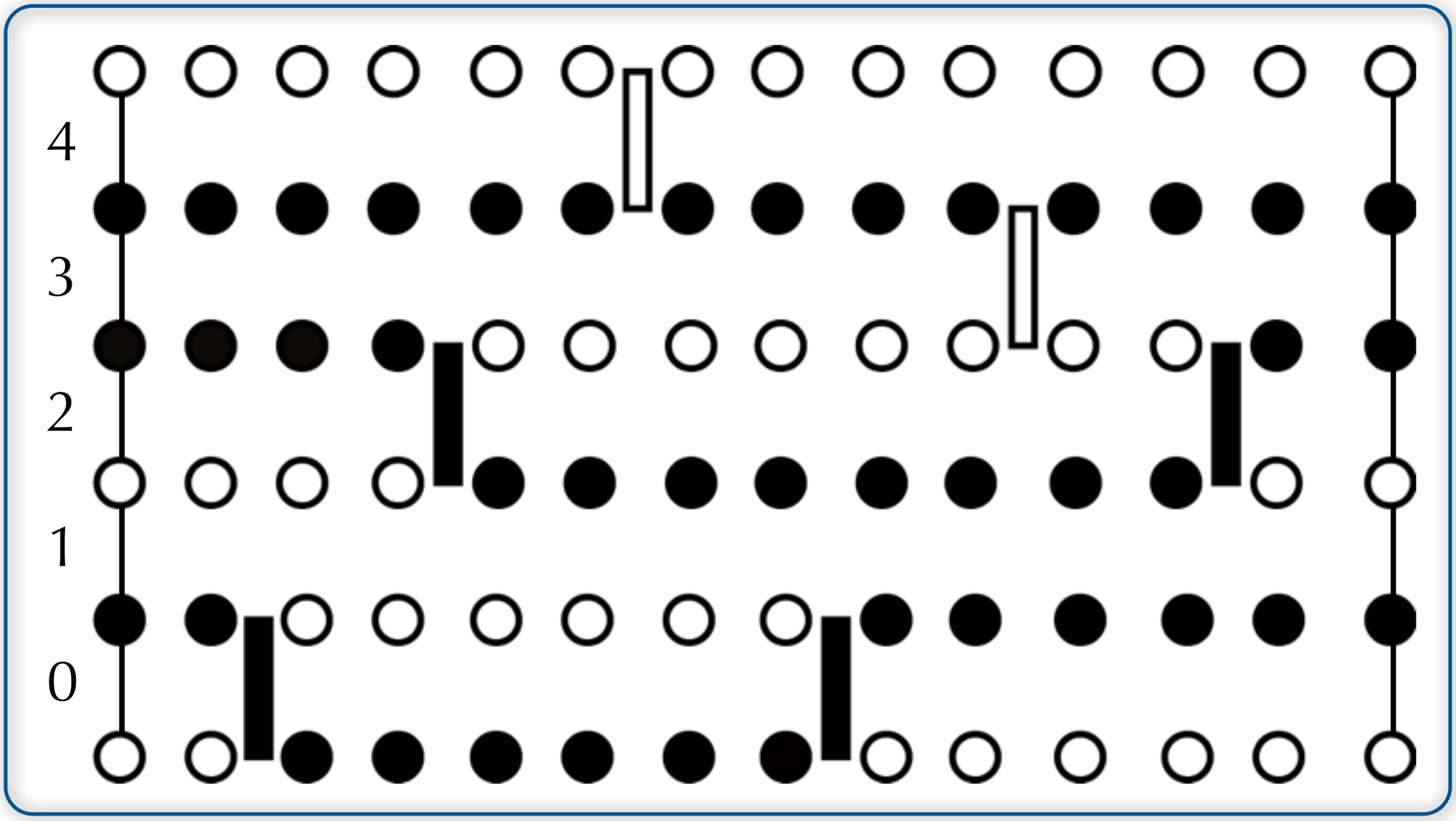
- A constant term 1/4 is added to the diagonal operator
- Spin operators are rotated by $\pi/2$ around the z-axis on one of the sublattices



All bond operators are positive

$$H_{1,a} = \frac{1}{4} - S_i^z S_j^z \qquad H_{2,a} = \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$$

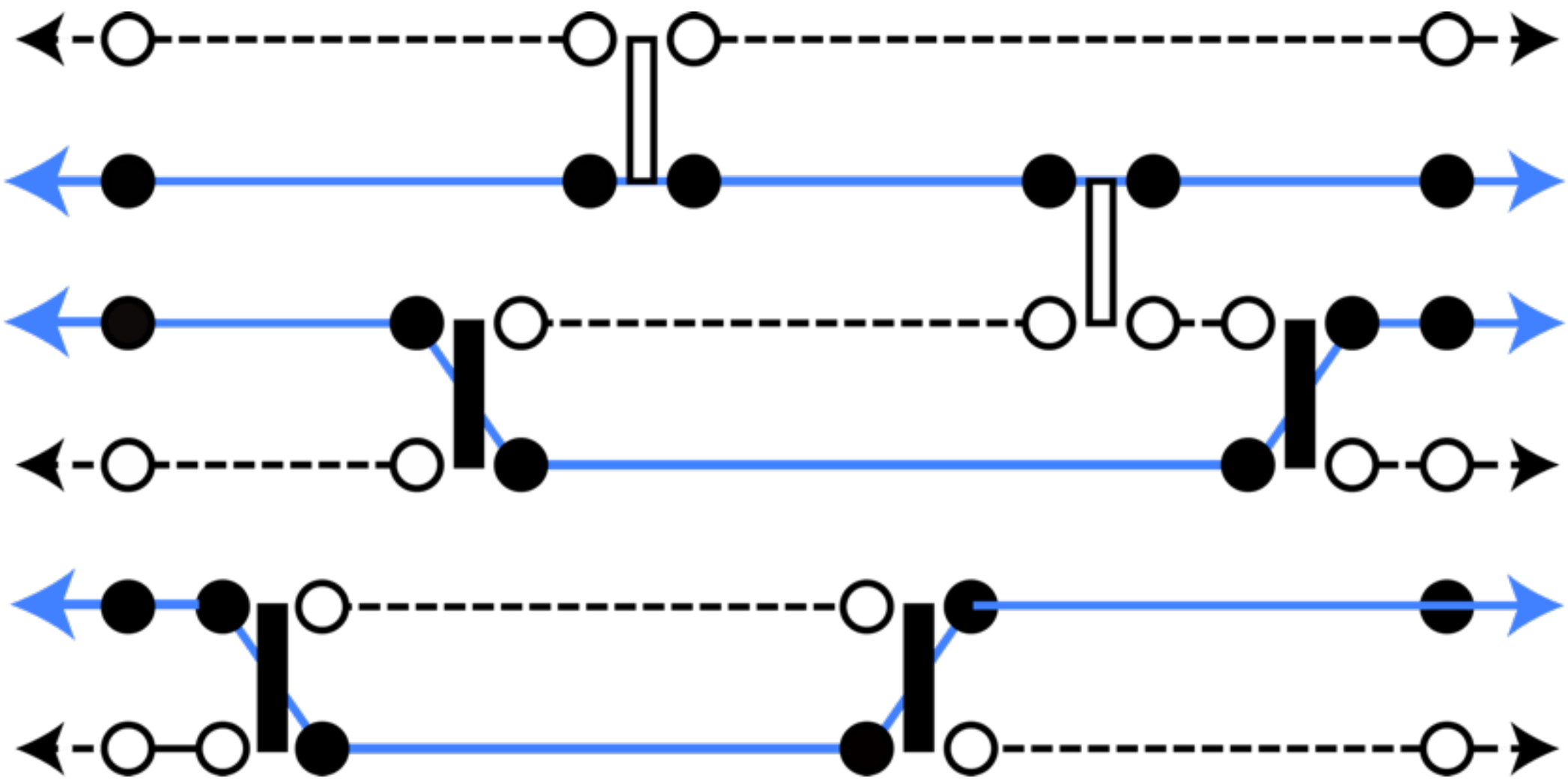
$n = 6 \quad M = 13$



$|\alpha_0\rangle$ $|\alpha_M\rangle = |\alpha_0\rangle$

$S_n = [0,0],[2,0],[0,0],[2,2],[0,0],[1,4],[0,0],[2,0],[0,0],[1,3],[0,0],[2,2],[0,0]$

resembles a world line picture:



The weight $W(x)$ of a sampled configuration x is proportional to the product of the positive matrix elements.

$$\langle \bullet \circ |H_{1,a}| \bullet \circ \rangle = \langle \circ \bullet |H_{1,a}| \circ \bullet \rangle = \frac{1}{2}$$

$$\langle \bullet \circ |H_{2,a}| \circ \bullet \rangle = \langle \circ \bullet |H_{2,a}| \bullet \circ \rangle = \frac{1}{2}$$

We now have a **representation**. From this we design **updates**:

- Local updates can be used to sample diagonal operators

$$H_{1,a} \leftrightarrow H_{0,0}$$

- Non-local updates needed to sample off-diagonal operators

$$H_{2,a} \leftrightarrow H_{1,a}$$

SSE "Diagonal" Updates

- Cycle through the operator list

- If a null operator is encountered, attempt to put a diagonal operator on a random bond $H_{0,0} \rightarrow H_{1,a}$

- If a diagonal operator is encountered, attempt to remove it (resulting in a null operator) $H_{1,a} \rightarrow H_{0,0}$

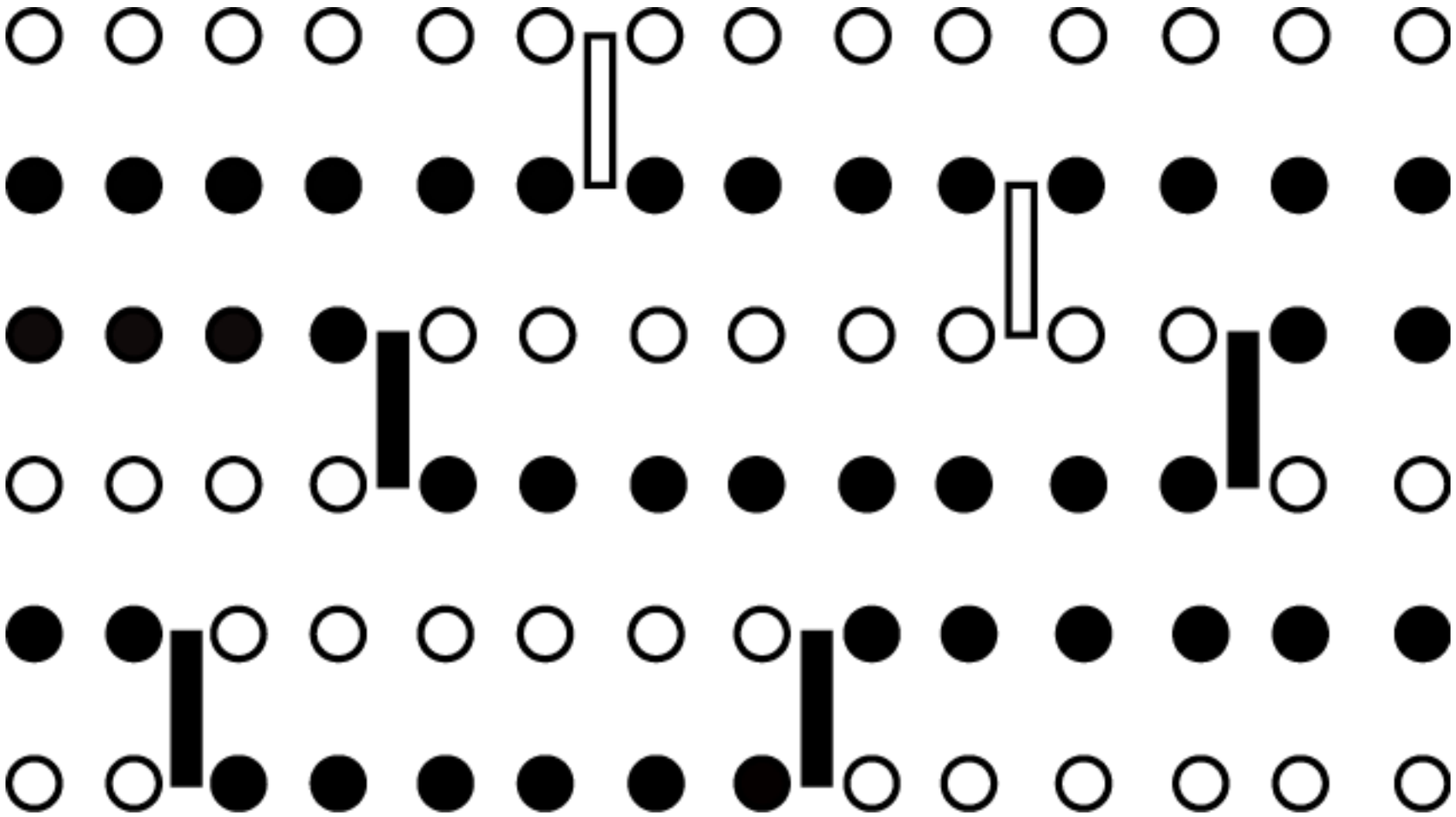
Like in classical Monte Carlo, we calculate the ratio of weights:

$$\frac{W(x')}{W(x)}$$

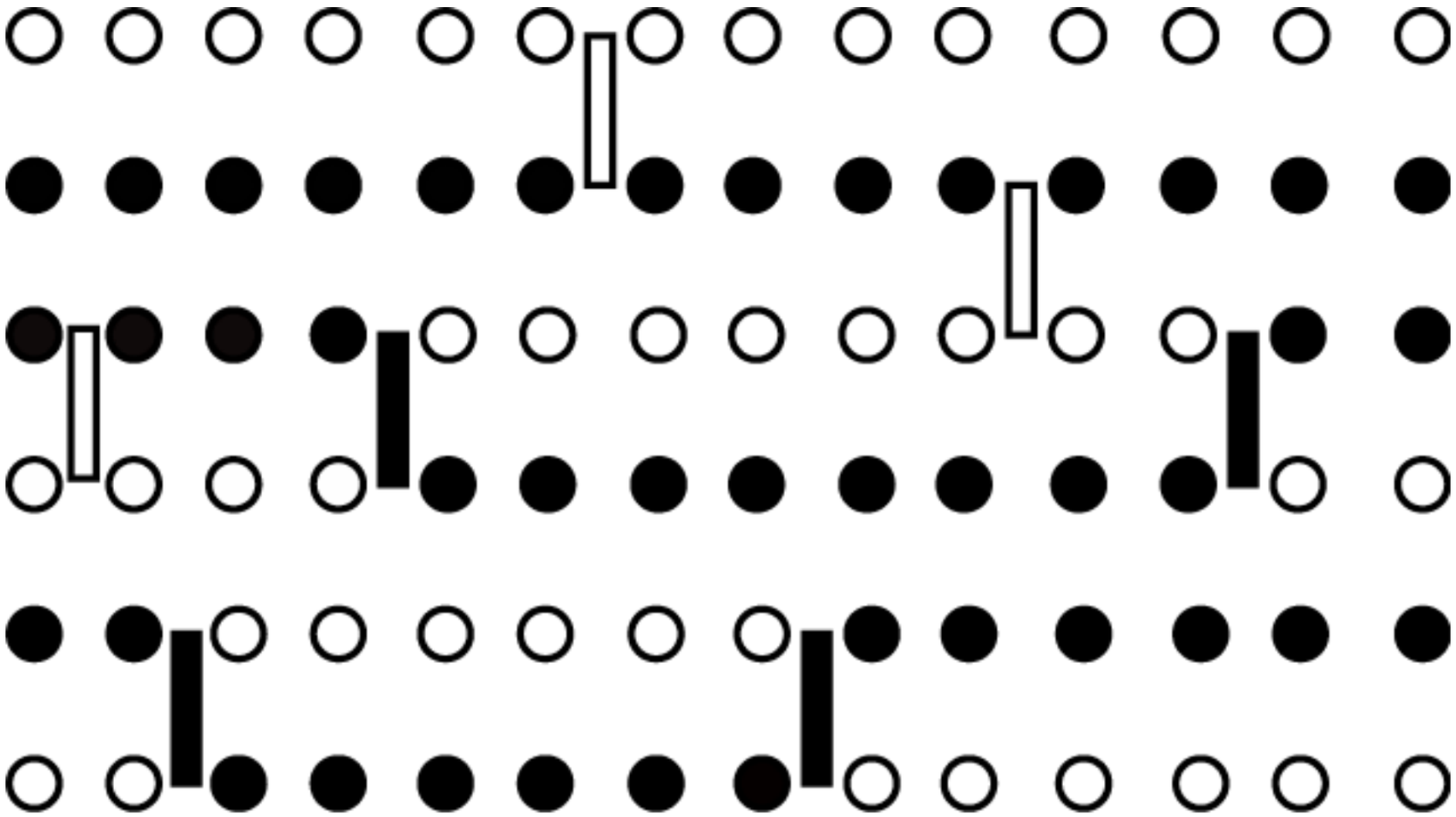
The transition probability is then obtained from detailed balance:

$$W(x)P(x \rightarrow x') = W(x')P(x' \rightarrow x),$$

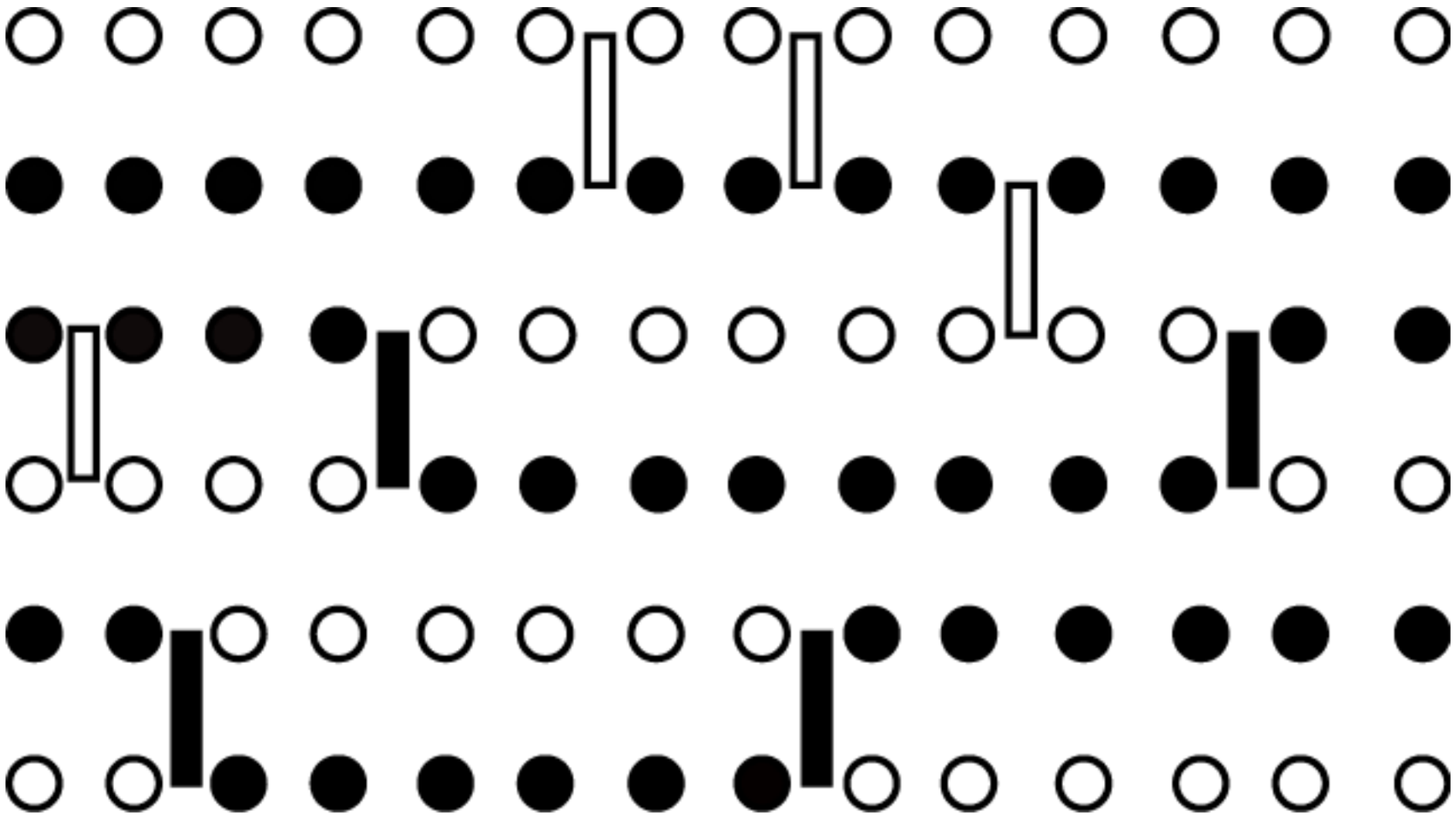
SSE “Diagonal” Updates



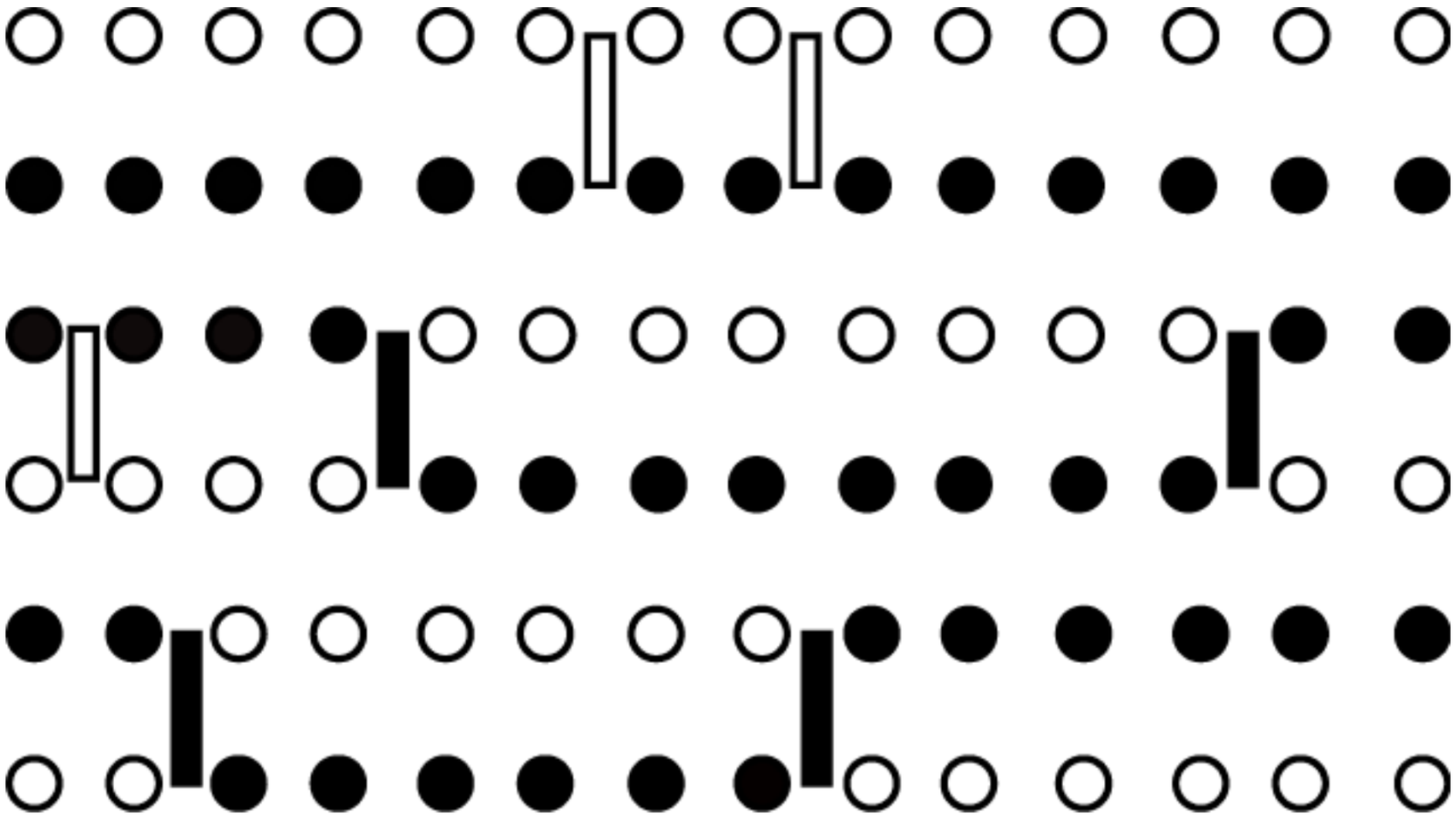
SSE “Diagonal” Updates



SSE “Diagonal” Updates



SSE “Diagonal” Updates



SSE "Diagonal" Updates

$$Z = \sum_{\alpha} \sum_{S_M} \frac{(\beta)^n (M-n)!}{M!} \prod_{i=1}^{M} \langle \alpha_{i-1} | H_{t_i,a_i} | \alpha_i \rangle$$

Transition probabilities for a Metropolis algorithm

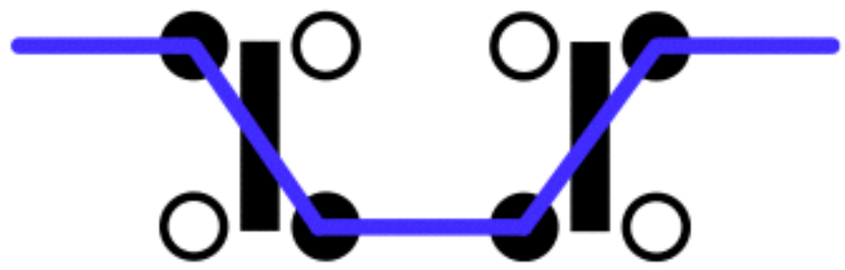
$$P(n \to n+1) = \min\left(\frac{1}{2}\frac{N_b \beta}{(M-n)}, 1\right)$$

- a lattice bond must be chosen at random for the insertion
- factor of 1/2 is the matrix element

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

SSE “Diagonal” Updates

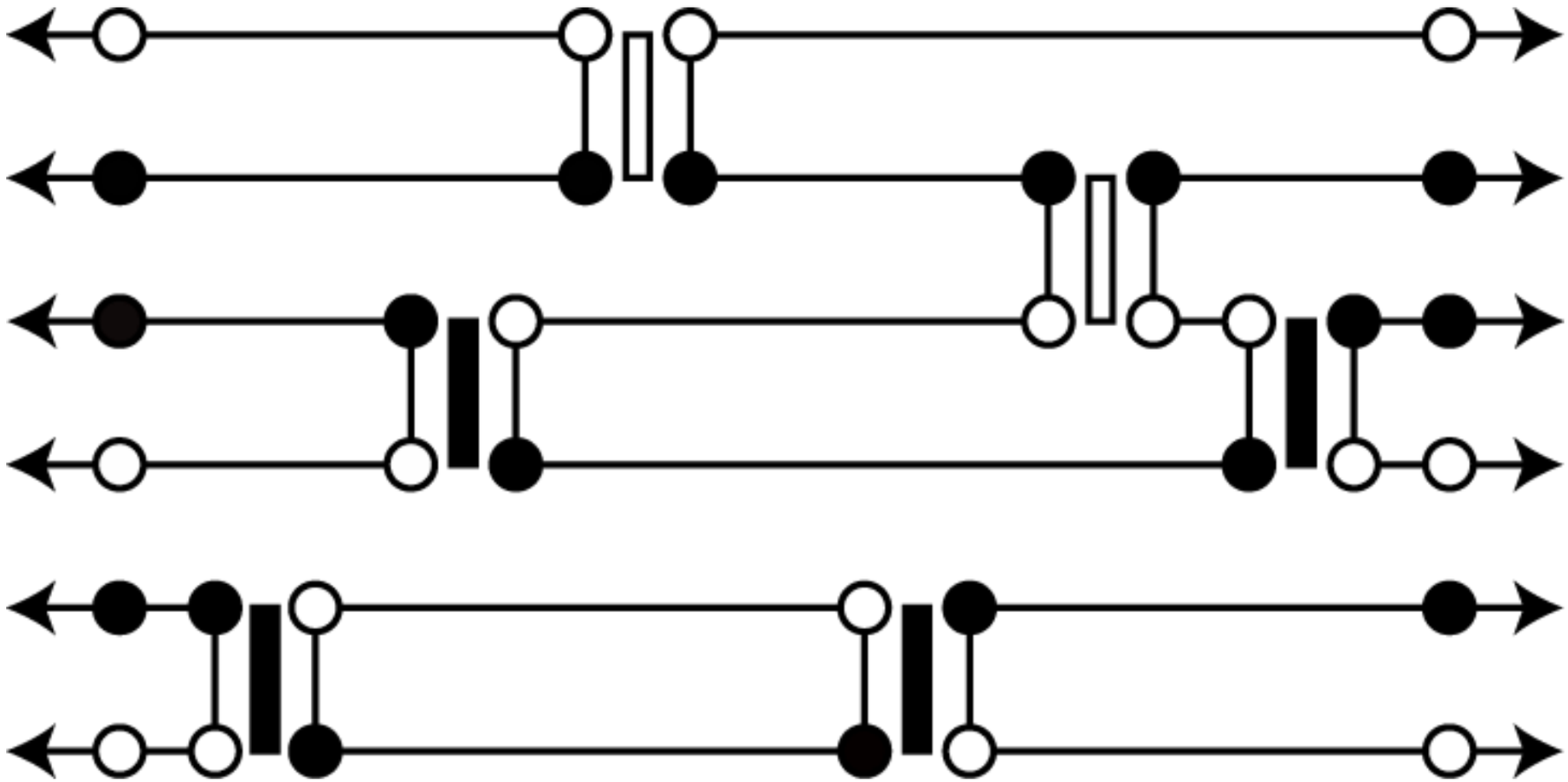
- Sample the power of the expansion effectively
- Easy to implement, local updates
- Do **not** result in an ergodic simulation: off-diagonal operators are not sampled



we require a method to change the type of more than one operator at once, if we are to preserve the periodic boundaries

SSE "Operator-Loop" Updates

The fact that all non-trivial matrix elements are 1/2 means that operator types can be changed without a change in weight



Closed "loops" are identified (in a linked list), then flipped with a Swendsen-Wang algorithm

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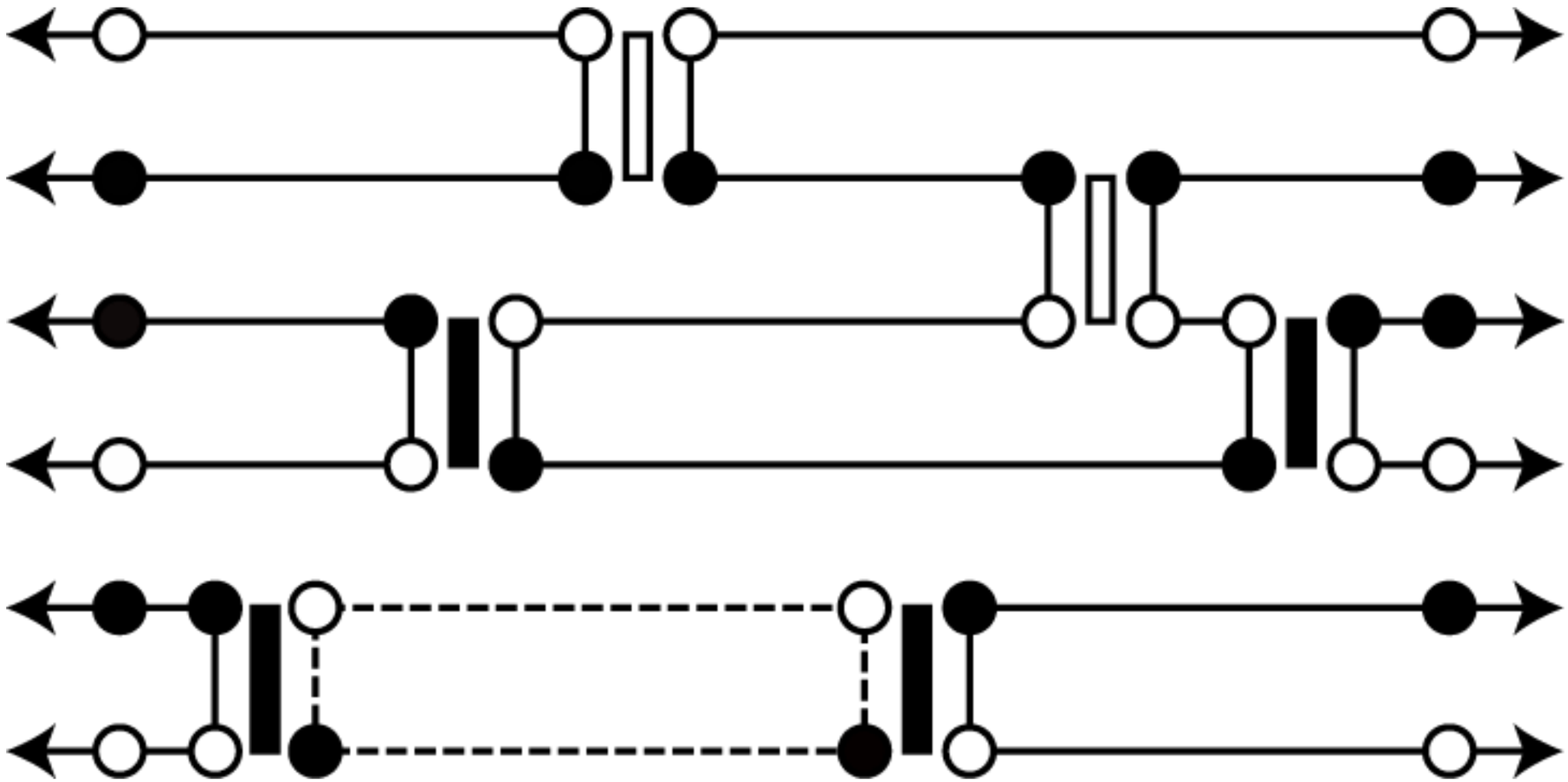

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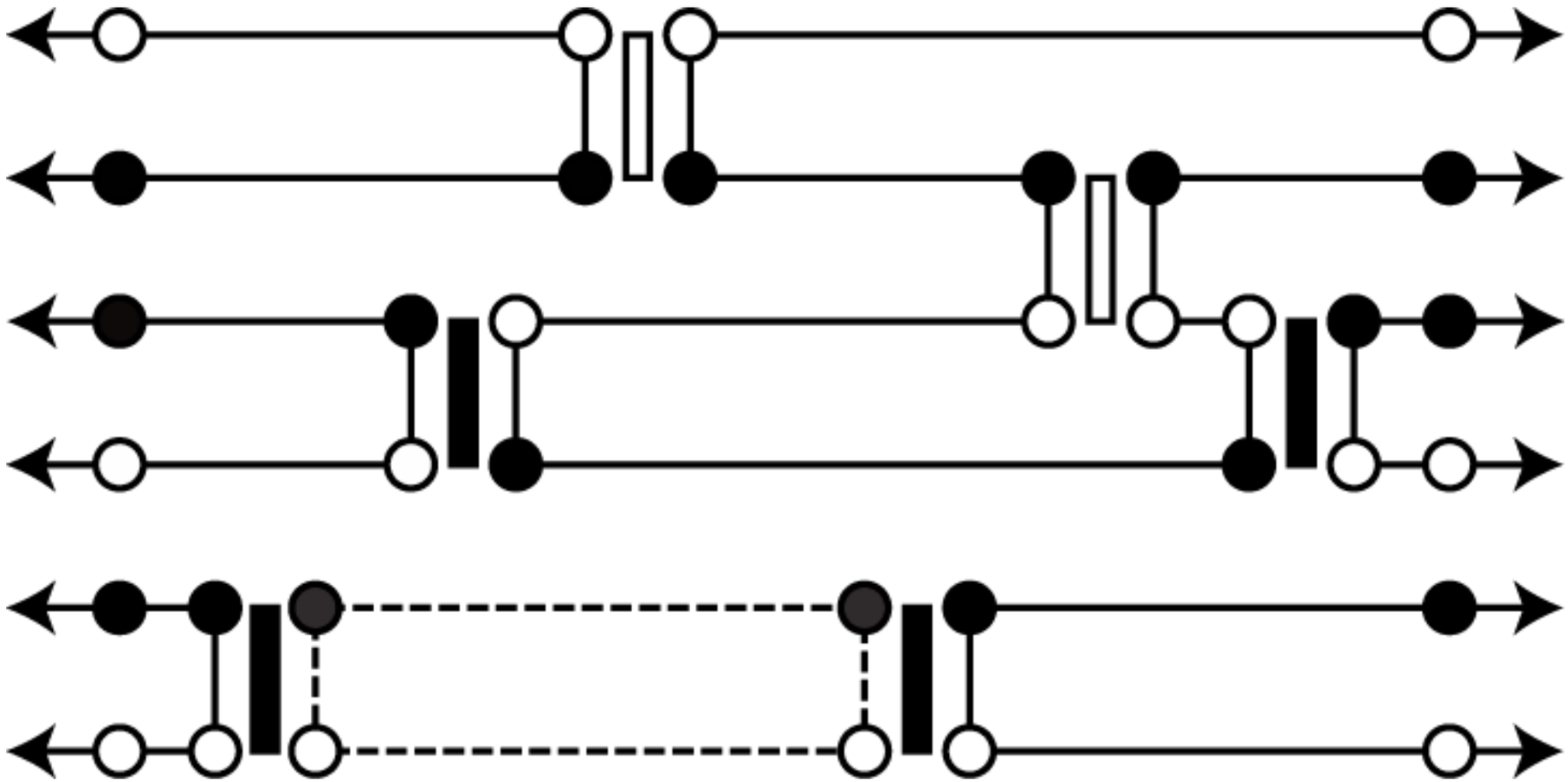

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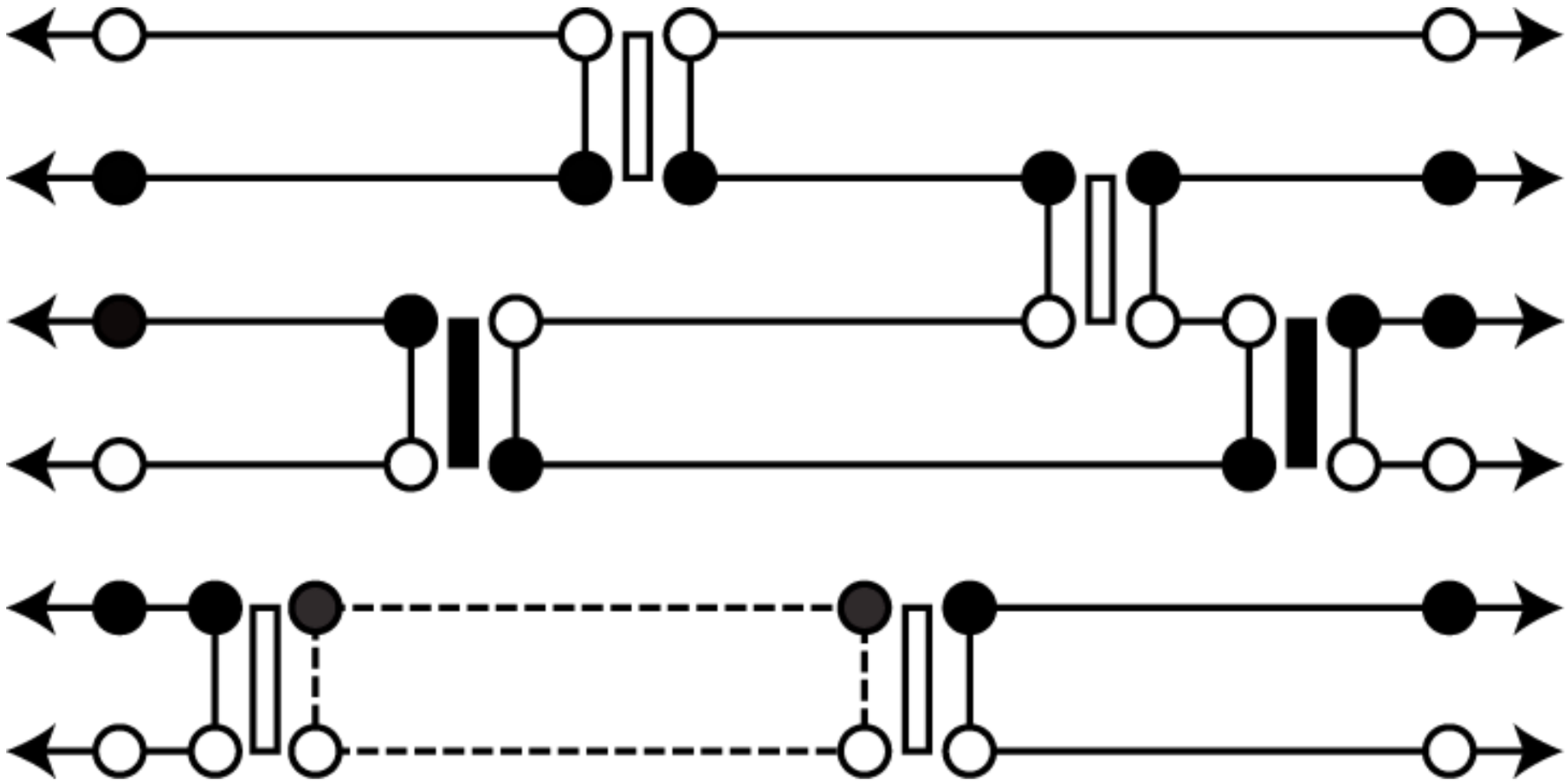

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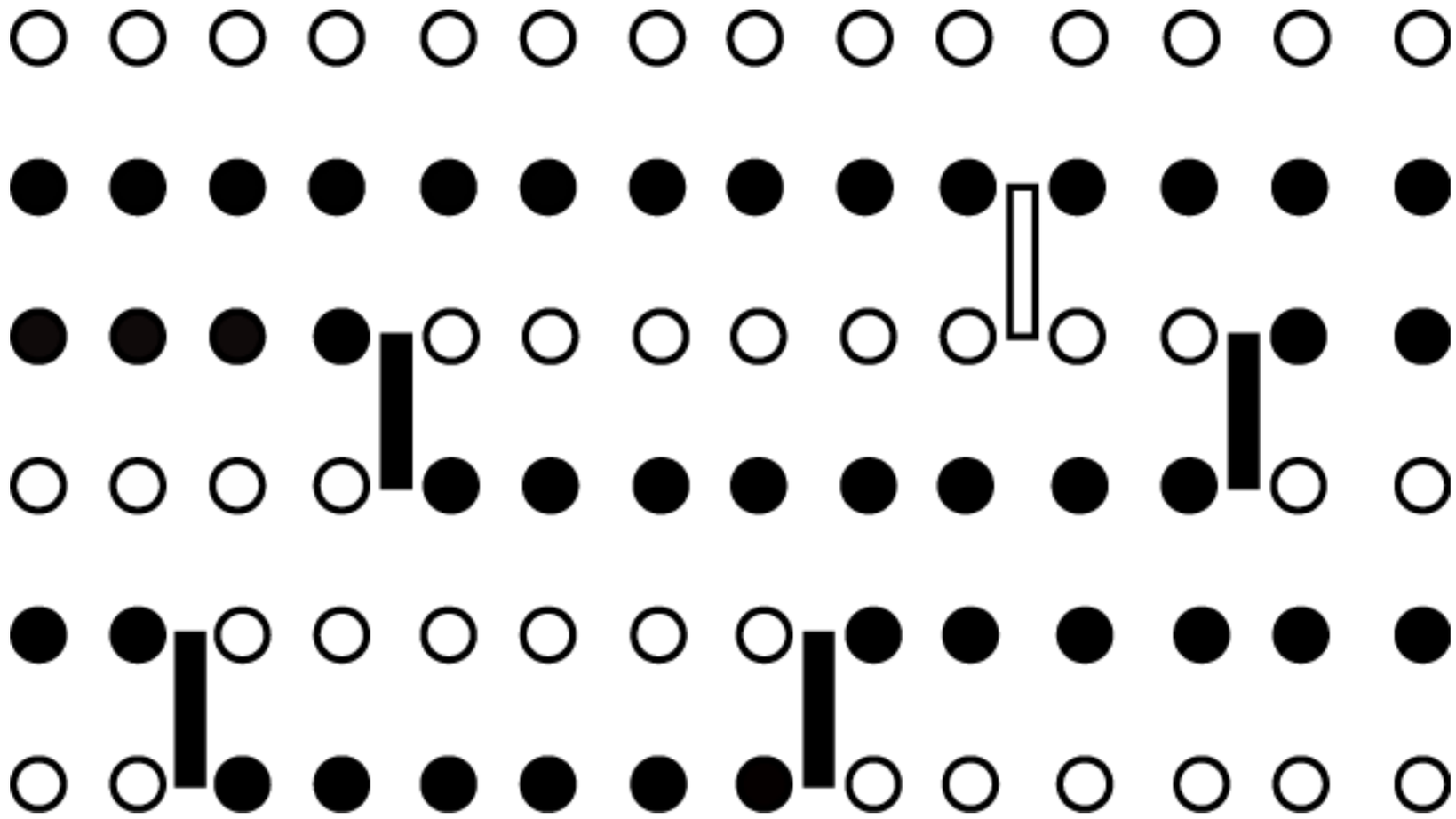
Other SSE updates:

- Spin-flips: required at high temperature



- Other more sophisticated operator loops possible
- Can be used in conjunction with Parallel Tempering, etc.

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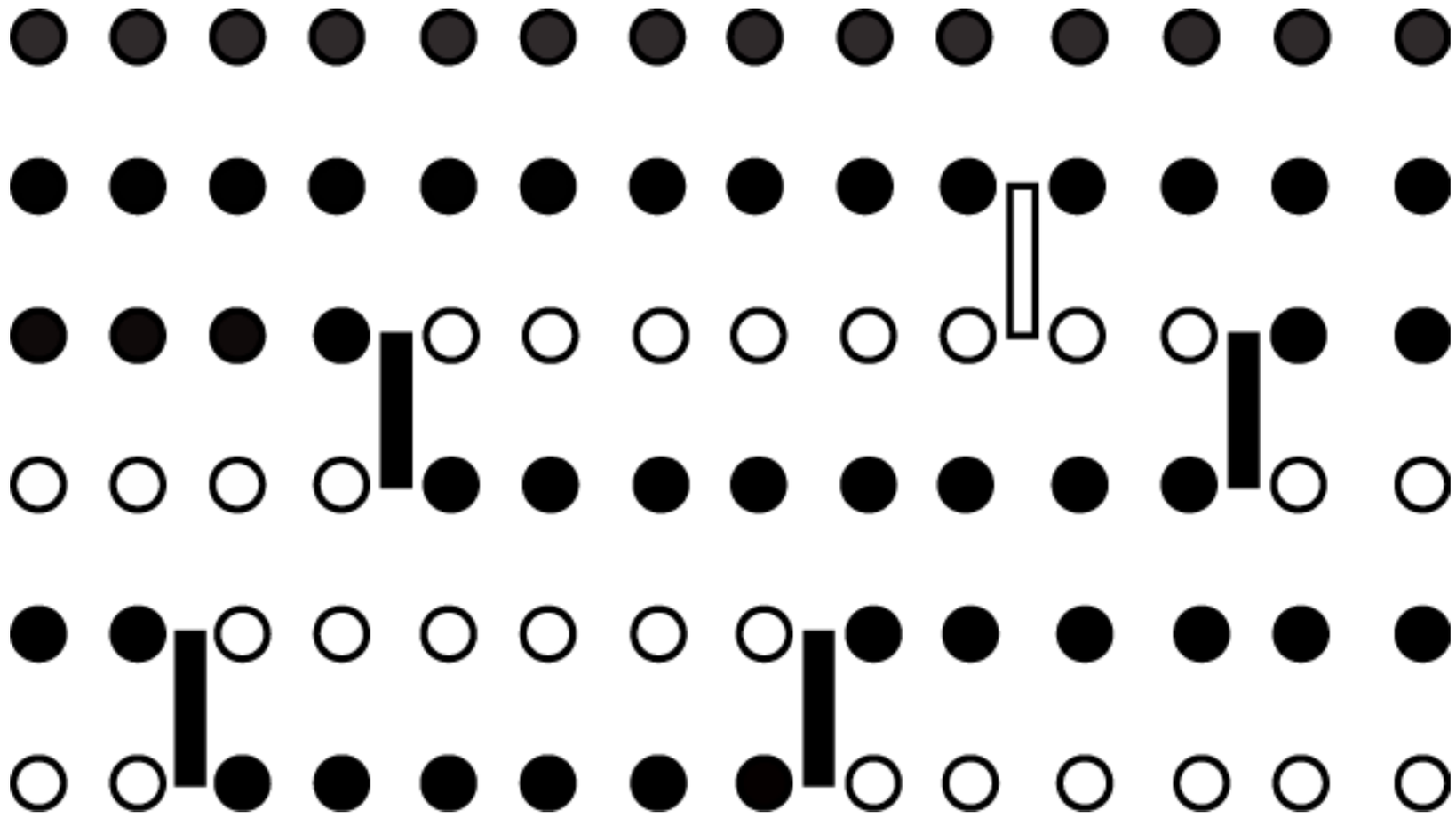

- Other more sophisticated operator loops possible
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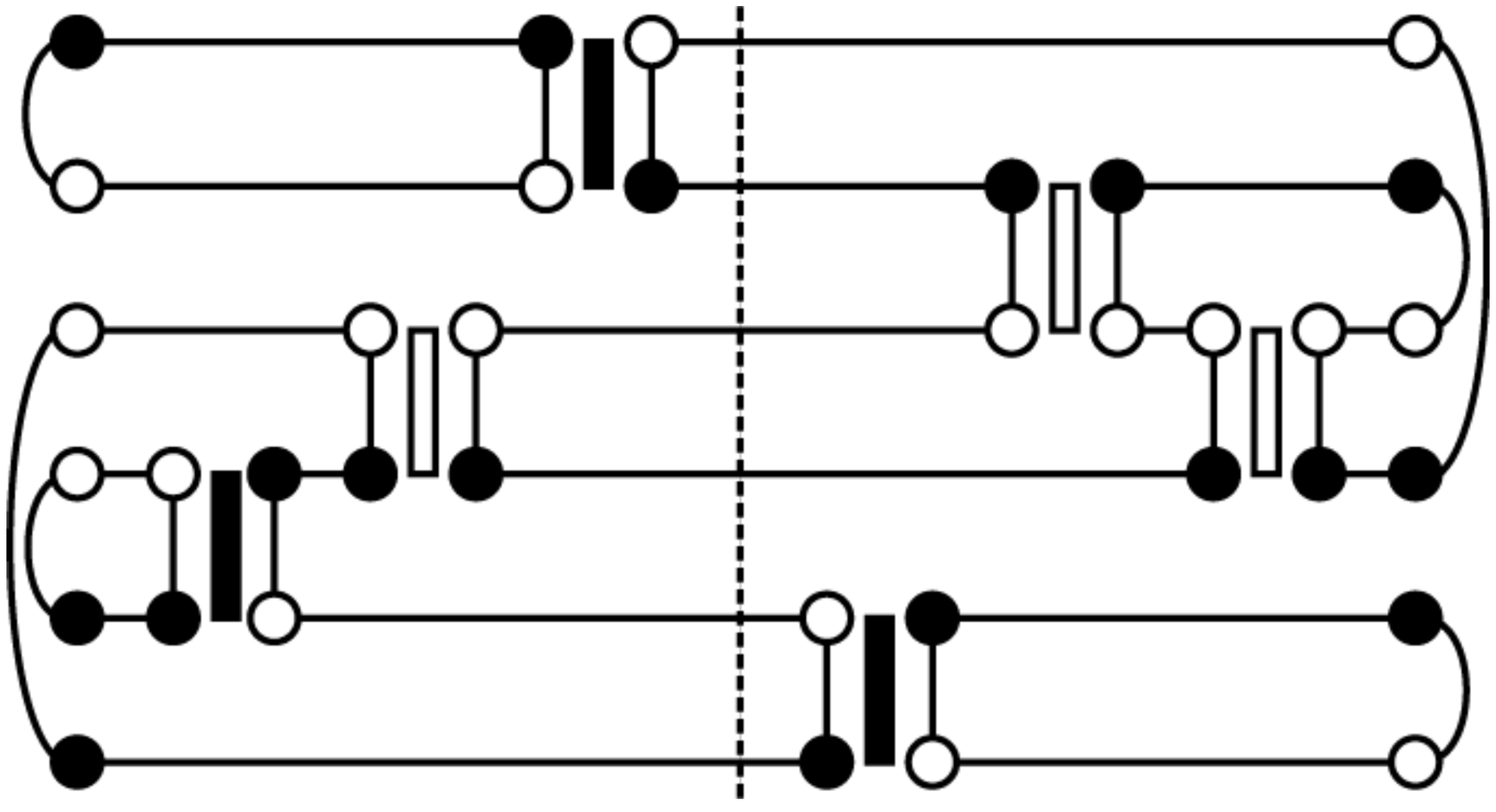
SSE T=0 representation

$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Remarkably, a very different representation can have essentially the same updating procedure



$$Z = \langle \alpha | (-H)^m (-H)^m | \alpha \rangle$$

another example: Transverse Field Ising Model

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

A convenient Hamiltonian decomposition: $H = -\sum_t \sum_a H_{t,a}$

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

The index a can label a bond, or a single lattice site. Note:

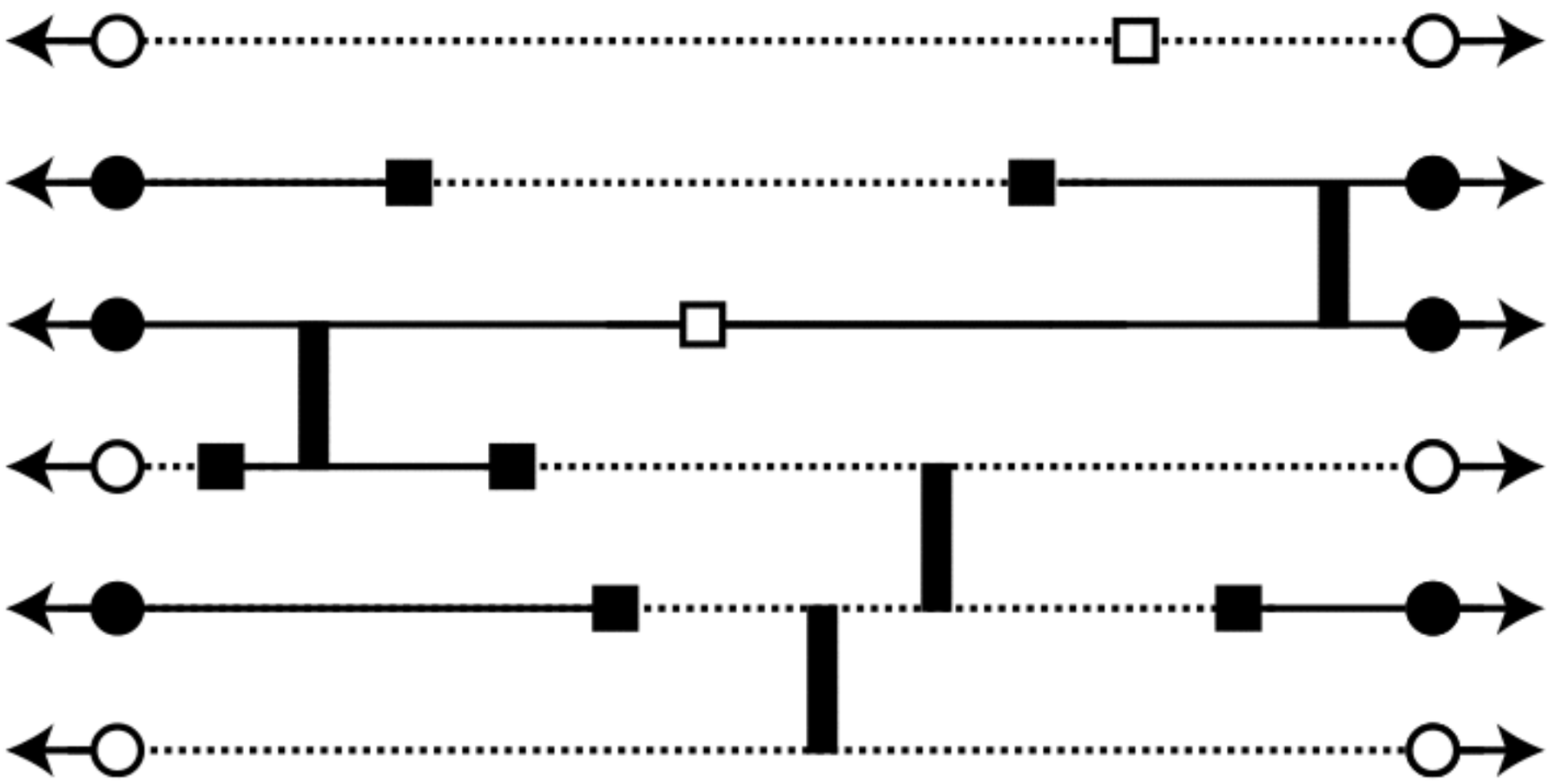
$$\begin{aligned} \langle \bullet | H_{-1,a} | \circ \rangle = \langle \circ | H_{-1,a} | \bullet \rangle = h, \\ \langle \bullet | H_{0,a} | \bullet \rangle = \langle \circ | H_{0,a} | \circ \rangle = h. \end{aligned}$$

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

another example: Transverse Field Ising Model

Finite-T representation

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



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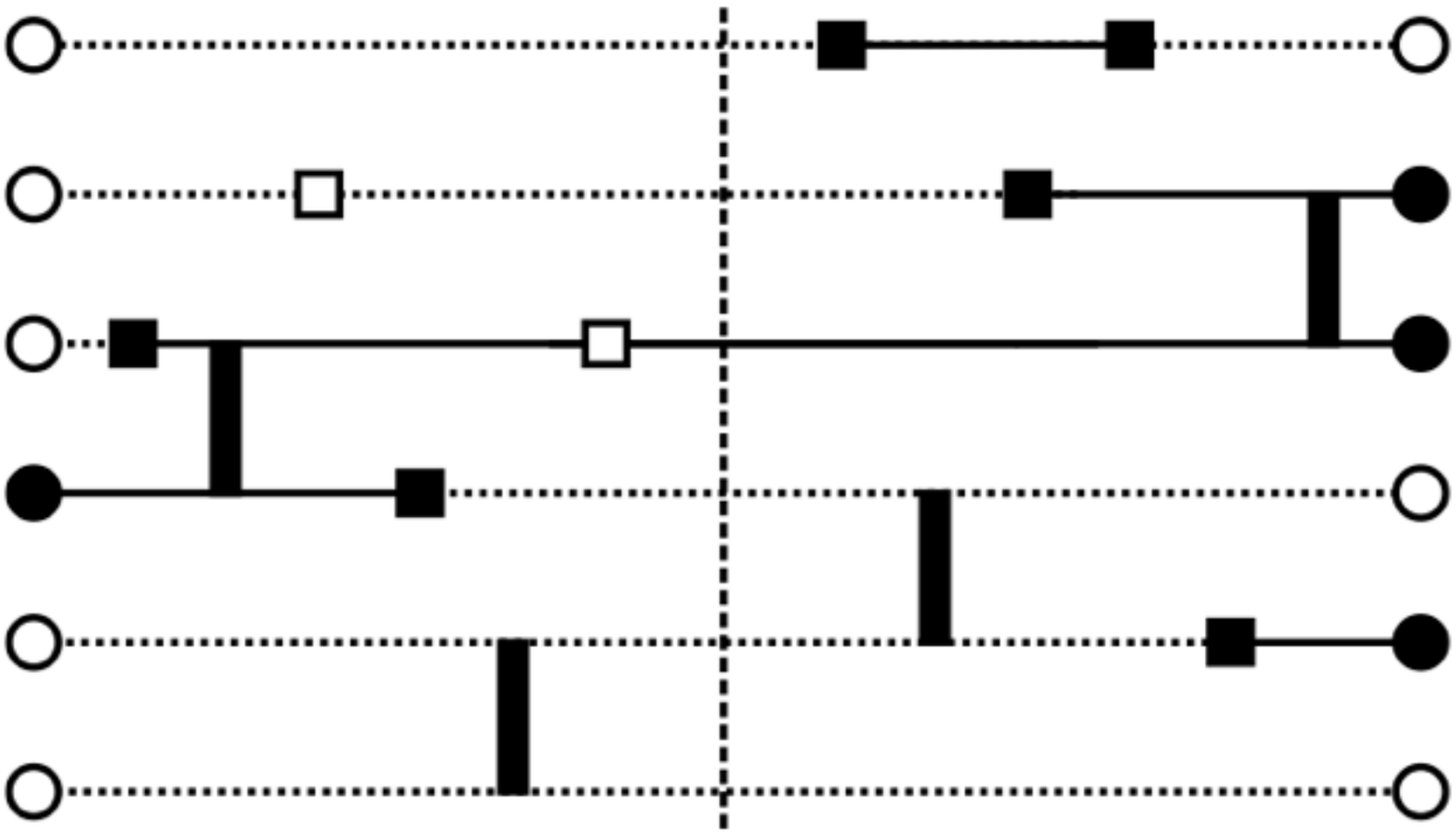
zero-T representation

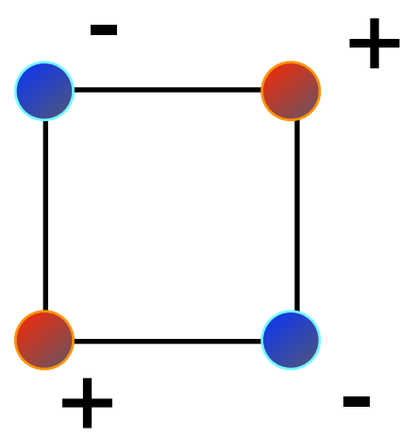
$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$



The Sign Problem in SSE

- Any constant term can be added to diagonal operators

- Spin operators are rotated by $\pi/2$
  around the z-axis on one of the sublattices ...



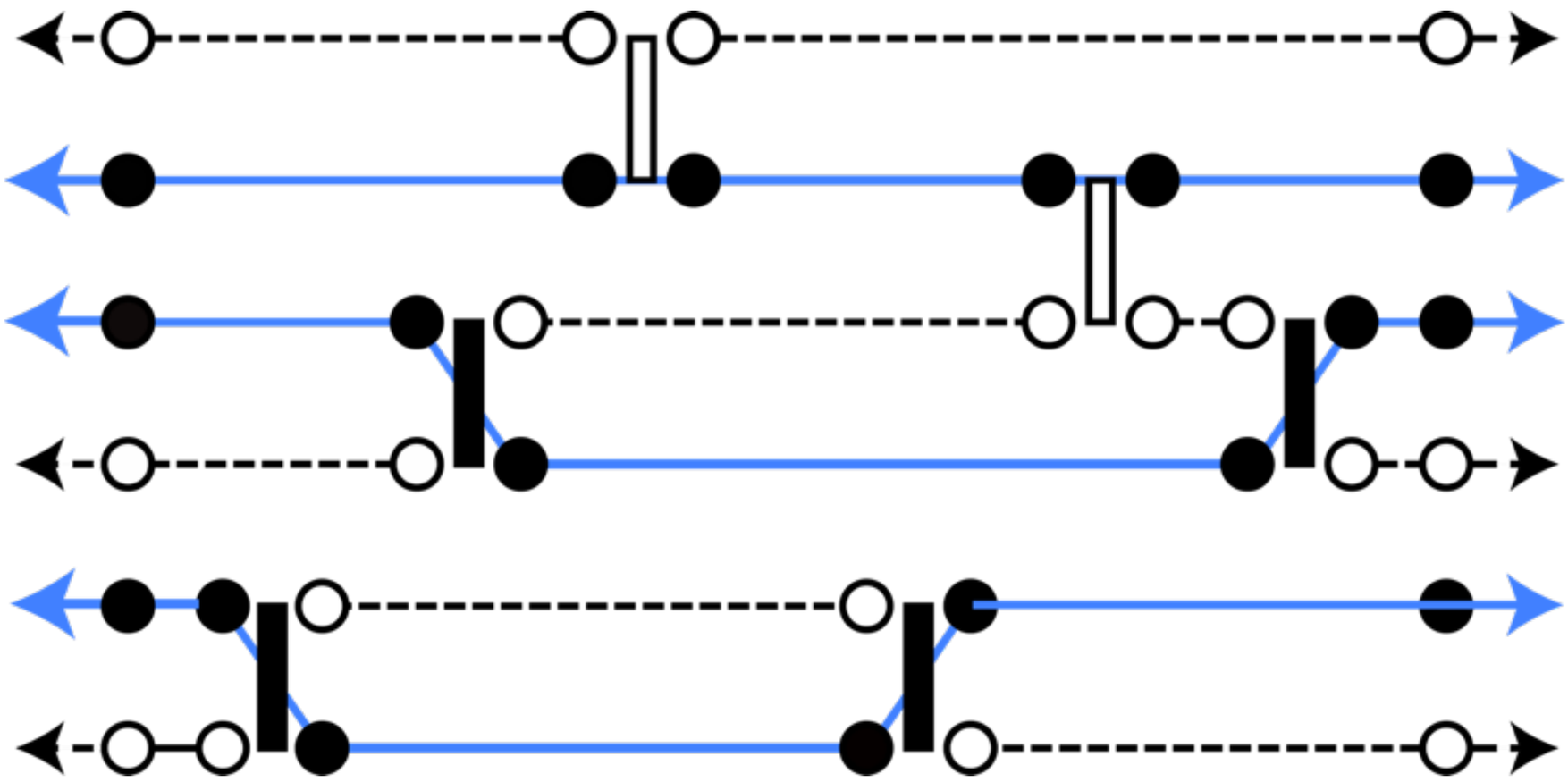
$$Z = \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha_0 | -H | \alpha_1 \rangle \langle \alpha_1 | -H | \alpha_2 \rangle \cdots \langle \alpha_{n-1} | -H | \alpha_n \rangle$$

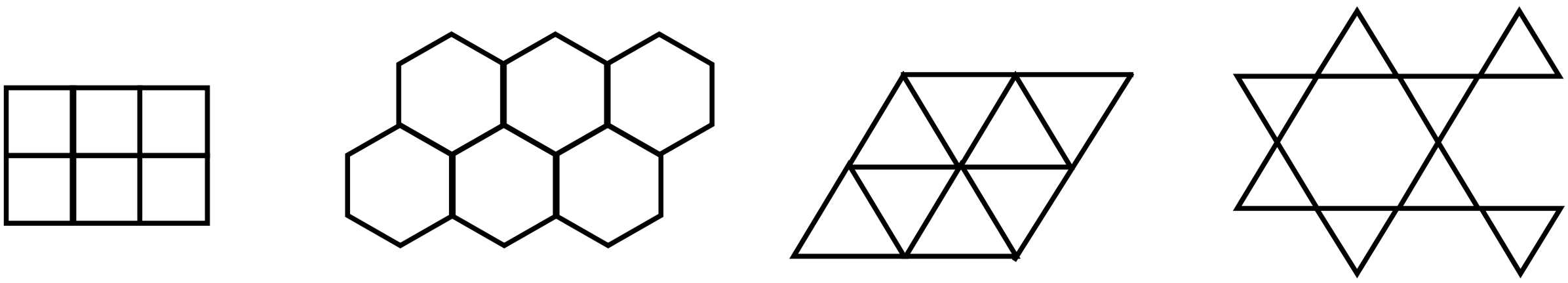
Alternatively, we can keep the matrix element unchanged, if we are confident that off-diagonal operators always occur in even numbers

$$H = -\sum_t \sum_a H_{t,a} \qquad\qquad H_{2,a} = -\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)$$

The Sign Problem in SSE

In the finite-T representation, periodic boundary condition in imaginary time enforce this:





Measurements in the SSE:

In general - expectation values of **operators** either:

- Diagonal in the basis $\langle S_i^z S_j^z \rangle$ $S(\mathbf{q})$

- Associated with the Hamiltonian

$\langle B_i B_j \rangle$ $B_i = S_i^+ S_j^- + S_i^- S_j^+$

example: $Z = \sum_{\alpha_0} \left\langle \alpha_0 \left| \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (-H)^n \right| \alpha_0 \right\rangle$ $E = -\frac{\partial \ln Z}{\partial \beta}$

$E = -\frac{1}{Z} \sum_{\alpha_0} \left\langle \alpha_0 \left| \sum_{n=0}^{\infty} \frac{n\beta^{(n-1)}}{n!} (-H)^n \right| \alpha_0 \right\rangle$ $E = -\frac{\langle n \rangle}{\beta}$

Quantum Monte Carlo

- A large class of Metropolis based Monte Carlo methods in D+1 dimension

- Extremely powerful, work well in higher D

- Inhibited by the "sign problem" for frustrated spins and fermions

- Algorithms are not static: new models, measurements, and tricks are discovered frequently

- At least one Nobel Prize lurking around to reward innovation