Quantum Monte Carlo

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DPG - School on Physics

supported by the Wilhelm and Else Heraeus-Foundation

Efficient Algorithms in Computational Physics

10 - 14 September 2012, Physikzentrum Bad Honnef, Germany

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:

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

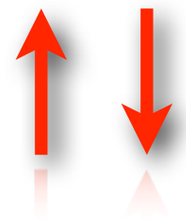
ie. we can solve all the model properties if we can solve the eigenvalue problem (i.e. diagonalize the Hamiltonian)

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 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

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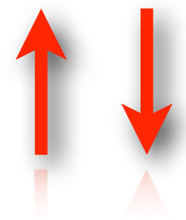

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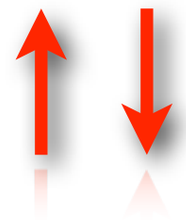

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Can we diagonalize “parts” of the Hamiltonian?

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

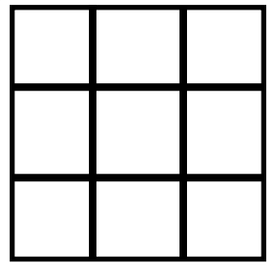
$\mathrm{e}^{\lambda(\hat{A}+\hat{B})}$ and $\mathrm{e}^{\lambda \hat{A}} \mathrm{e}^{\lambda \hat{B}}$

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

Numerical Methods for Quantum Systems

- Exact diagonalization

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



obtain full spectrum

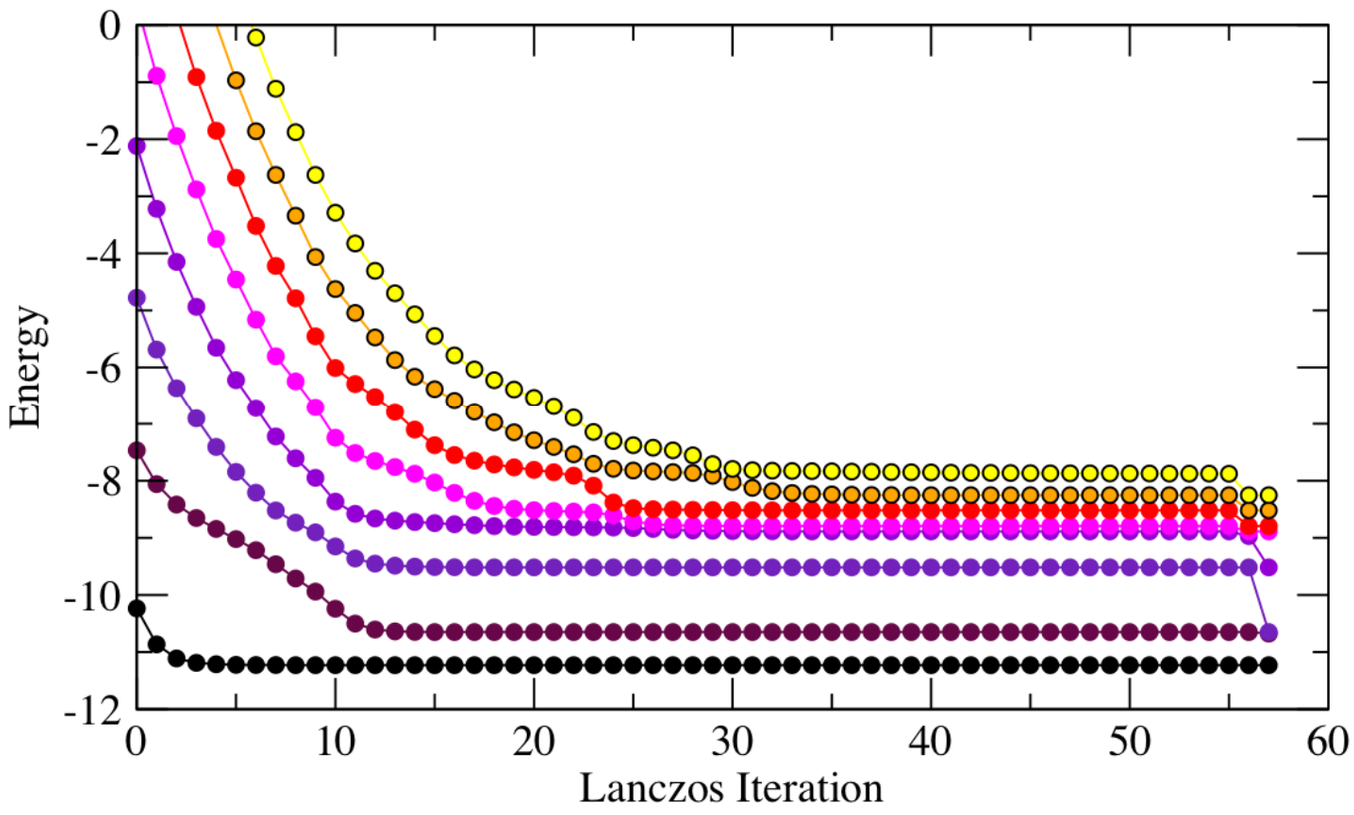
$N \approx 16 - 20$

- Lanczos diagonalization

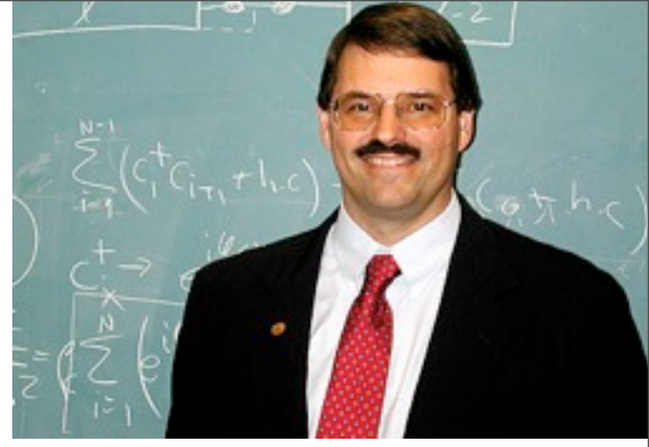
iterative: groundstate only

$|\Psi_0\rangle$

$N \approx 40$



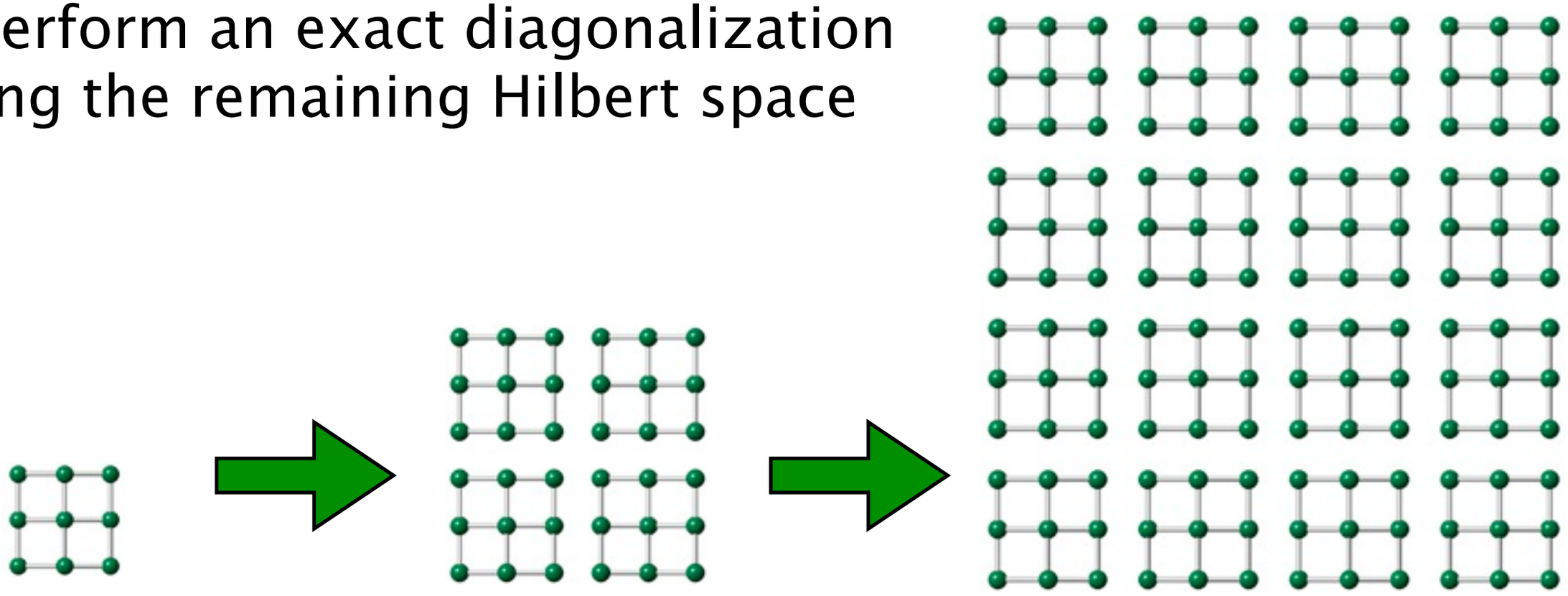
Density Matrix Renormalization Group (very basic idea)



- Reduce the size of the Hilbert space through some clever decimation procedure

- Keep only the “important” information

- Perform an exact diagonalization using the remaining Hilbert space



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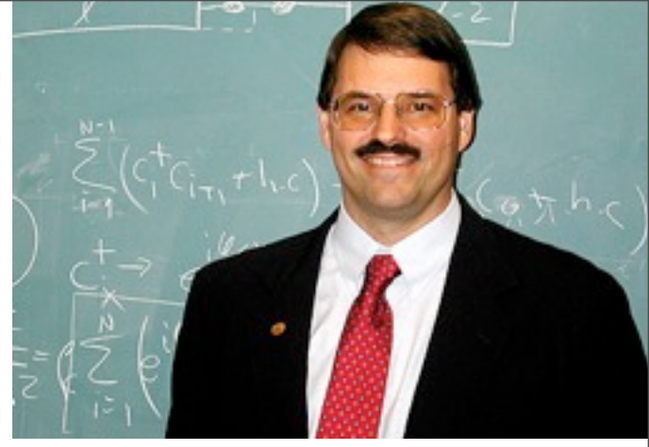

- Early success: the Haldane Gap

PHYSICAL REVIEW B VOLUME 48, NUMBER 6 1 AUGUST 1993-II

Numerical renormalization-group study of low-lying eigenstates of the antiferromagnetic $S = 1$ Heisenberg chain

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David A. Huse
AT&T Bell Labs, Murray Hill, New Jersey 07974

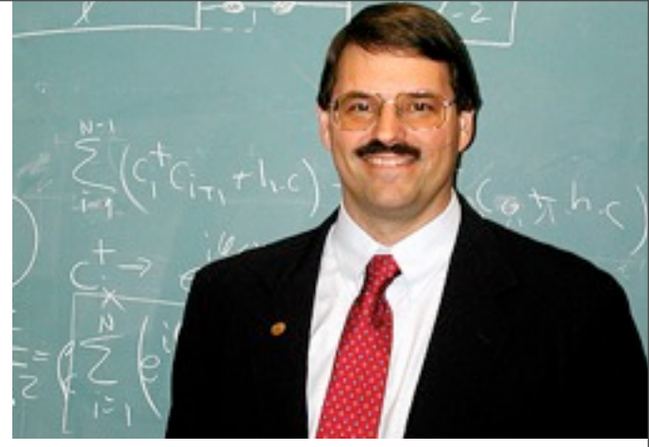
(Received 3 February 1993; revised manuscript received 23 April 1993)

We present results of a numerical renormalization-group study of the isotropic $S = 1$ Heisenberg chain. The density-matrix renormalization-group techniques used allow us to calculate a variety of properties of the chain with unprecedented accuracy. The ground state energy per site of the infinite chain is found to be $e_0 \cong -1.401\,484\,038\,971(4)$

The excitation energy of the first excited state, a state with one magnon with momentum $q = \pi$, is the Haldane gap, which we find to be $\Delta \cong 0.410\,50(2)$.

$S = 1$

Density Matrix Renormalization Group (very basic idea)

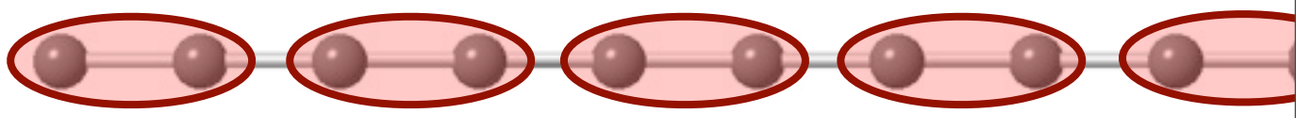


- The DMRG works, because truncating the eigenvalues of the reduced density matrix is able to preserve the entanglement properties of typical 1D systems

$$S = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

$$S = \ln(2)$$

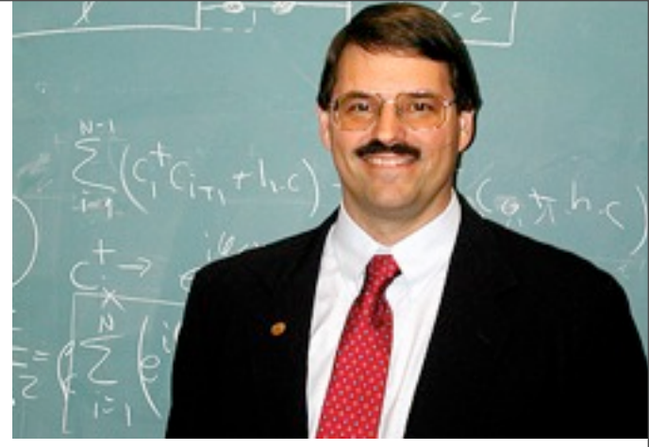
AKLT



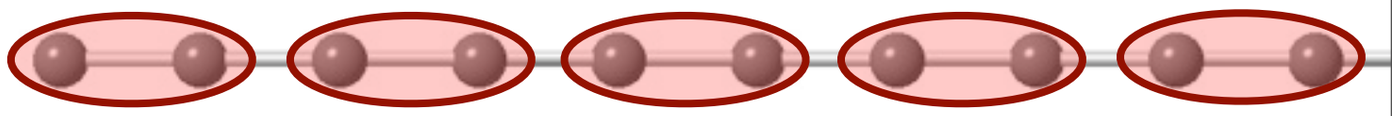
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$S(x) = \frac{c}{3} \cdot \ln[x'] + \text{const.}$$

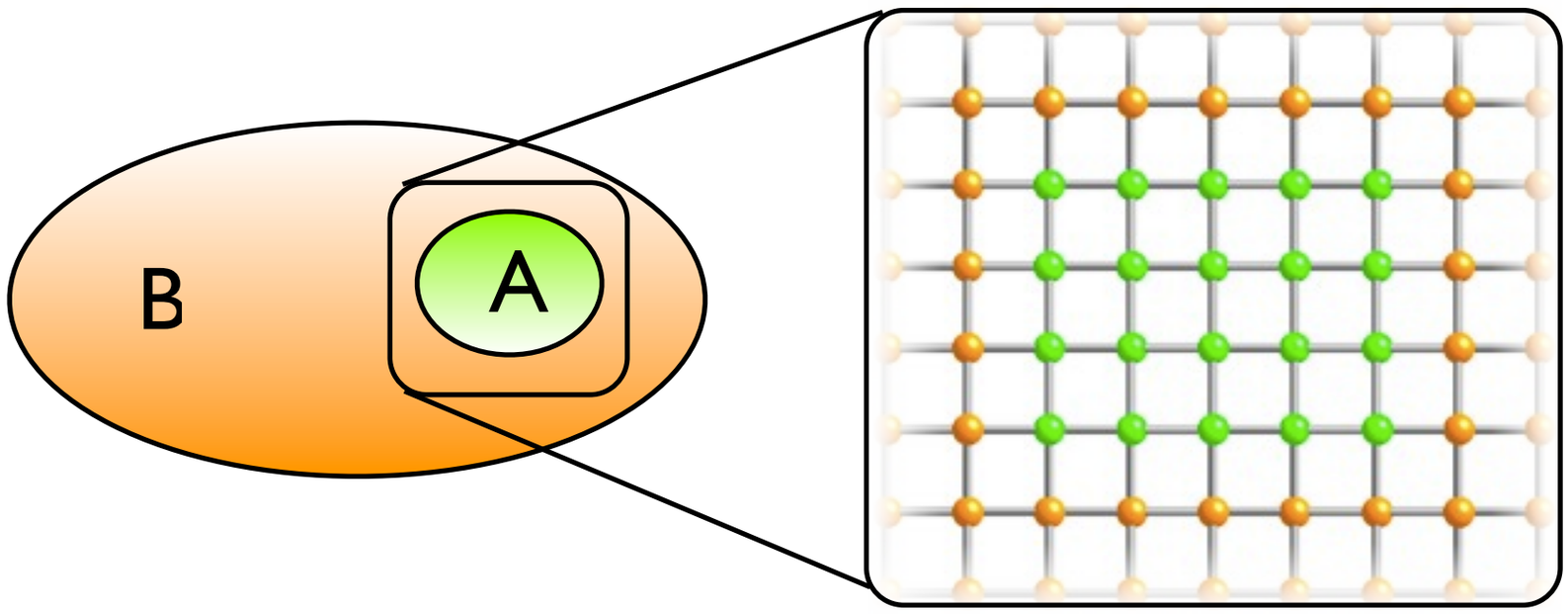
Density Matrix Renormalization Group (very basic idea)



- The DMRG doesn't work in D>1, because it doesn't capture typical entanglement properties...



$$S_A = aL + c\ln(L) + \cdots$$



Quantum Monte Carlo

Suzuki, 1993

Avoids the storage problem by **importance sampling**

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

- lattice or continuum
- free of systematic errors or bias
- often 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

A “zoo” of QMC methods, depending on which model 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

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

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

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

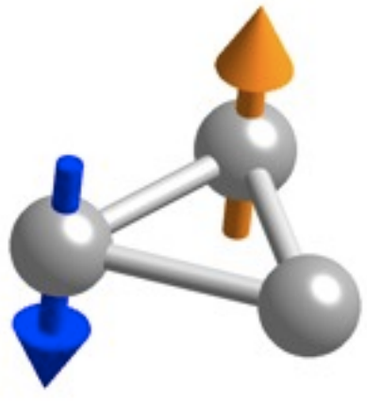
Auxiliary field Monte Carlo — Assaad, Evertz

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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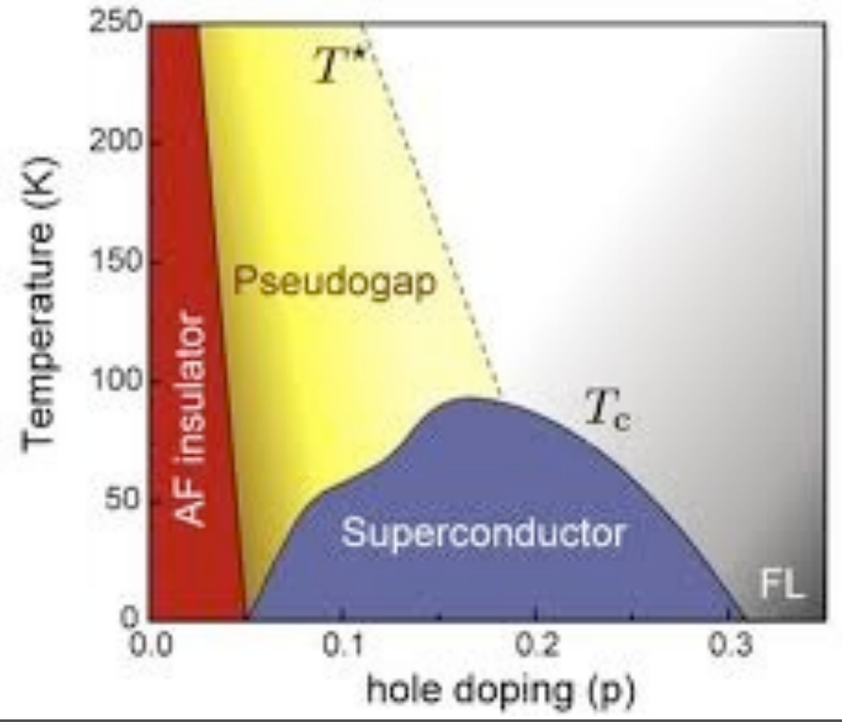
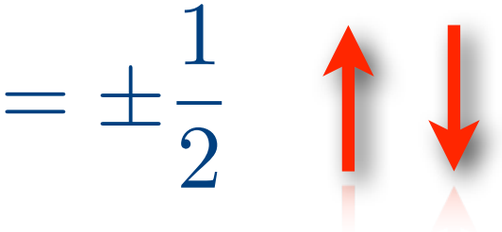


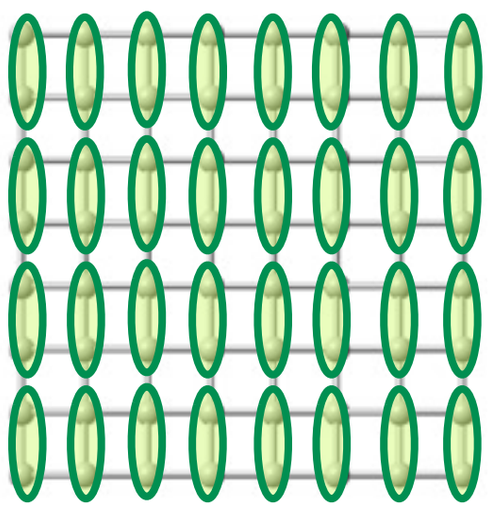
Quantum Monte Carlo consists of three ingredients

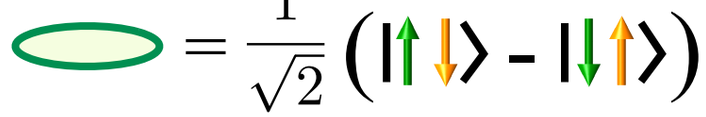
- A $D+1$ dimensional "representation" on the computer
- A procedure for updating configurations of the representation
- A way of devising measurements

The first thing you need is a choice of basis:

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







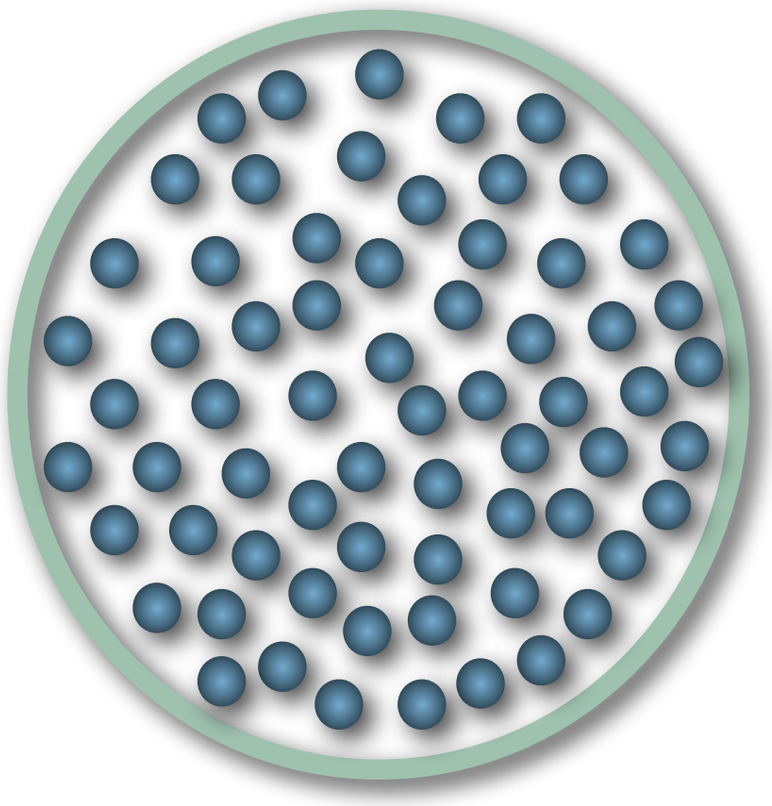
Example: Path Integral Monte Carlo

D. M. Ceperly, RMP **67**, 279 (1995)

Say you want to simulation N particles in the continuum:

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

$$\hat{H} = \hat{T} + \hat{V}$$



Naturally choose a position basis

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

$$\int \mathcal{D}R\, |R\rangle\langle R| = 1$$

Example: Path Integral Monte Carlo

The partition function is:

$$\begin{aligned}\mathcal{Z} &= \mathrm{Tr}\, \mathrm{e}^{-\beta \hat{H}} \\ &= \int dr_1 \cdots \int dr_N \, \langle r_1, \ldots r_N | \mathrm{e}^{-\beta \hat{H}} | r_1, \ldots, r_N \rangle \\ &= \int \mathcal{D}R \, \langle R | \mathrm{e}^{-\beta \hat{H}} | R \rangle\end{aligned}$$

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

But, the Hamiltonian commutes with itself

$$e^{-(\beta/2+\beta/2)\hat{H}} = e^{-\beta/2\hat{H}} e^{-\beta/2\hat{H}}$$

Example: Path Integral Monte Carlo

$$\mathcal{Z} = \int \mathcal{D}R \, \langle R | \mathrm{e}^{-\beta \hat{H}} | R \rangle$$

$$\mathcal{Z} = \int \mathcal{D}R \, \langle R | \mathrm{e}^{-\frac{\beta}{M}\hat{H}} \mathrm{e}^{-\frac{\beta}{M}\hat{H}} \mathrm{e}^{-\frac{\beta}{M}\hat{H}} \ldots \mathrm{e}^{-\frac{\beta}{M}\hat{H}} | R \rangle$$

insert *M-1* resolutions of the identity

$$\mathcal{Z} = \int \mathcal{D}R_0 \mathcal{D}R_1 \cdots \mathcal{D}R_{M-1} \langle R_0 | \mathrm{e}^{-\frac{\beta}{M}\hat{H}} | R_1 \rangle \langle R_1 | \mathrm{e}^{-\frac{\beta}{M}\hat{H}} | R_2 \rangle \langle R_2 | \mathrm{e}^{-\frac{\beta}{M}\hat{H}} | R_3 \rangle \cdots$$

$$\cdots \langle R_{M-1} | \mathrm{e}^{-\frac{\beta}{M}\hat{H}} | R_0 \rangle$$

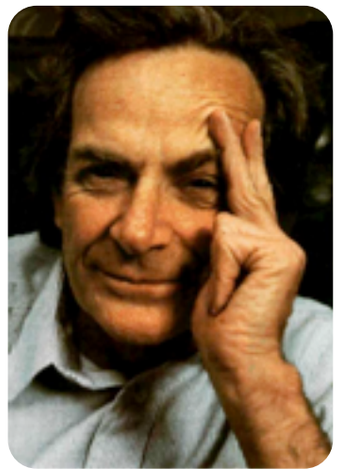
we usually define $\tau = \dfrac{\beta}{M}$

Example: Path Integral Monte Carlo

notice that

$$\langle R_{\ell-1}|\mathrm{e}^{-\tau\hat{H}}|R_\ell\rangle = \langle R_{\ell-1}|\hat{U}(-i\hbar\tau)|R_\ell\rangle$$

We can imagine that each Hamiltonian operator evolves the state of the system by a single imaginary time step, and after M such steps, we return to the initial state!



"Discrete Path Integral" picture of Feynmann

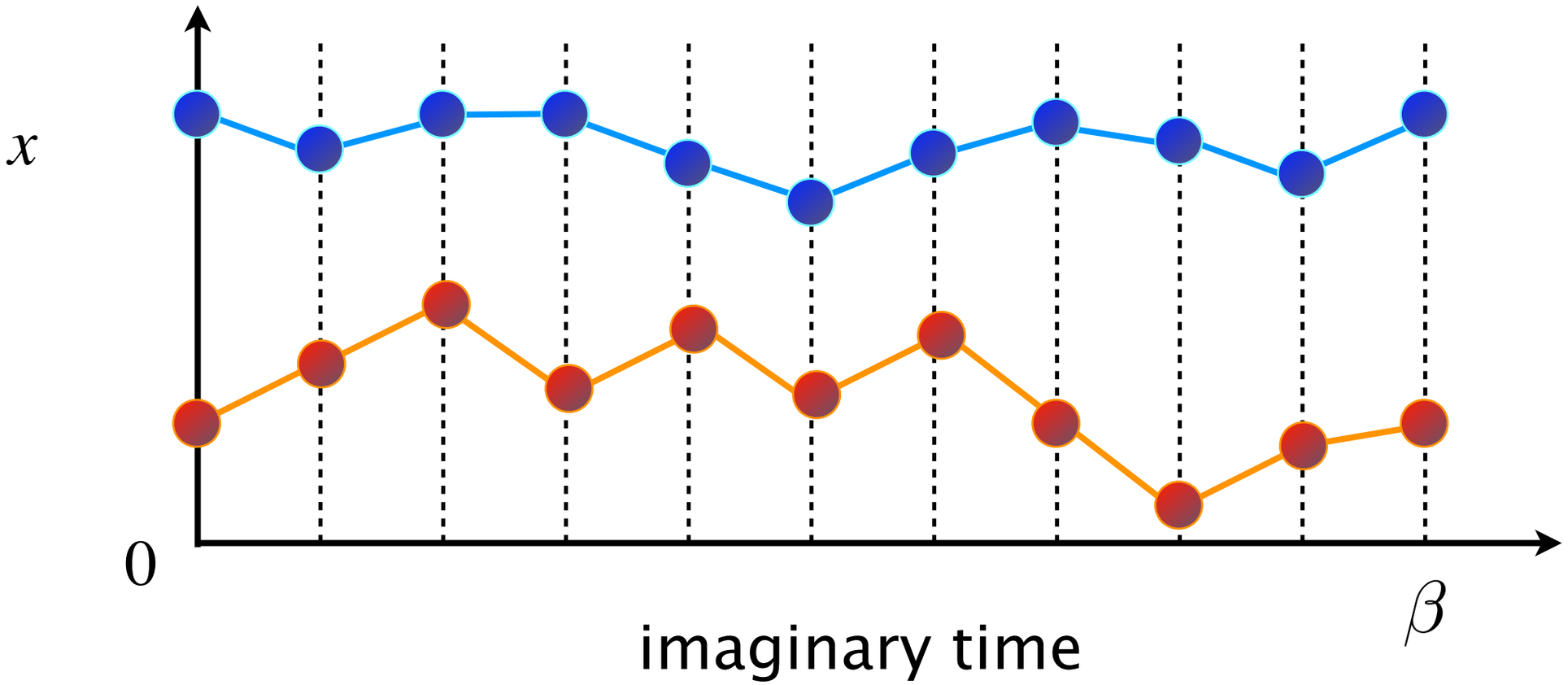
- A D-dimensional quantum model has a $D+1$ dimensional representation on the computer

Example: Path Integral Monte Carlo

Consider a 1D system, consisting of N = 2 particles with M = 10:

$$\mathcal{Z} = \int \mathcal{D}R_0 \cdots \int \mathcal{D}R_9 \, \langle R_0 | \mathrm{e}^{-\tau \hat{H}} | R_1 \rangle \cdots \langle R_9 | \mathrm{e}^{-\tau \hat{H}} | R_0 \rangle$$

$R_0 = \{x_{1,0}, x_{2,0}\}$ $\qquad$ $R_{10} = R_0 = \{x_{1,0}, x_{2,0}\}$



Example: Path Integral Monte Carlo

Examine one imaginary time "transition amplitude":

$$\langle R_{\ell-1}|\mathrm{e}^{-\tau(\hat{T}+\hat{V})}|R_{\ell}\rangle$$

One needs a way to solve this matrix element. Use the "primitive approximation"

$$\mathrm{e}^{-\tau(\hat{T}+\hat{V})} = \mathrm{e}^{-\tau\hat{T}}\mathrm{e}^{-\tau\hat{V}} + O(\tau^2)$$

This is the "Trotter error"

It gets smaller for increasing M: $\tau = \dfrac{\beta}{M}$

In practice, higher order terms included: $O(\tau^4)$

Example: Path Integral Monte Carlo

ie. We can approximate the high-temperature transition amplitudes to high order in τ (exact in the limit $M \to \infty$):

$$\langle R_{\ell-1}|\mathrm{e}^{-\tau(\hat{T}+\hat{V})}|R_\ell\rangle \approx \langle R_{\ell-1}|\mathrm{e}^{-\tau\hat{T}}|R'\rangle\langle R'|\mathrm{e}^{-\hat{V}}|R_\ell\rangle$$

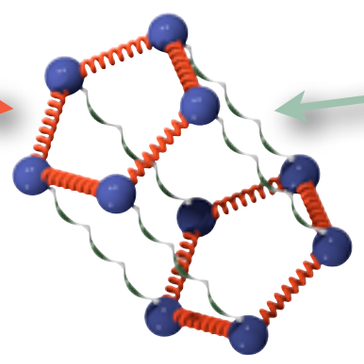
Gaussian integral

$\mathrm{e}^{-\tau\hat{V}(R_\ell)}\delta(R'-R_\ell)$

$$\mathcal{Z} \sim \frac{1}{N!}\sum_P \prod_{m=0}^{M-1} \int \mathcal{D}R_m \ \exp\left[-\frac{(R_m - R_{m+1})^2}{4\lambda\tau} - \tau\hat{V}(R_m)\right]$$

kinetic: connects time steps

potential: connects particles

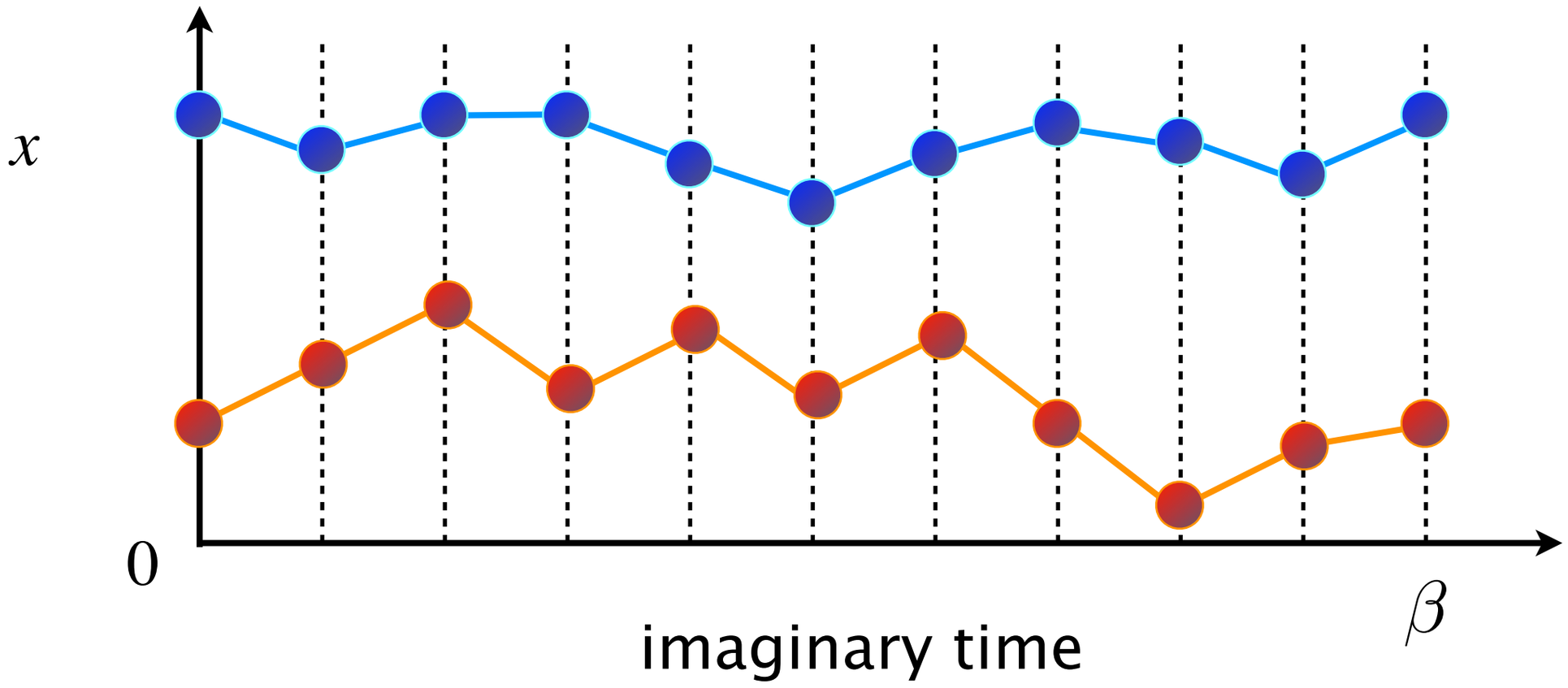


D. M. Ceperly, RMP **67**, 279 (1995)

Quantum Monte Carlo:

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

- A procedure for updating configurations of the representation



Quantum Monte Carlo:

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

- A procedure for updating configurations of the representation

Path Integral Monte Carlo: "Worm Updates"

The University of Vermont

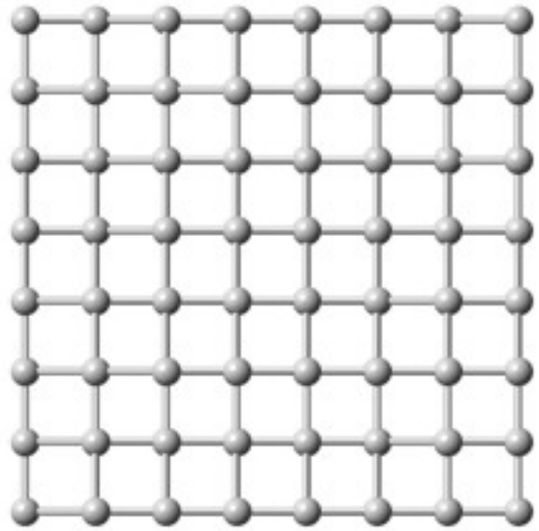
http://www.delmaestro.org/adrian

Stochastic Series Expansion QMC

Anders Sandvik

A simple to implement, powerful QMC method for lattice models

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



- Scales linearly in system size (and inverse temperature)
- Sign problem prevents simulation of fermions, frustrated spins
- 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;

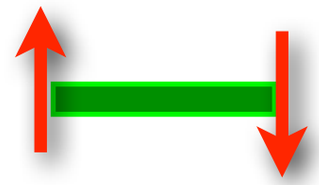
- proportional to the product of n matrix elements
- each $\langle \alpha_i | -H | \alpha_{i+1} \rangle$ is a real number
- must be positive to be interpreted as a probability for use in a Metropolis condition: otherwise get the "sign problem"

The Hamiltonian is broken into elementary lattice operators

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

"type"

lattice unit (e.g. bond)



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

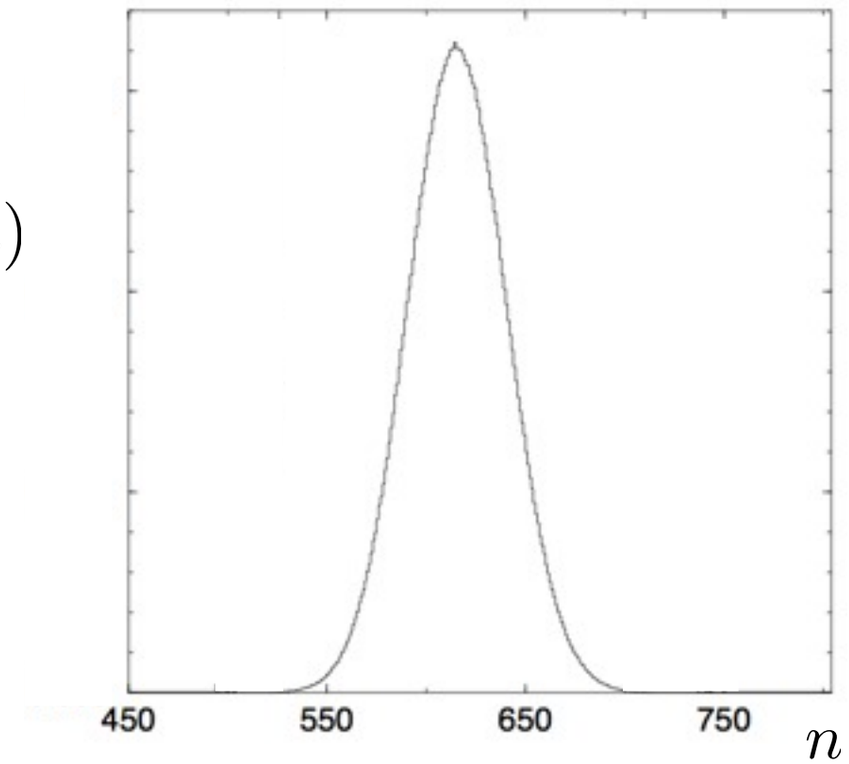
sequence of operator indices

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

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

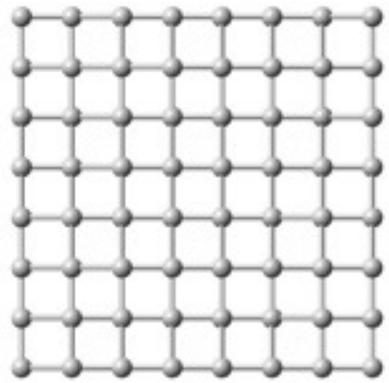
Thermal Expectation value $$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\ \ e^{-\beta \hat{H}} \mathcal{O}}{\mathrm{Tr}\ \ e^{-\beta \hat{H}}}$$

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

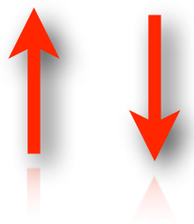
$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



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

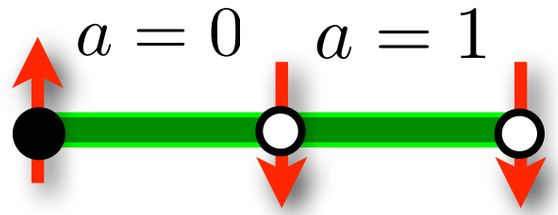
$$H = -\sum_t \sum_a H_{t,a}$$

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

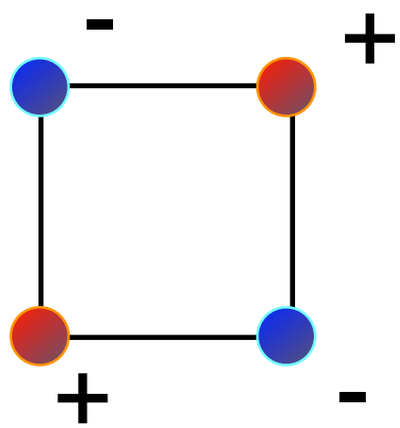
diagonal $\quad H_{1,a} = \frac{1}{4} - S_i^z S_j^z,$

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

“type” bond label



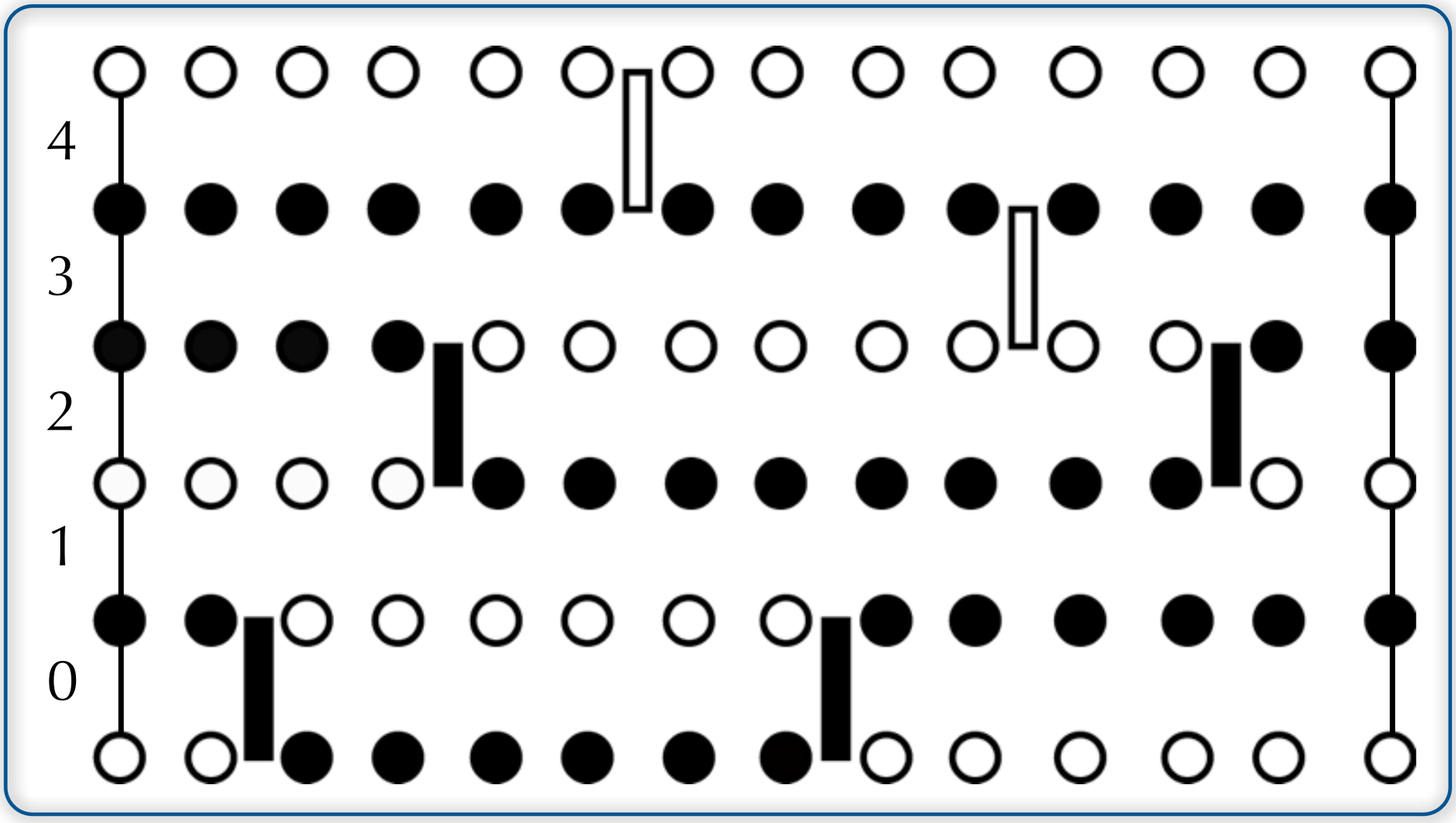
- A constant term 1/4 is added to the diagonal operator
- Spin operators are rotated by $\pi/2$ around the z-axis on one of the sublattices



All bond operators are positive

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

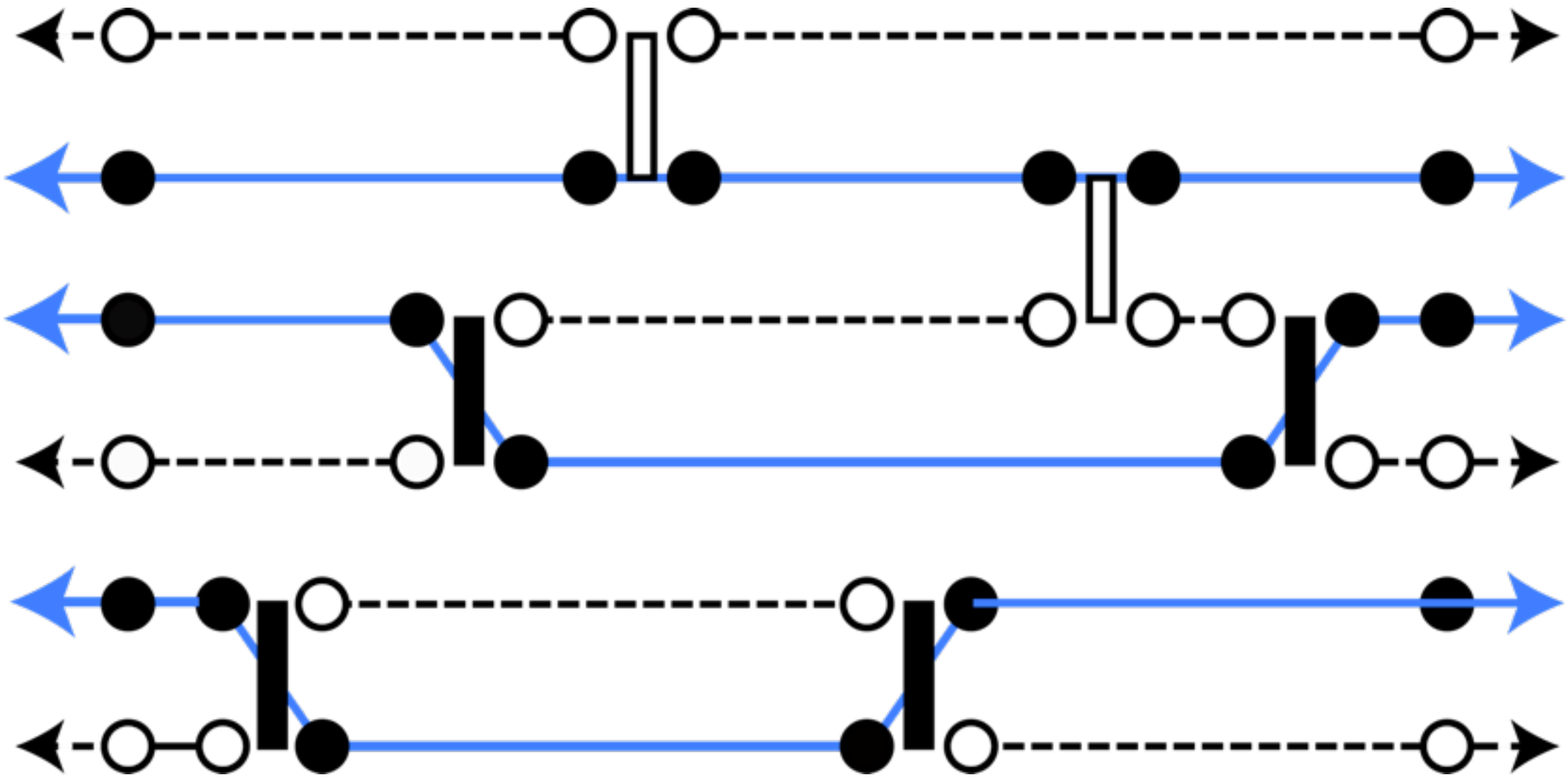
$n = 6 \quad M = 13$



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

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

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) $H_{1,a} \rightarrow H_{0,0}$

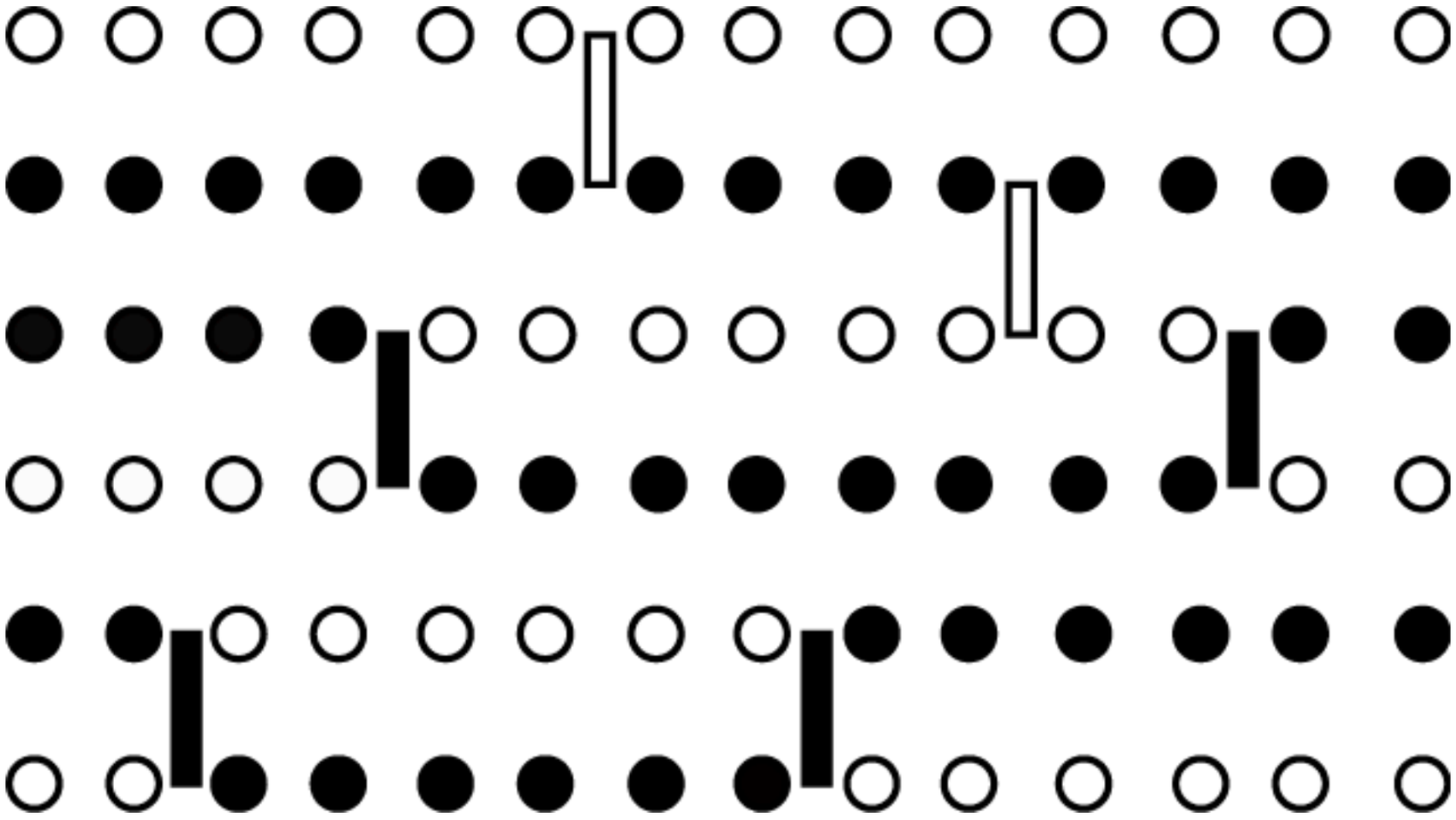
Like in classical Monte Carlo, we calculate the ratio of weights:

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

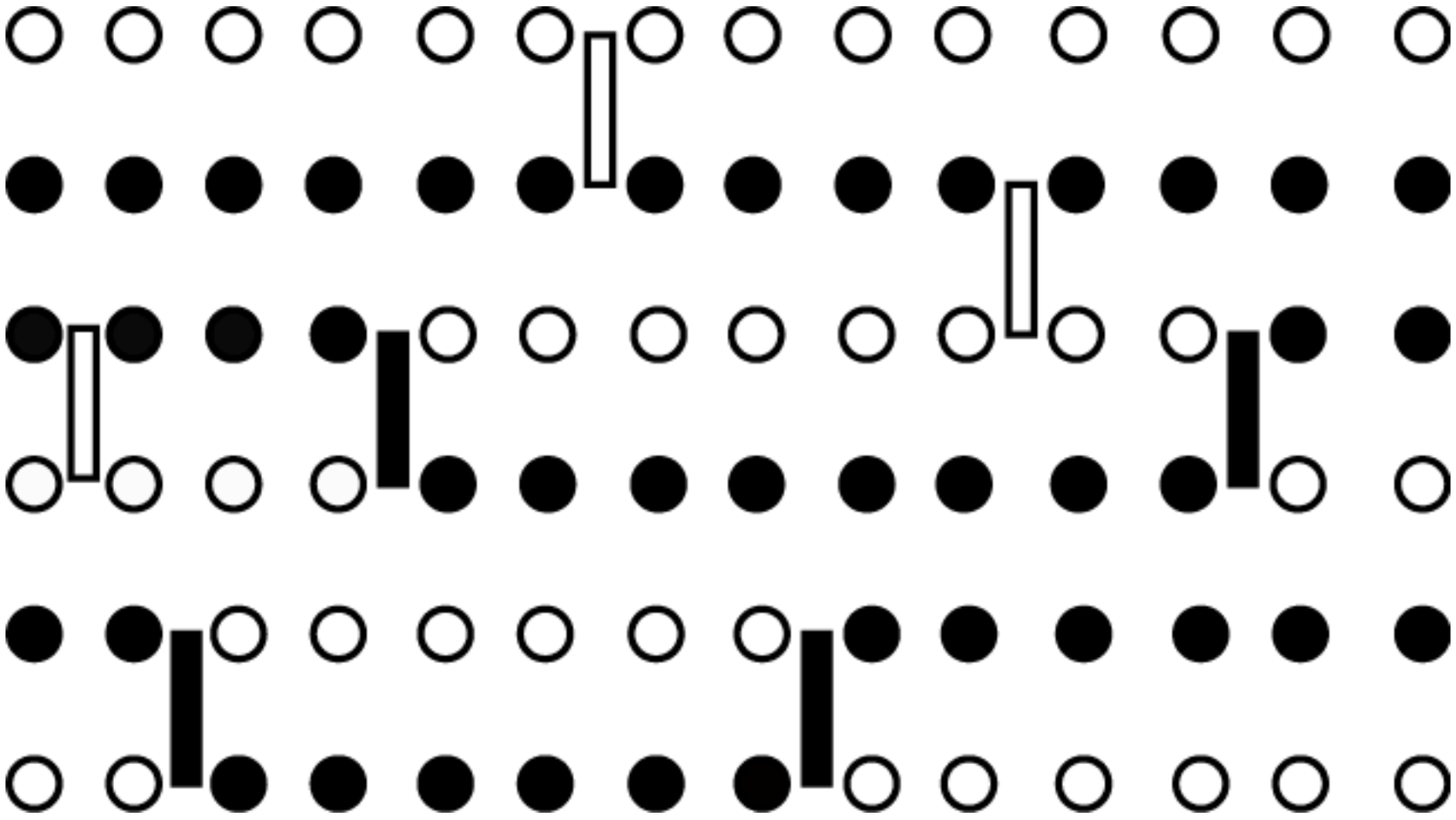
The transition probability is then obtained from detailed balance:

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

SSE “Diagonal” Updates



SSE “Diagonal” Updates



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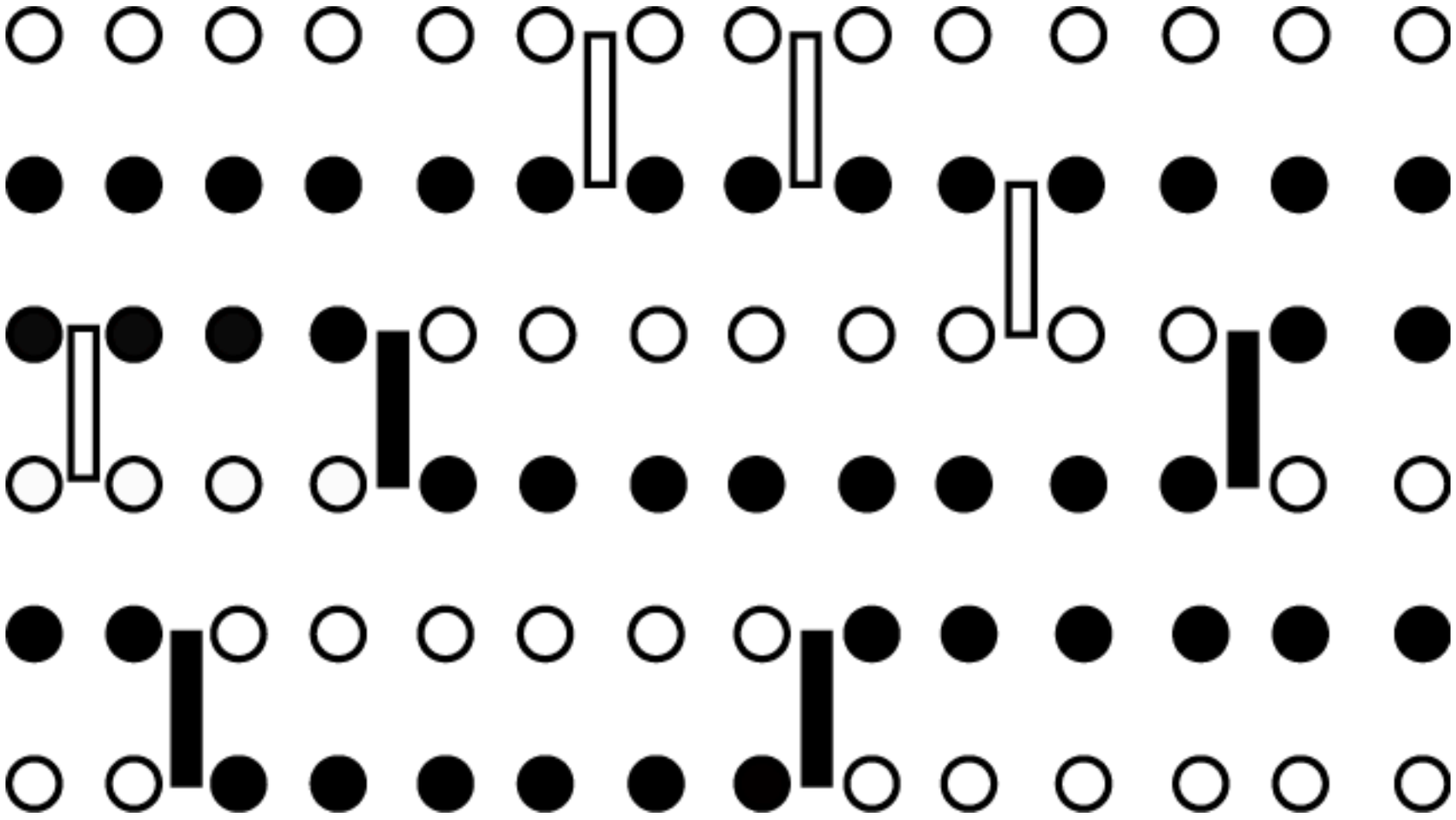

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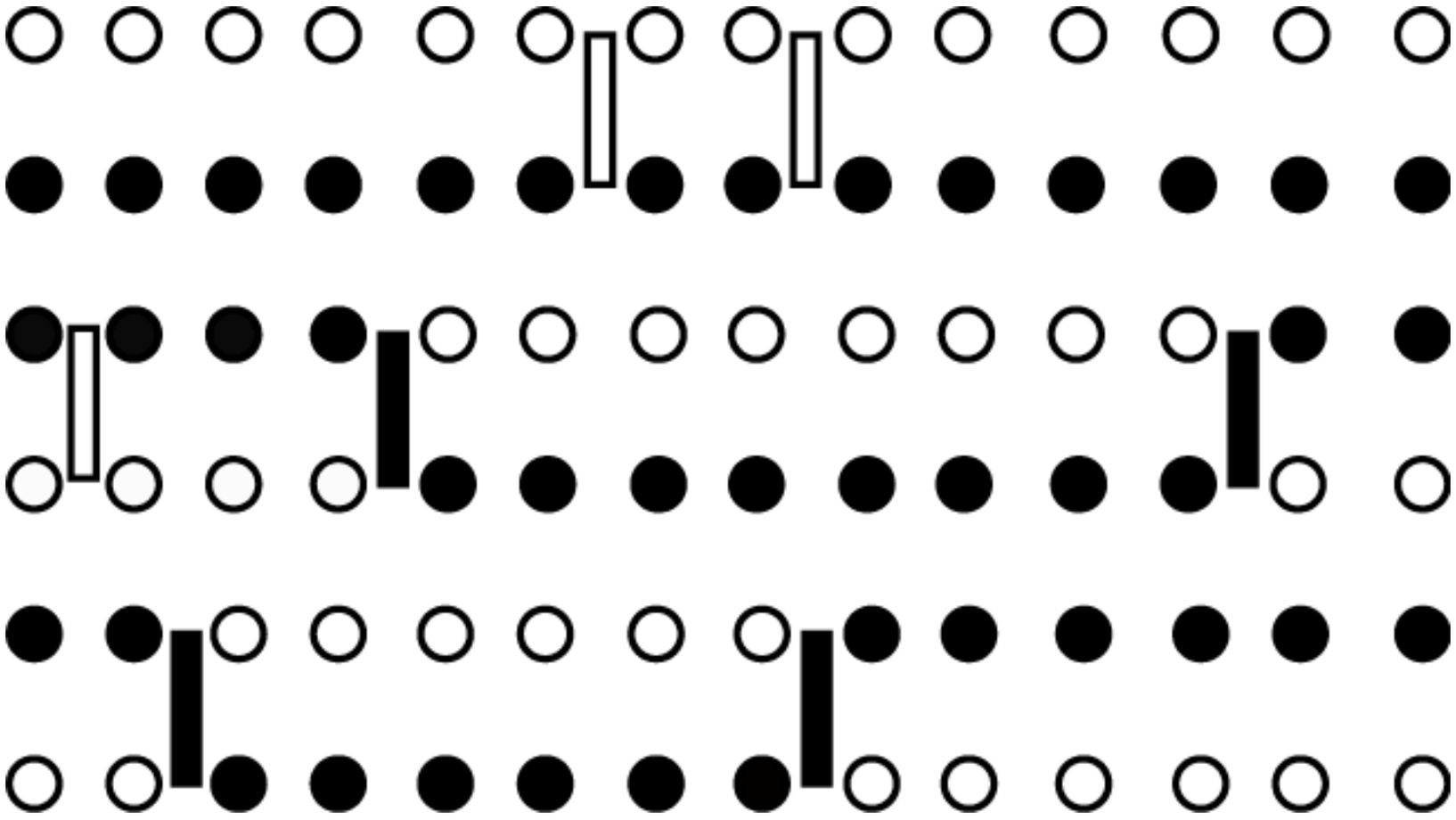


SSE "Diagonal" Updates

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

Transition probabilities for a Metropolis algorithm

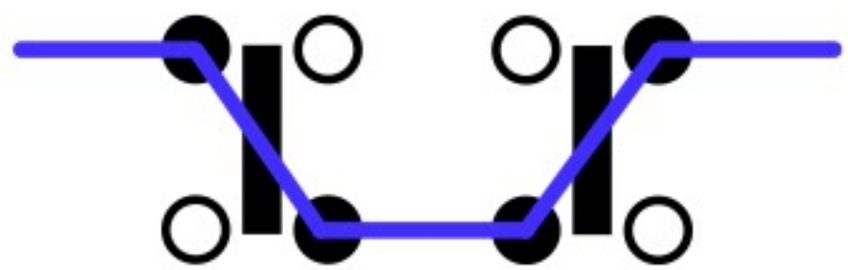
$$P(n \to n+1) = \min\left(\frac{1}{2}\frac{N_b \beta}{(M-n)}, 1\right)$$

- 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

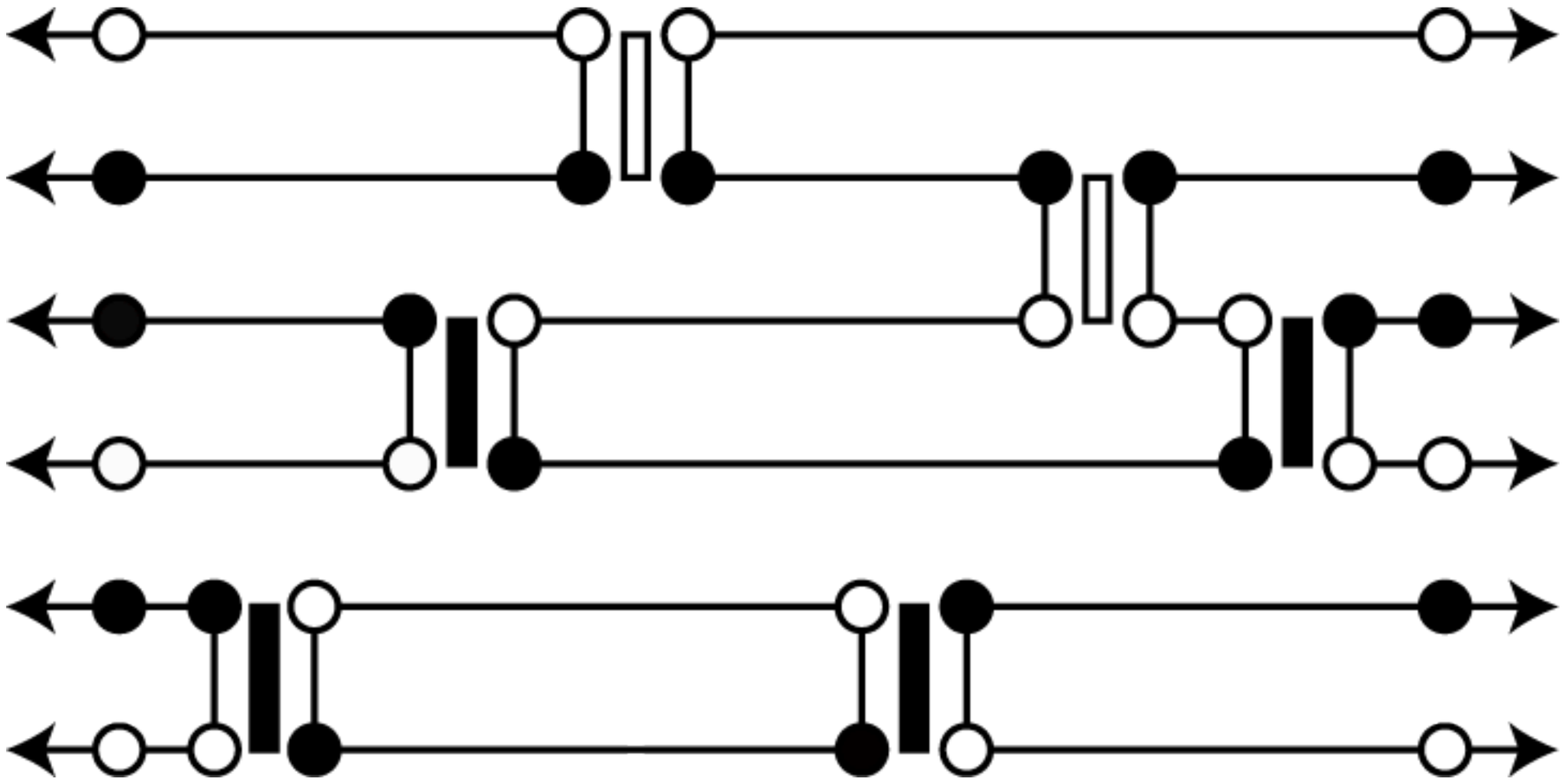
- Sample the power of the expansion effectively
- Easy to implement, local updates
- Do **not** result in an ergodic simulation: off-diagonal operators are not sampled



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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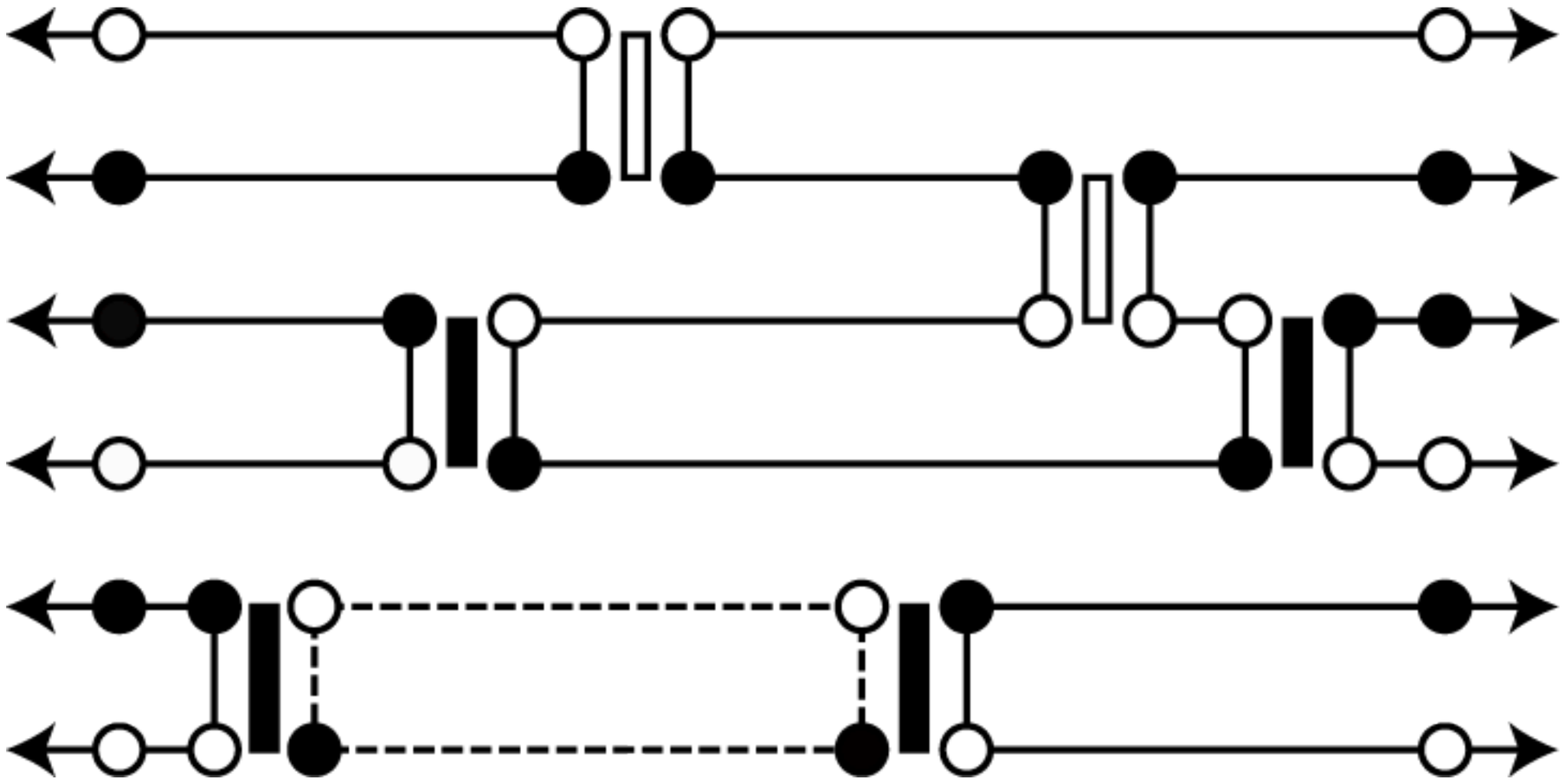

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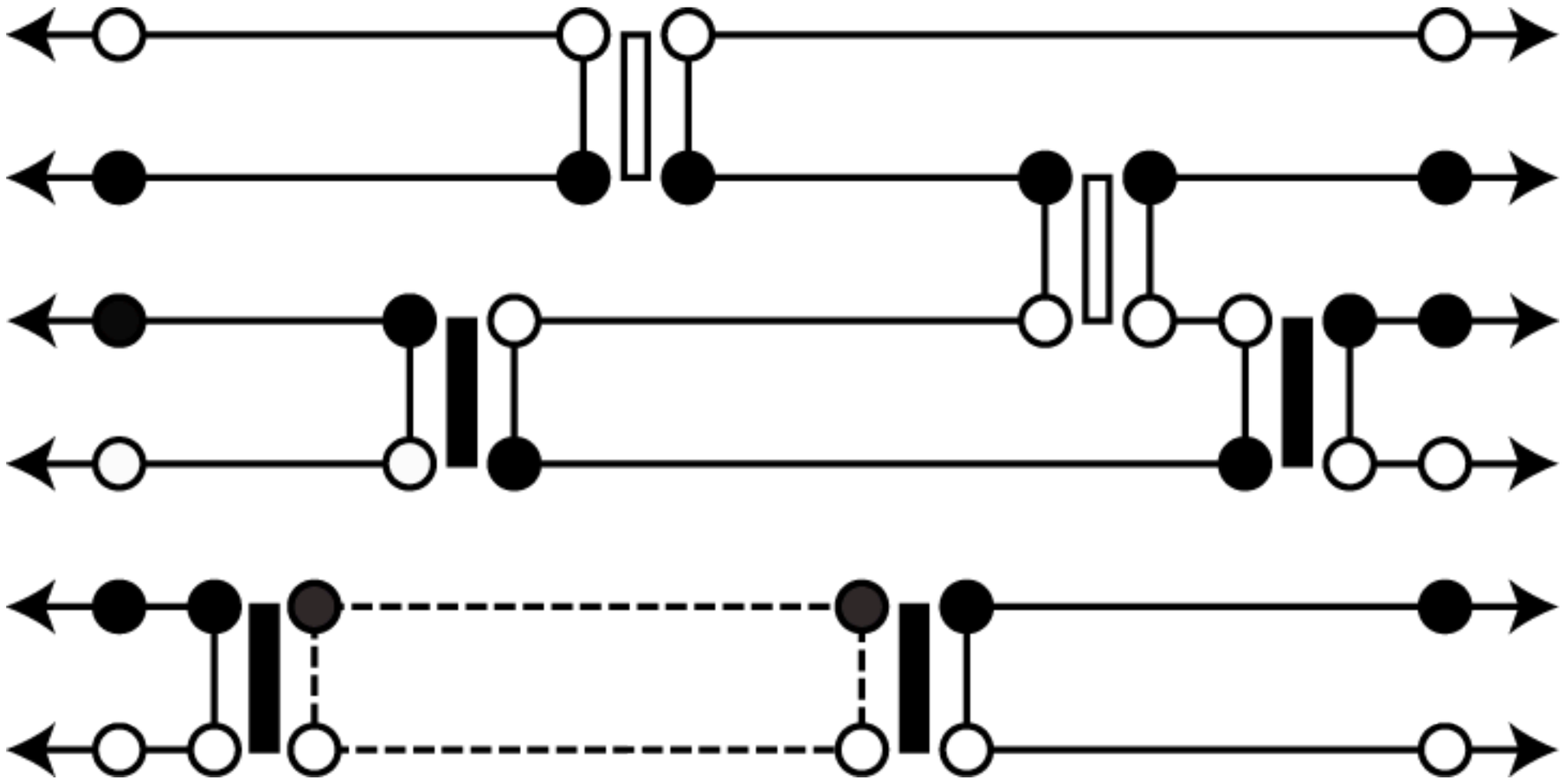

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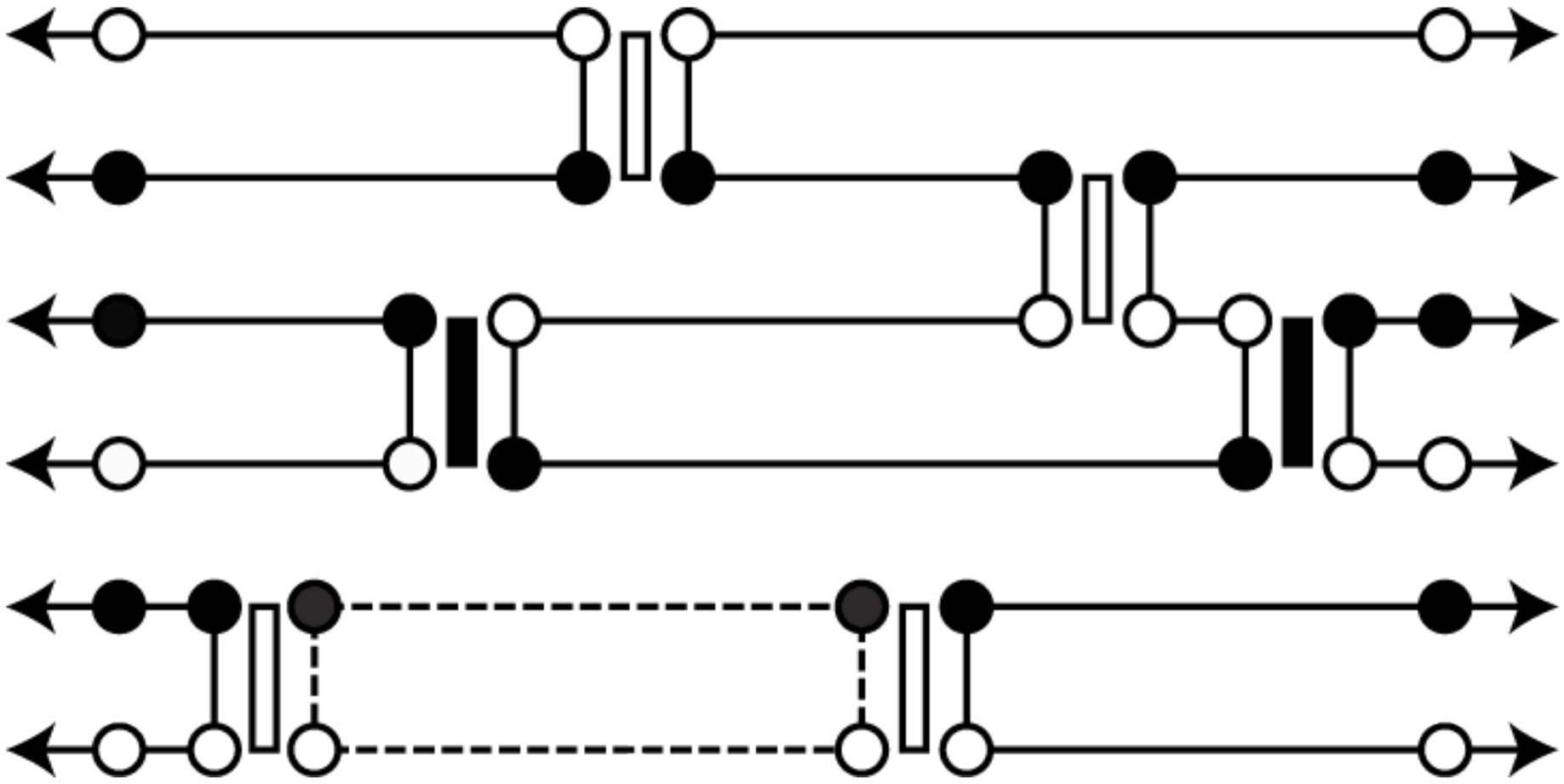

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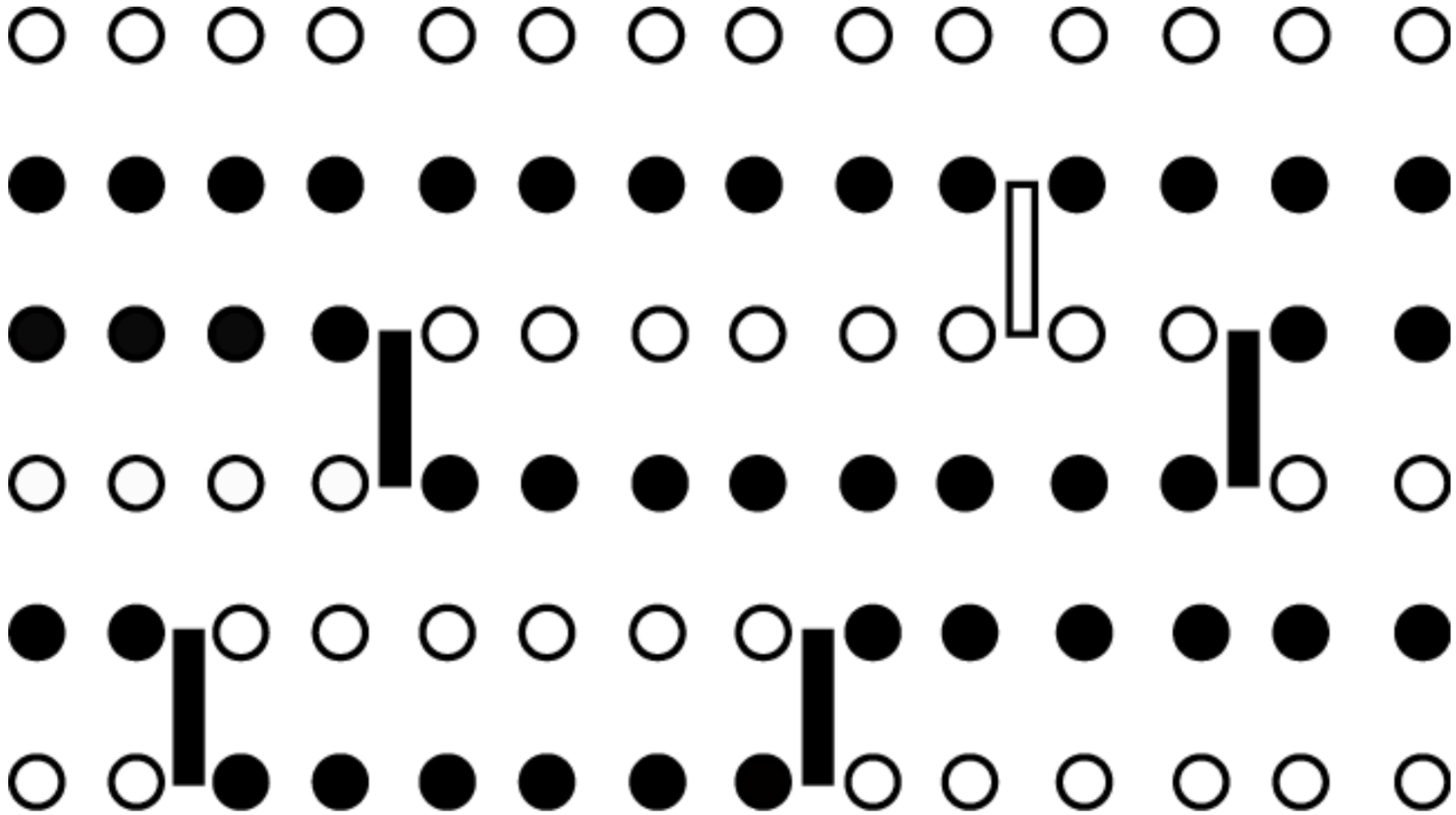
Other SSE updates:

- Spin-flips: required at high temperature



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

Other SSE updates:

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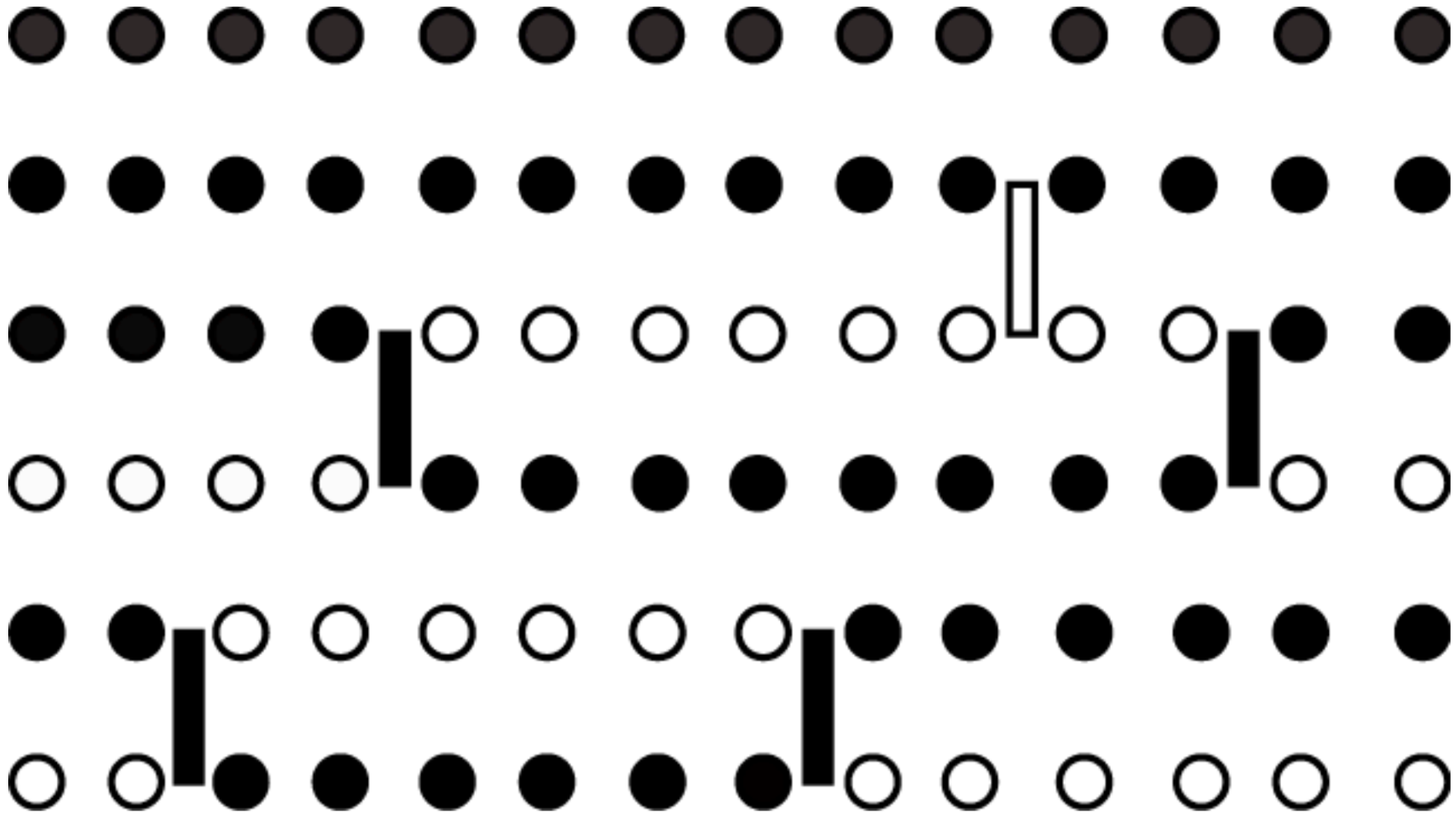
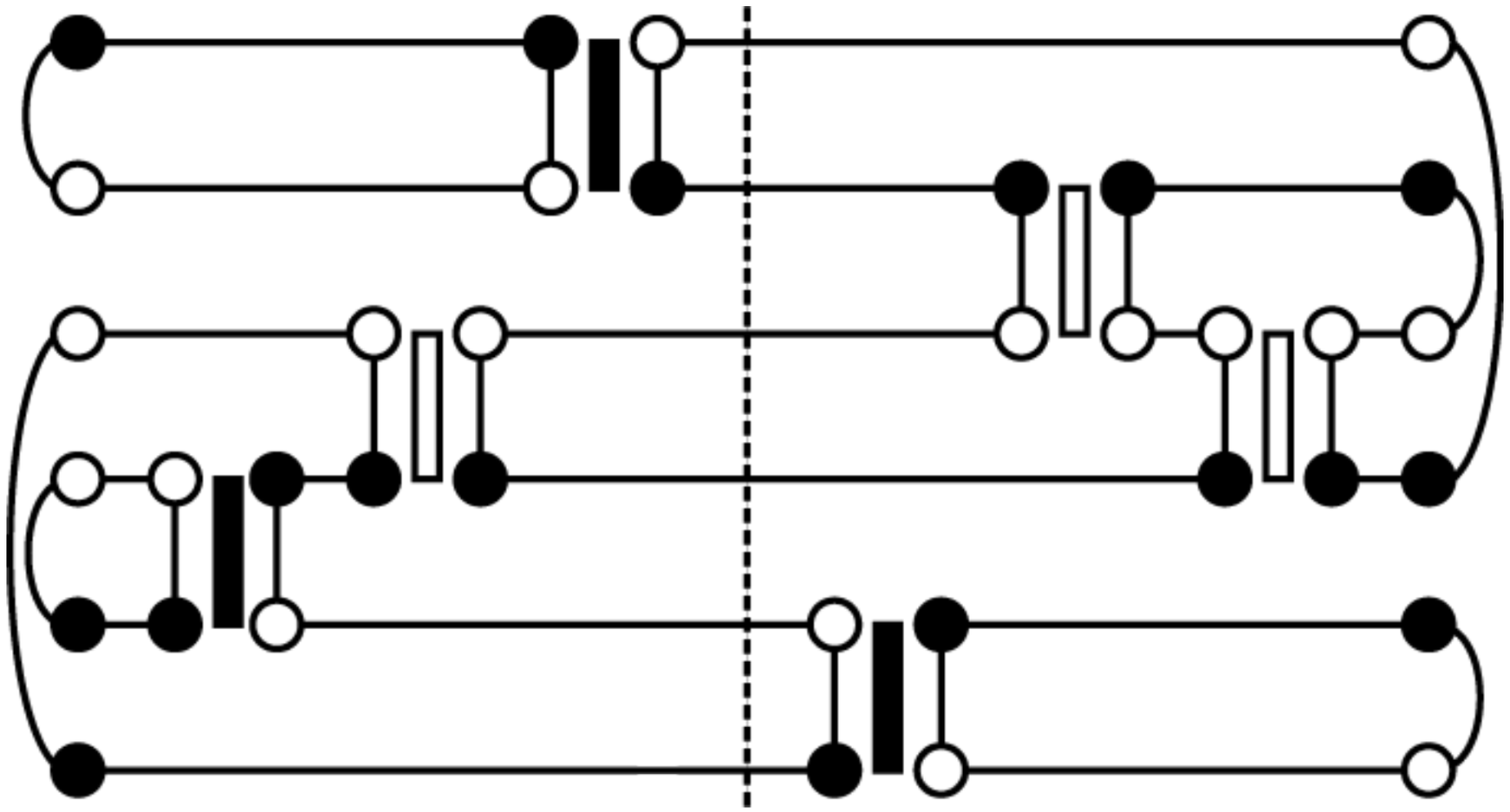


- Other more sophisticated operator loops possible
- Can be used in conjunction with Parallel Tempering, etc.

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:

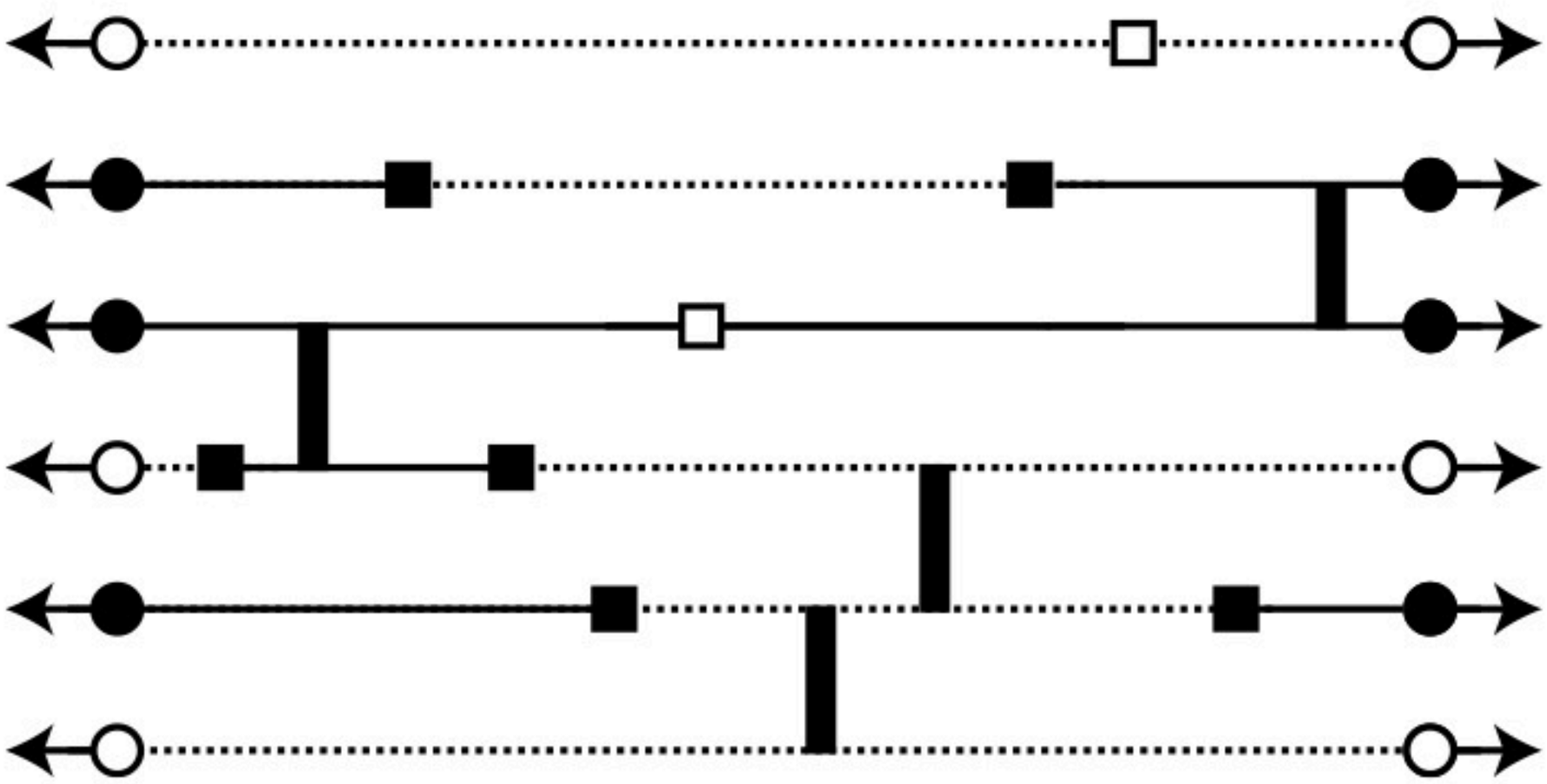
$$\begin{aligned} \langle \bullet | H_{-1,a} | \circ \rangle = \langle \circ | H_{-1,a} | \bullet \rangle = h, \\ \langle \bullet | H_{0,a} | \bullet \rangle = \langle \circ | H_{0,a} | \circ \rangle = h. \end{aligned}$$

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

another example: Transverse Field Ising Model

Finite-T representation

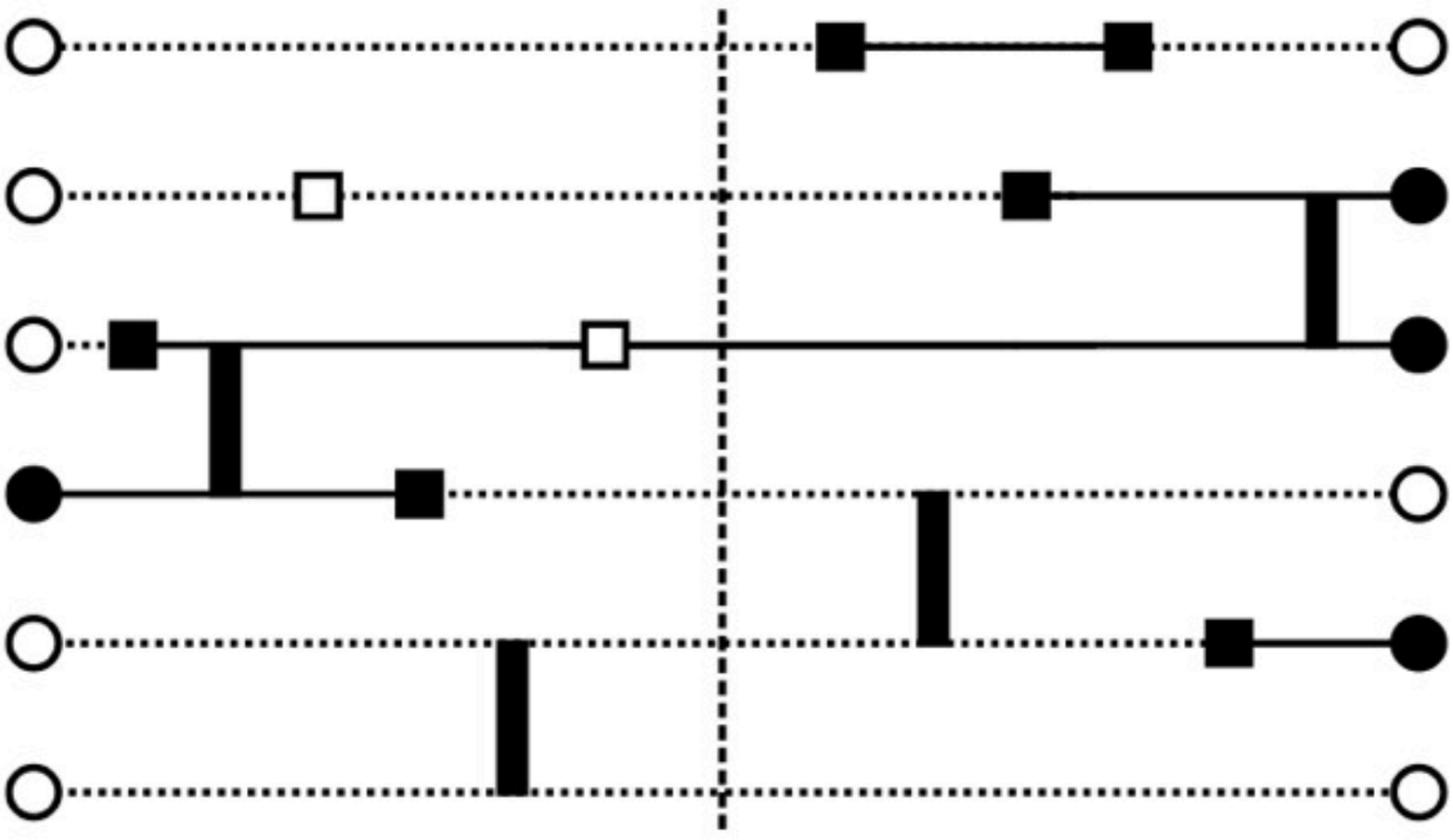
$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$



another example: Transverse Field Ising Model

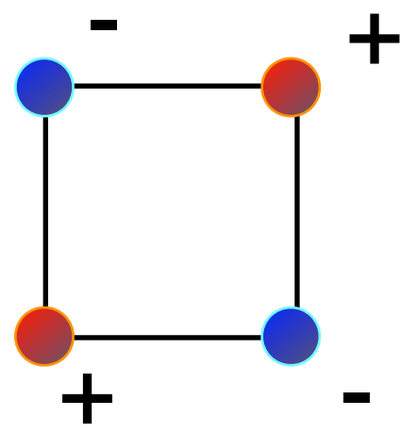
zero-T representation

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



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 ...



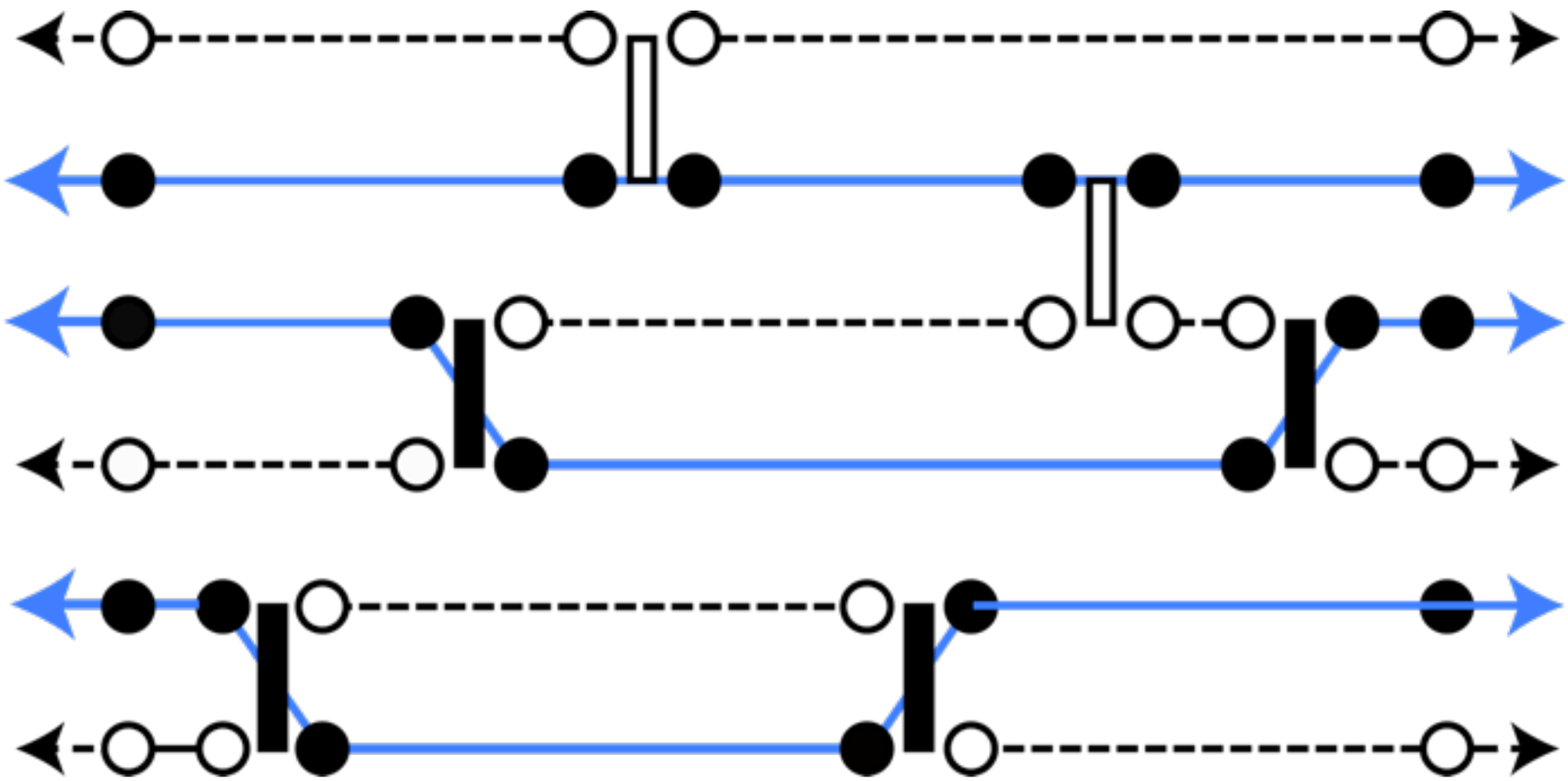
$$Z = \sum_{\{\alpha_i\}} \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \langle \alpha_0 | - H | \alpha_1 \rangle \langle \alpha_1 | - H | \alpha_2 \rangle \cdots \langle \alpha_{n-1} | - H | \alpha_n \rangle$$

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

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

The Sign Problem in SSE

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



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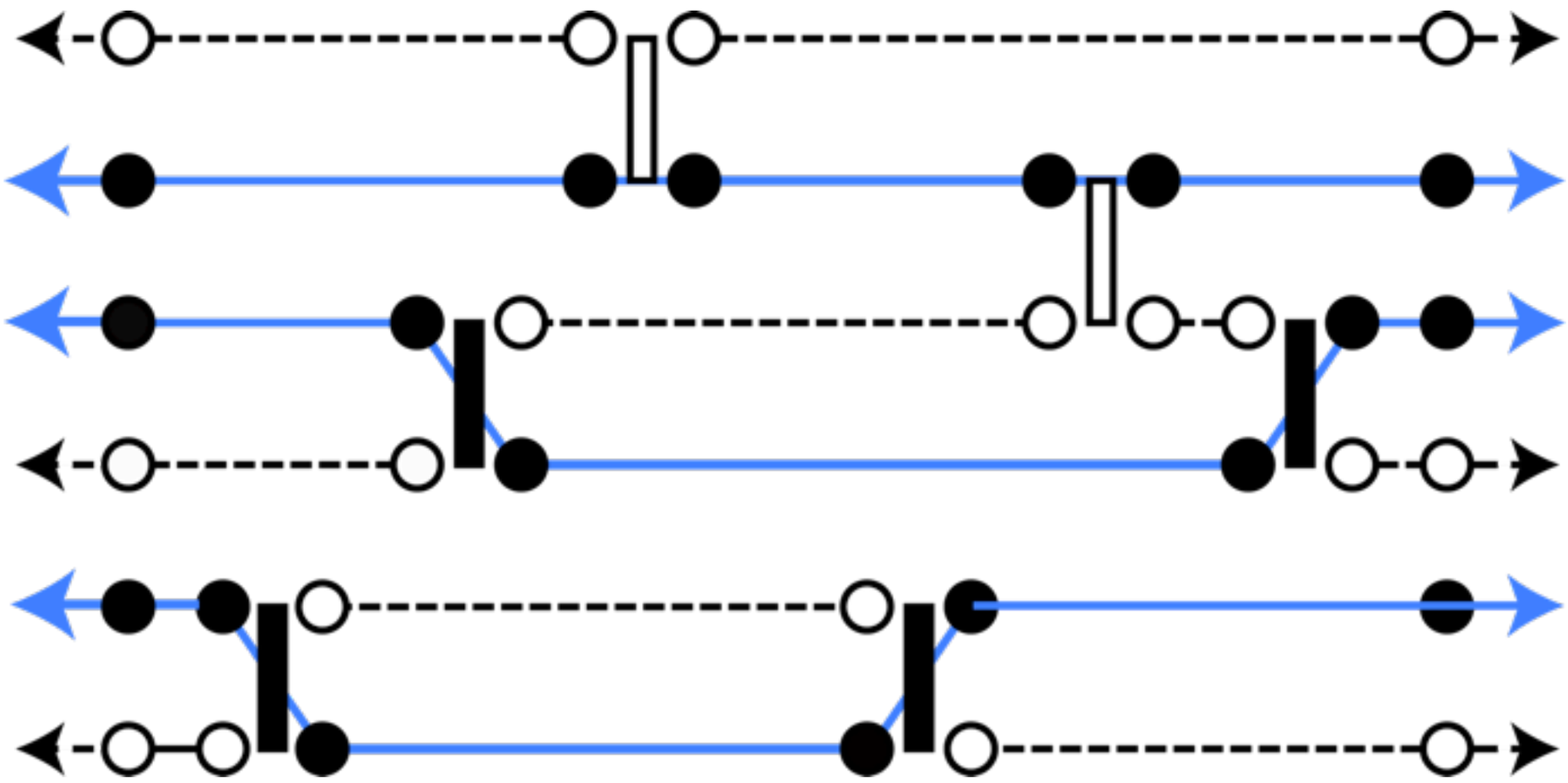

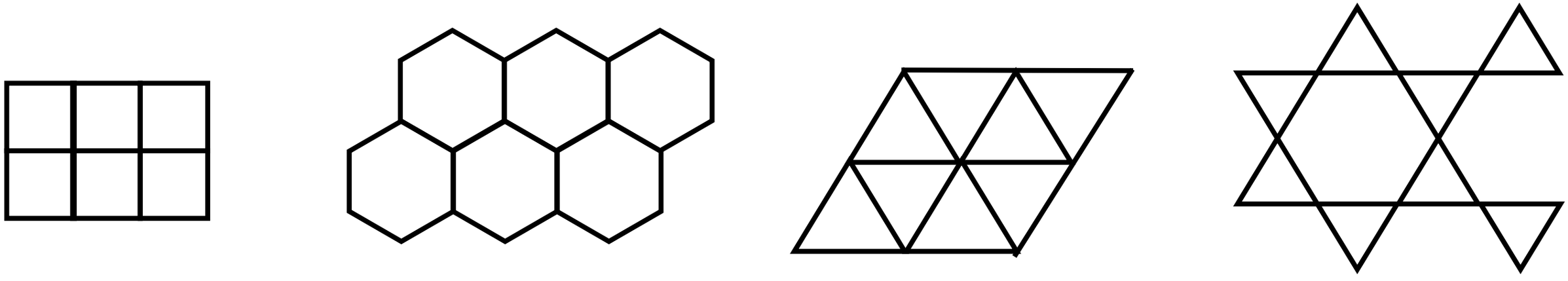

Measurements in the SSE:

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

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

- Associated with the Hamiltonian

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

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

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

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...