Monte Carlo simulations of the Ising model

The Monte Carlo idea

- Task: Compute

$$\langle \mathcal{O} \rangle = \sum_s \mathcal{O}_s W_s \qquad W_s = \frac{e^{-\beta H}}{Z}$$

Number of terms is an exponential function of system size.

- Instead, do as in an experiment:

Generated with prob. dist. W

$$\overline{\mathcal{O}} = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}_{s_i}$$

- Monte Carlo idea:
Generate configurations distributed as W, and replace the ensemble average by the "experimental" average:

$$\langle \mathcal{O} \rangle = \overline{\mathcal{O}}$$

P(s->s') is the prob. that the MC machine goes from s to s'

- Detailed balance:

$$P(s \to s')W(s) = W(s')P(s' \to s)$$

- Consider a long string of measurements:

$$s_1 \to s_2 \ldots s_i \to s_{i+1} \ldots s_j \to s_{j+1} \cdots$$

- Pick out measurement samples obtained at several distant places in the chain. For simplicity lets assume there are only two possible ~~measurement results~~ configurations (s and s'). Consider the next step in the chain: Number of samples going from state s to s' is

$$N_{s \to s'} = N_s P(s \to s') = N_s P(s' \to s)\frac{W(s')}{W(s)}$$

while the number of samples going from s' to s is:

$$N_{s' \to s} = N_{s'} P(s' \to s)$$

The net flux from s to s' is

$$\frac{N_{s\to s'} - N_{s'\to s}}{N_s} = P(s' \to s)\left(\frac{W(s')}{W(s)} - \frac{N_{s'}}{N_s}\right)$$

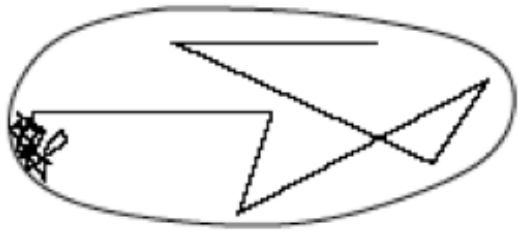
In equilibrium:

$$\frac{N_{s'}}{N_s} = \frac{W(s')}{W(s)}$$

So the detailed balance condition ensures that the relative frequency of occurence of the different spin configurations follows the distribution W.

Ergodicity

- Detailed balance is not enough to ensure $\overline{\mathcal{O}} = \langle \mathcal{O} \rangle$
- Need also: finite probability that any allowed configuration is measured.
- In "real life": $N = \text{finite}$.
  Motion in phase space should be sufficiently fast



- Avoid slowing down in a corner of phase space.

Monte Carlo simulations

- Start with a random spin configuration
- Equilibriation: Do N_{eq} MC updates until the observables (magnetization, energy etc.) cease to depend systematically on N_{eq} . N_{eq} is typically 1000-100000 sweeps of the whole lattice.
- Measurement: Do N_{meas} MC updates where the observables are recorded and accumulated after each update. After N_{meas}, divide the accumulated results by N_{meas} and record the result. N_{meas} is typically 1000-10000. Then repeat this N_{bin} times. This will produce N_{bin} statistically independent results from which one can calculate the total average and estimate the statistical uncertainty based on their variations. N_{bin} is typically 10-100.

Detailed balance

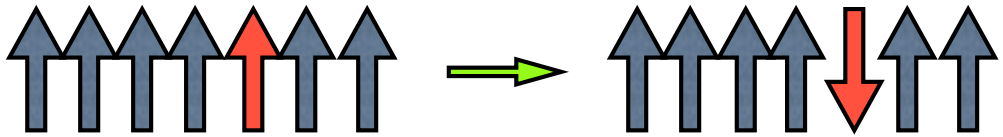
$$W(s)P(s \to s') = P(s' \to s)W(s')$$

- $P(s \to s')$? Algorithm!
- Common factors in W cancels out.

Metropolis algorithm

$$W(s)P(s \to s') = P(s' \to s)W(s')$$

- Metropolis algorithm: $P(s \to s') = \min(\frac{W(s')}{W(s)}, 1)$



Detailed balance and Metropolis

Detailed balance: $W(s)P(s \to s') = P(s' \to s)W(s')$

Metropolis: $\begin{cases} P(s \to s') = \min(\frac{W(s')}{W(s)}, 1) \\ P(s' \to s) = \min\left(\frac{W(s)}{W(s')}, 1\right) \end{cases}$

$$W(s) \cdot \min\left(\frac{W(s')}{W(s)}, 1\right) = W(s') \cdot \min\left(\frac{W(s)}{W(s')}, 1\right)$$

$W(s') < W(s) : \text{l.h.s.} = W(s'), \text{r.h.s.} = W(s')$ ✓

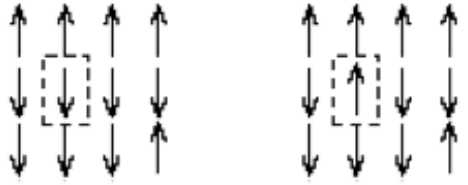
$W(s') > W(s) : \text{l.h.s.} = W(s), \text{r.h.s.} = W(s)$ ✓

Ising model, Metropolis algorithm

- Ising model:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

- Metropolis algorithm (Metropolis *et al.* J.Chem. Phys. 21, 1087 (53)):



  - Given a configuration, flip an arbitrary spin.
  - If new config. is lower in energy, accept it.
    if higher accept it with a probability $e^{-\beta(E'-E)}$
  - repeat

- Detailed balance:

$$P(s \to s') = \min\left(1, W(s')/W(s)\right)$$

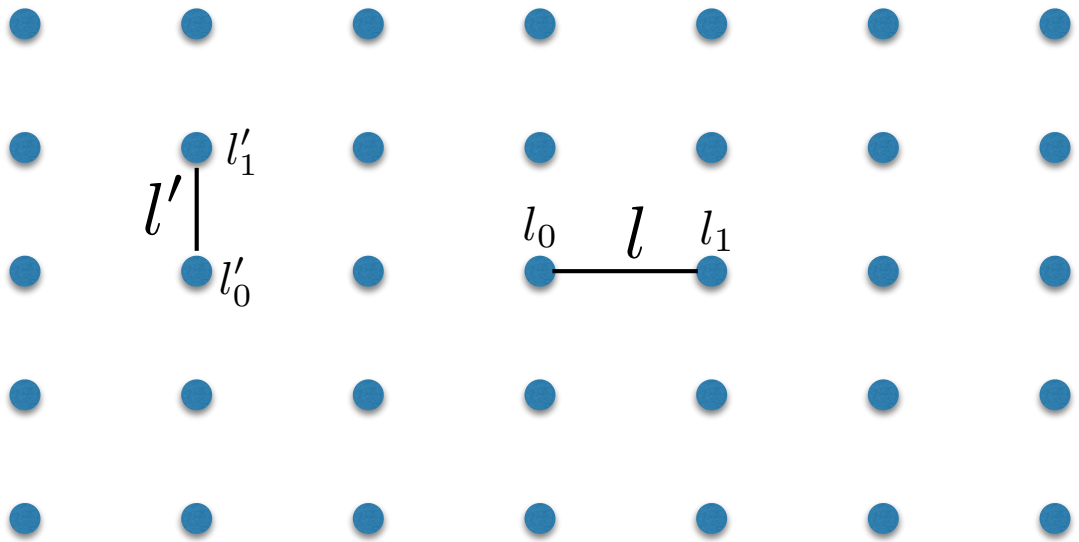
Swendsen-Wang algorithm

R.H.Swendsen, J.-S. Wang, PRL **58**,86 (1987)

$$Z = \sum_{\{\sigma\}} \prod_{l} e^{\beta J \sigma_{l_0} \sigma_{l_1}}$$

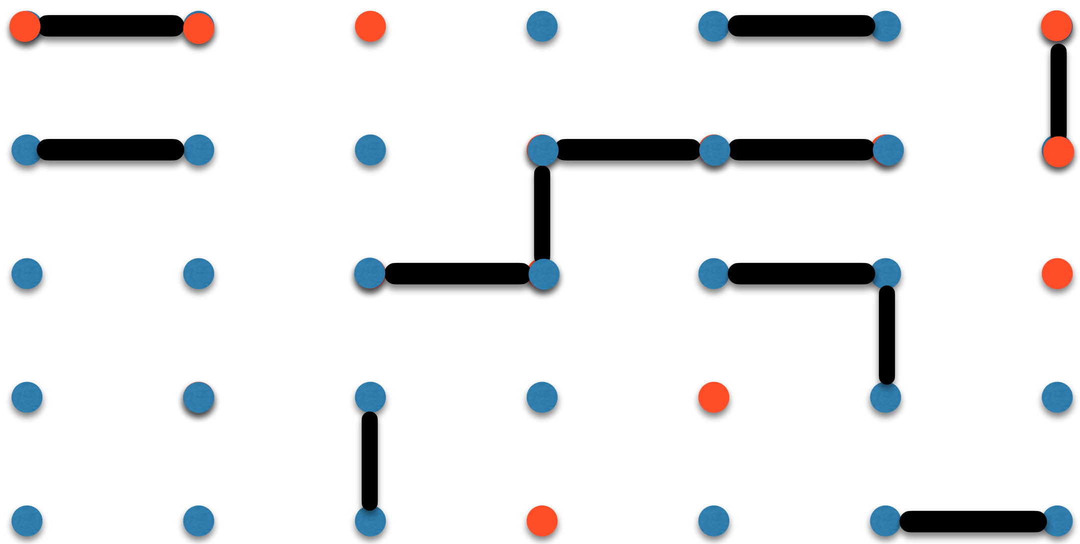
No magnetic field!

Links between nearest neighbors



Swendsen-Wang algorithm

R.H.Swendsen, J.-S. Wang, PRL **58**,86 (1987)



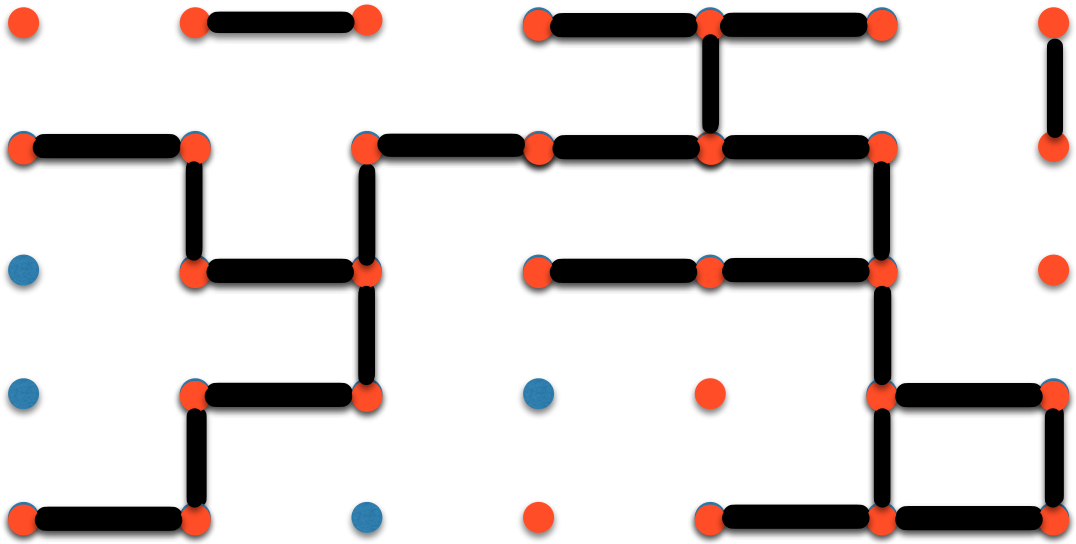
$\sigma = -1$

$\sigma = +1$

1. Assign "bonds" with probability between aligned spins
2. Flip clusters with probability 1/2
3. Remove bonds, and start over

Swendsen-Wang algorithm

R.H.Swendsen, J.-S. Wang, PRL **58**,86 (1987)



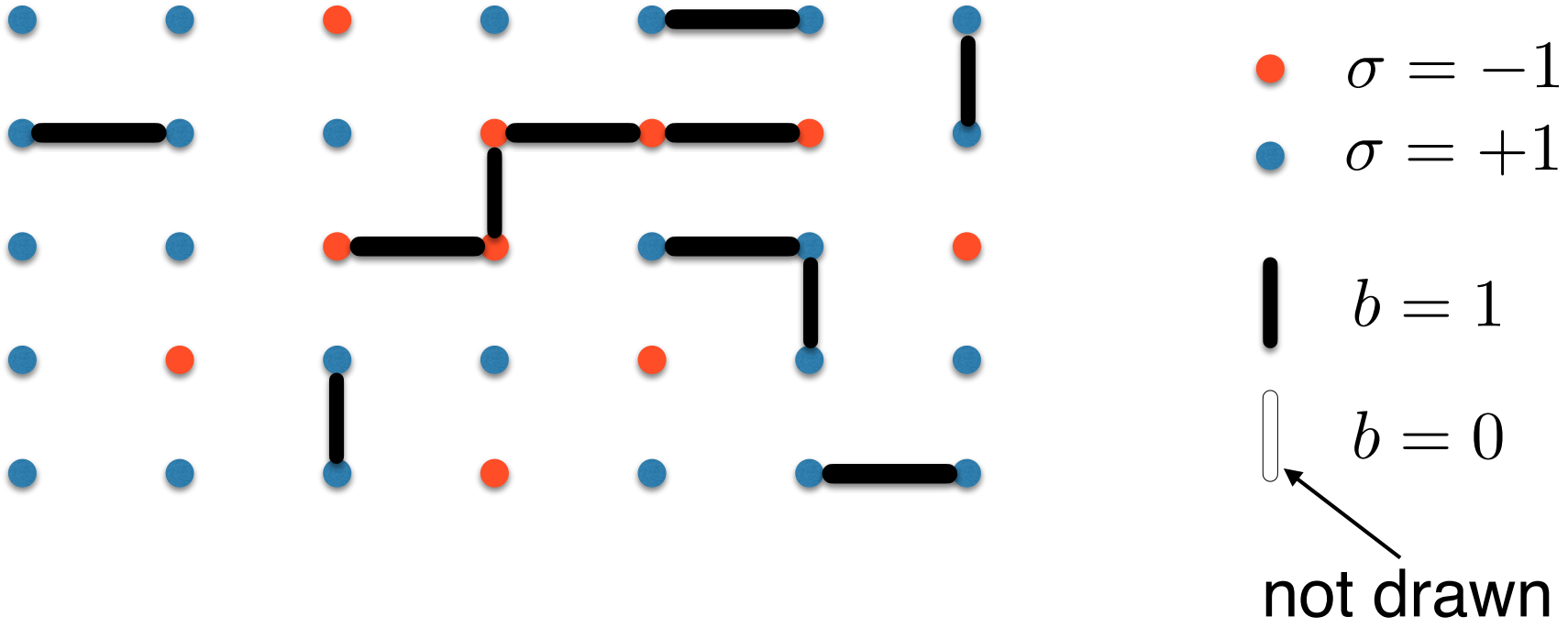
$\sigma = -1$

$\sigma = +1$

Swendsen-Wang

$$Z = \sum_{\{\sigma\}} \prod_{l} e^{\beta J \sigma_{l_0} \sigma_{l_1}}$$

Introduce: Bond variables b that lives on links and takes values b=1 or b=0



Swendsen-Wang

$$Z = \sum_{\{\sigma\}} \prod_{l} e^{\beta J \sigma_{l_0} \sigma_{l_1}}$$

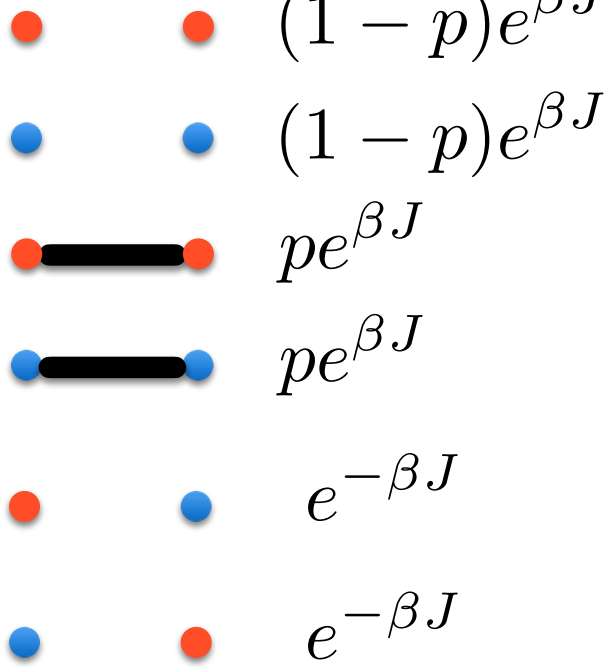
$$= \sum_{\{\sigma\}} \sum_{\{b\}} \prod_{l} \left[e^{\beta J} \delta_{\sigma_{l_0}, \sigma_{l_1}} \left(p \delta_{b_l, 1} + (1-p) \delta_{b_l, 0} \right) + e^{-\beta J} \left(1 - \delta_{\sigma_{l_0} \sigma_{l_1}} \right) \delta_{b_l, 0} \right]$$

New weights: $W(\sigma) \to W(\sigma, b)$

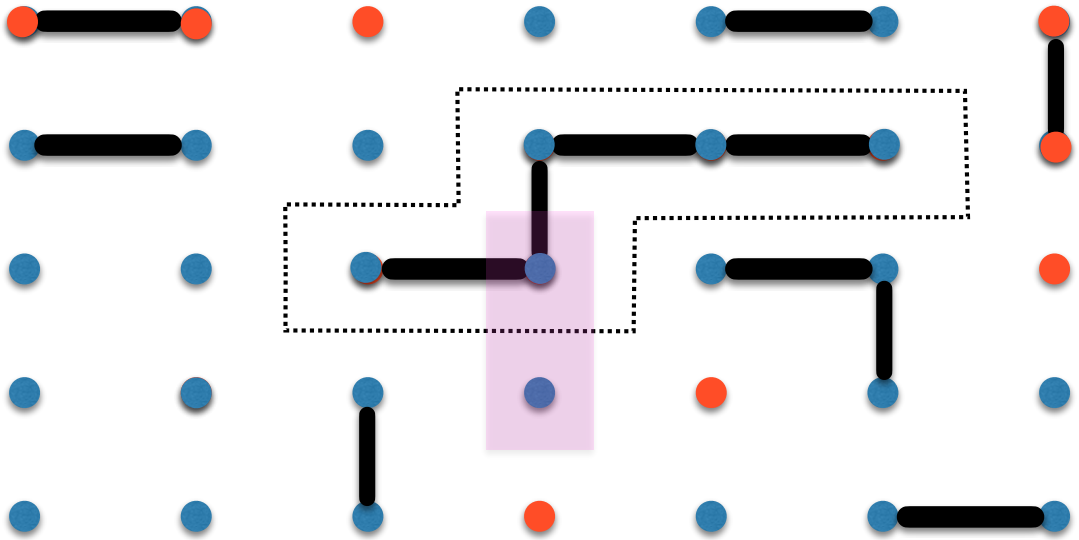
Swendsen-Wang

$$Z = \sum_{\{\sigma\}} \sum_{\{b\}} \prod_{l} \left[e^{\beta J} \delta_{\sigma_{l_0},\sigma_{l_1}} \left(p\delta_{b_l,1} + (1-p)\delta_{b_l,0} \right) + e^{-\beta J} \left(1 - \delta_{\sigma_{l_0}\sigma_{l_1}} \right) \delta_{b_l,0} \right]$$

Table of $W(\sigma, b)$



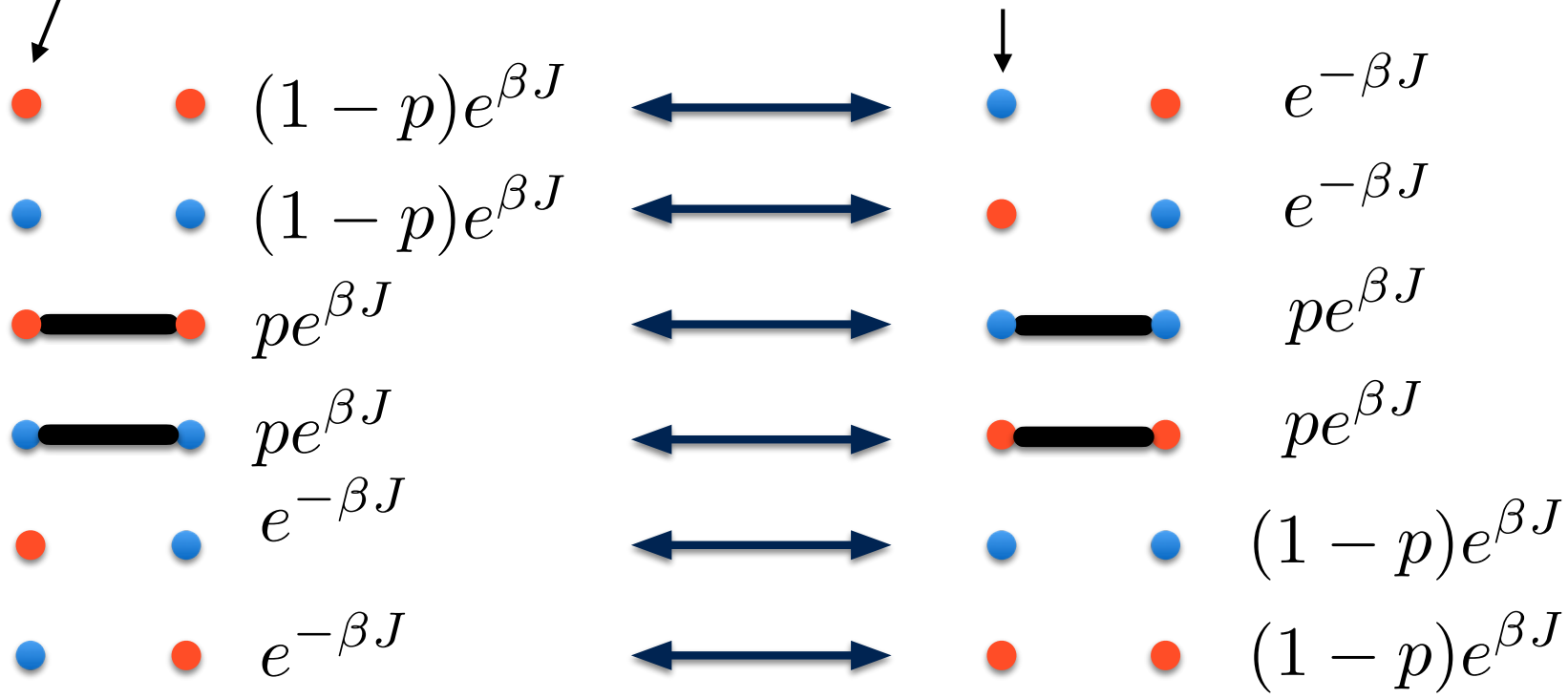
Swendsen-Wang



On flipping all spins on a cluster, only spins on links with no bonds change alignment with each other.

Swendsen-Wang

Flipping one of the spins (both if b=1) gives new configurations:



Swendsen-Wang

Detailed balance: $W(\sigma)P(\sigma \to \sigma') = W(\sigma')P(\sigma' \to \sigma)$

Split P into two stages, 1) assign bonds, 2) flip spins:

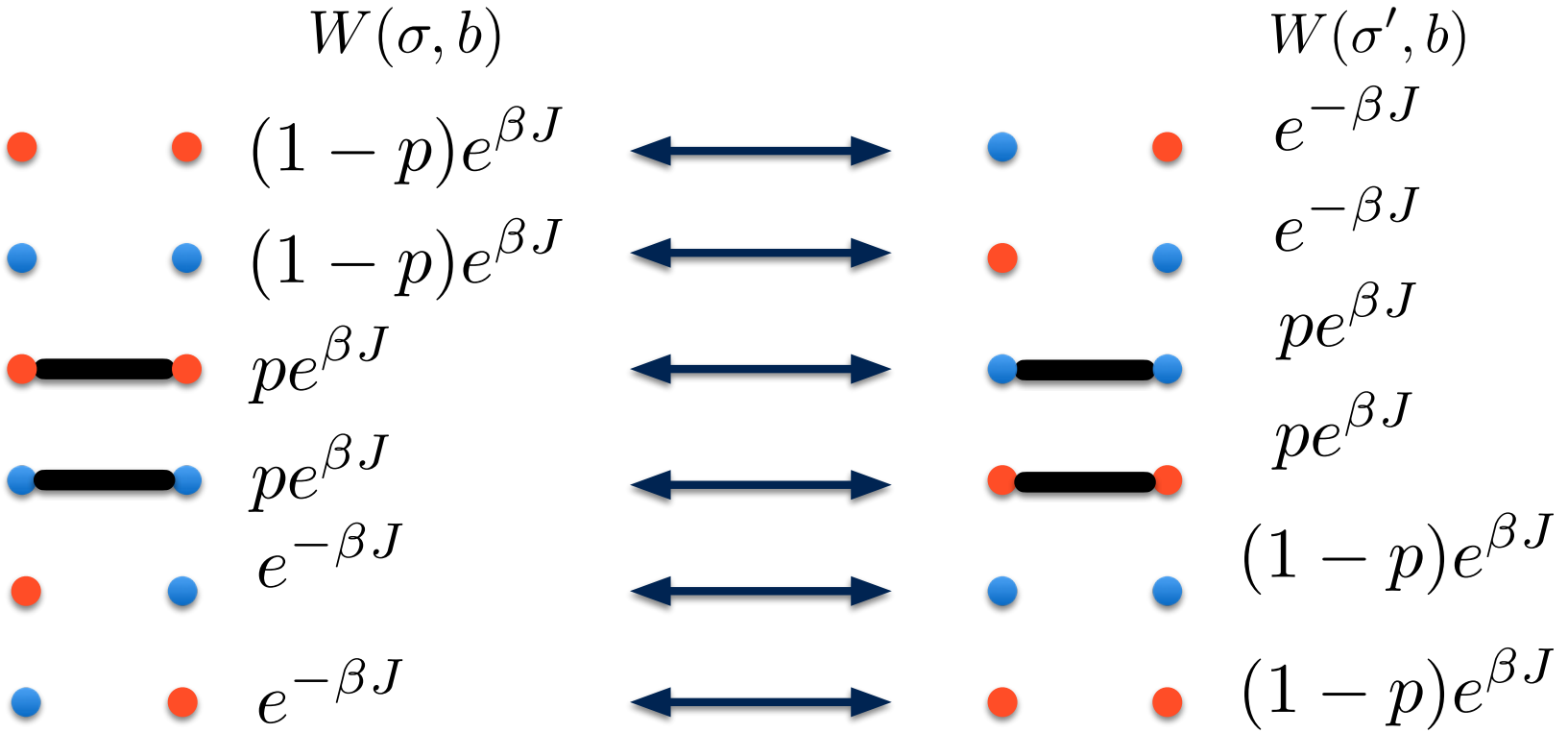
$$P(\sigma \to \sigma') = P(\sigma \to \sigma, b)\tilde{P}(\sigma, b \to \sigma', b)$$

Choose: $\tilde{P}(\sigma, b \to \sigma', b) = \frac{1}{2}$

Then detailed balance is:

$$\underbrace{W(\sigma)P(\sigma \to \sigma, b)}_{W(\sigma, b)} = \underbrace{W(\sigma')P(\sigma' \to \sigma', b)}_{W(\sigma', b)}$$

Swendsen-Wang

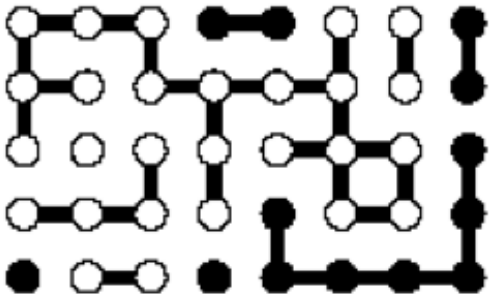


$$W(\sigma, b) = W(\sigma', b) \implies (1-p)e^{\beta J} = e^{-\beta J}$$

$$p = 1 - e^{-2\beta J}$$

Swendsen-Wang algorithm

- Swendsen-Wang algorithm (R.H. Swendsen J.-S. Wang PRL, 58,86 (87)):
  - Given a spin config. Go thru all links between spins and assign bonds with prob. p:
    - Equal spins: $p = 1 - e^{-2\beta J}$
    - Different spins: $p = 0$.
  - Flip resulting clusters with prob. $1/2$.
  - Measure observables
  - Erase bonds and repeat.



Wolff cluster algorithm

U. Wolff, Phys. Lett. B **228**, 379 (1989)

- A single-cluster variant of Swendsen-Wang. Can be implemented easily using recursion.
- 1. Pick a site on random, label it the SITE
- 2. Flip the spin on SITE.
- 3. Consider each neighbor of SITE, one at a time.
  - If the neighboring spin is antialigned with SITE spin, assign SITE to be the neighboring spin with prob. p (same p as in SW). Goto 2.
  - else if not moving SITE do next neighbor. When out of neighbors go back to previous SITE and do the rest of the neighbors there. When all neighbors on all sites visited have been considered, the update is done.

Wolff cluster algorithm