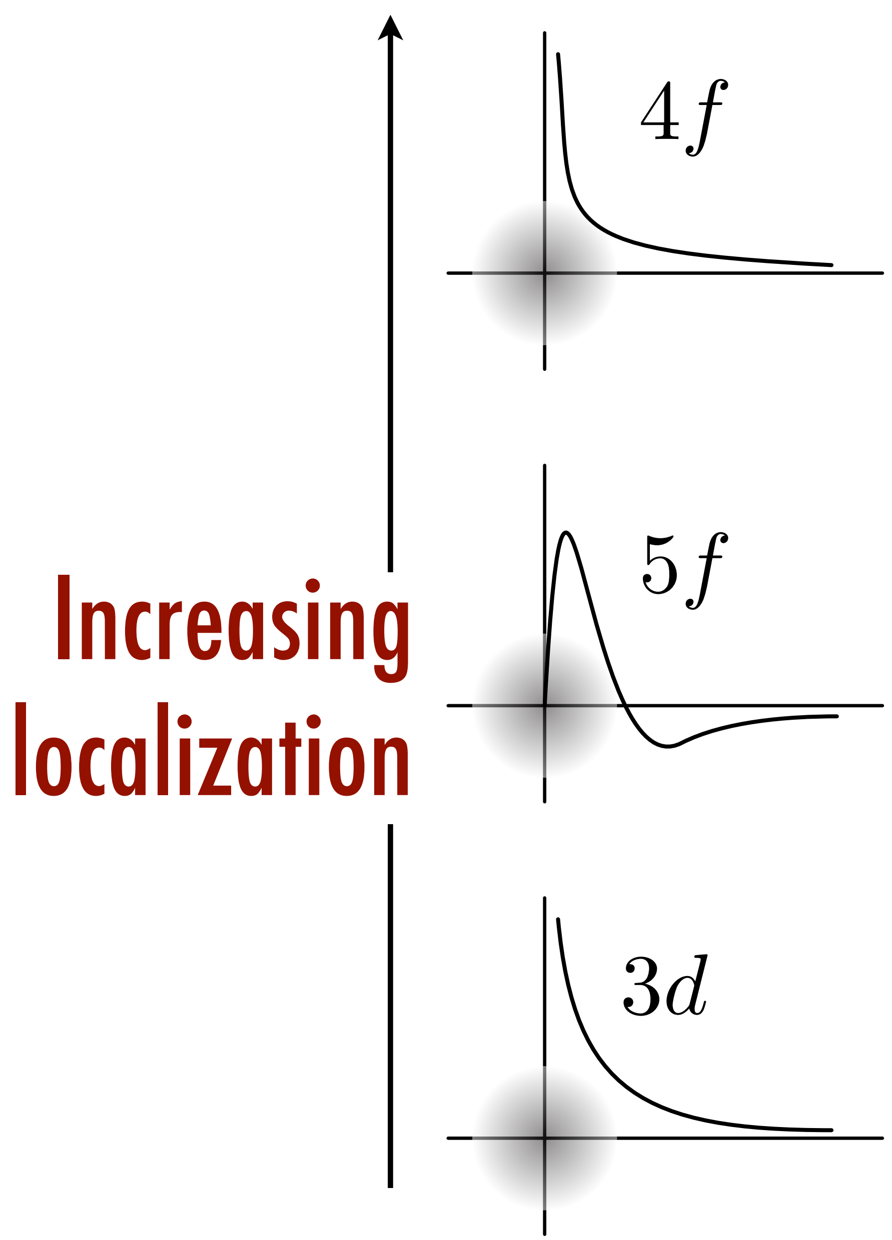
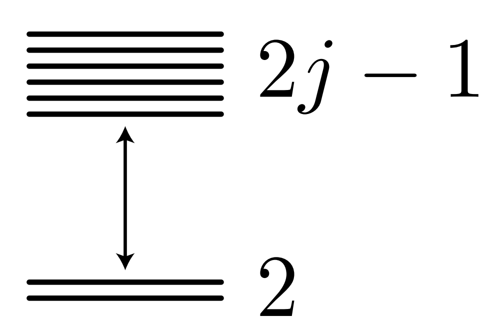
Ising model

Phys 750 Lecture 18

Electronic moments in solids



- In the core levels of real atoms (e.g., transition metals, rare earths, actinides)
- Highly localized orbitals
- $(2j+1)$-fold degenerate; combination of orbital and intrinsic angular momenta
- Possible crystal field splitting into Kramer's doublet



Microscopic magnetism

- Consider effective $\mathrm{SU}(2)$ degrees of freedom

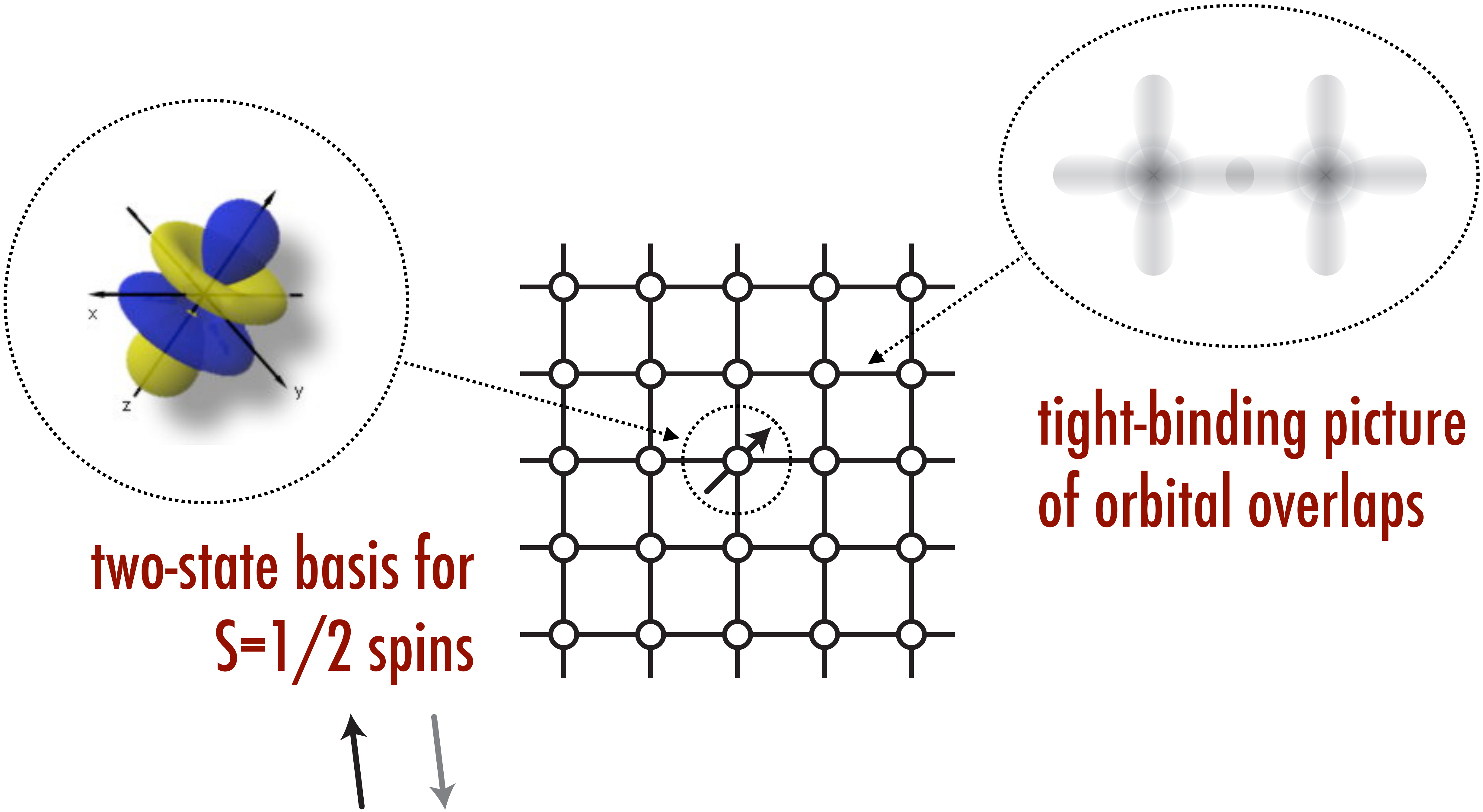
Paul matrices

$$\mathbf{S} = (S^x, S^y, S^z) = \frac{\hbar}{2}(\sigma^x, \sigma^y, \sigma^z)$$

- Long range dipole interactions only play a role on the macroscopic level (e.g., in domain formation)
- This quantum object – a "spin" – interacts with other nearby spins via the exchange interaction

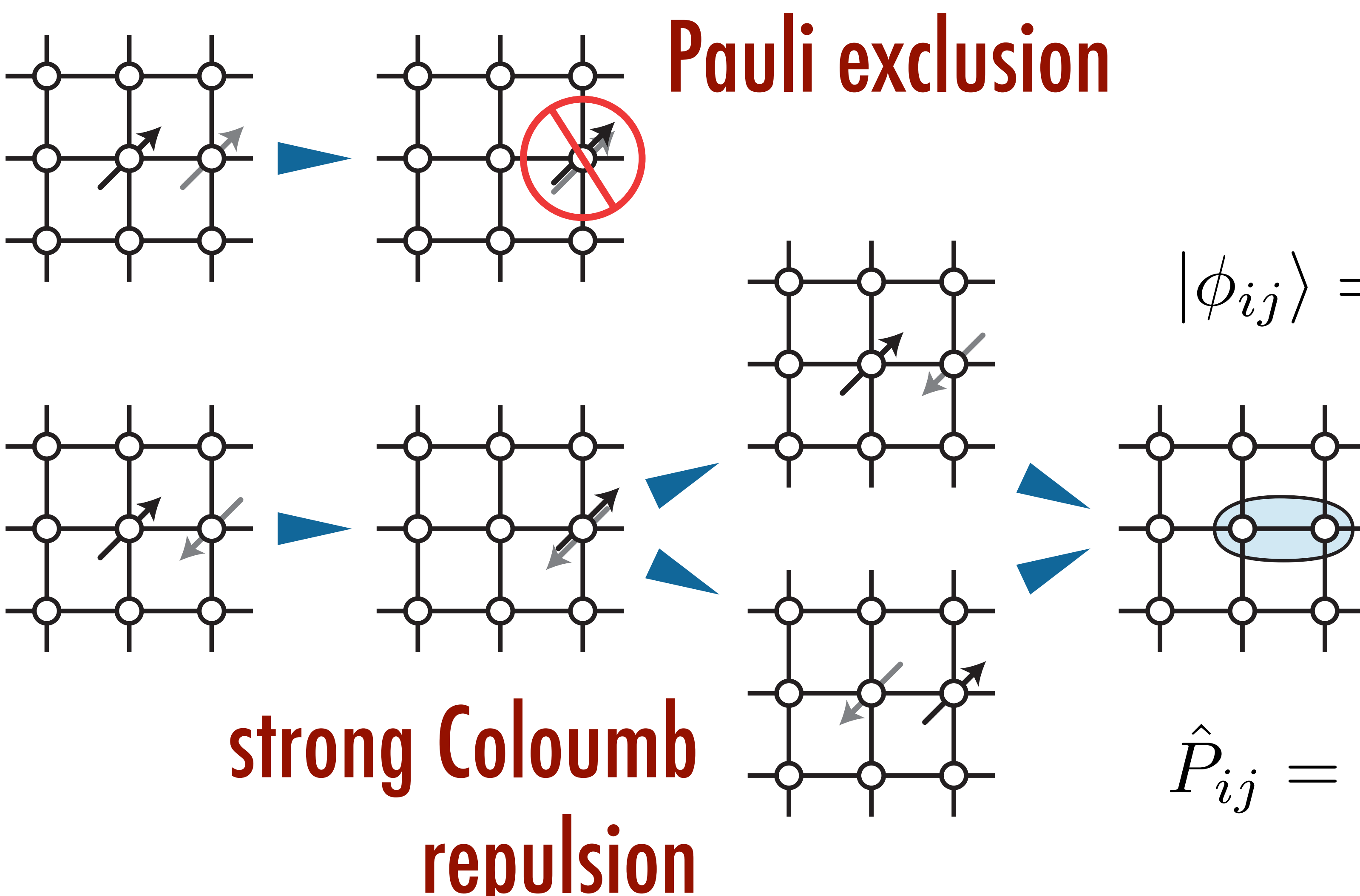
$$S_i^a I_{ij}^{ab} S_j^b = \frac{1}{2} I^{\perp} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + I^{\parallel} S_i^z S_j^z$$

Simplified view



Virtual exchange processes

- E.g., a spin-isotropic antiferromagnetic coupling:



$$|\phi_{ij}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle\right)$$

$$\hat{P}_{ij} = |\phi_{ij}\rangle\langle\phi_{ij}| = \tfrac{1}{4} - \mathbf{S}_i \cdot \mathbf{S}_j$$

Ising model

- If, in addition, the exchange coupling is highly spin-anisotropic (e.g., $I^{\|} \gg I^{\perp}$) and short ranged then interaction depends only on the local alignment of adjacent spins

$$\mathcal{H}[s] = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i$$

sum once over all nn bonds

allow for an external field

- Change of notation

$$I^{\|} = -\frac{4J}{\hbar^2}, \quad \sigma^z = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix} \longrightarrow s_i \in \{-1, +1\}$$

Ising model thermodynamics

- All thermodynamics follows from the partition function in the canonical ensemble:

$$Z = \sum_{\{s_i\}} e^{-\beta\mathcal{H}[s]} \longrightarrow E = \frac{\sum \mathcal{H} e^{-\beta\mathcal{H}}}{\sum e^{-\beta\mathcal{H}}}$$

internal energy

$$= -\frac{\partial Z/\partial\beta}{Z} = -\frac{\partial \ln Z}{\partial\beta} = \frac{\partial(\beta F)}{\partial\beta}$$

$$= -T^2\frac{\partial(F/T)}{T} = F - T\frac{\partial F}{\partial T}$$

free energy

$$F = -kT\ln Z$$

$$= E - TS$$

entropy $S = -\dfrac{\partial F}{\partial T}$

Ising model thermodynamics

- The specific heat and the magnetic susceptibility are related to fluctuations of the configurational energy and fluctuations of the total magnetization:

$$C = \frac{\partial E}{\partial T} = \frac{\partial E}{\partial \beta}\frac{\partial \beta}{\partial T}$$

$$= \frac{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}{kT^2}$$

$$\chi = \frac{\partial M}{\partial H} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{kT}$$

$$M = \sum_i s_i = \frac{1}{\beta}\frac{\partial \ln Z}{\partial H}$$

derivatives of primary quantities

Ising model thermodynamics

- In dimension $d > 1$, the Ising model exhibits a continuous (or second order) phase transition between ferromagnetic and magnetically disordered phases
- Recall the Ehrenfest classification:
  - 1st order: discontinuities in F'
  - 2nd order: continuous F', discontinuities in F''

$M \sim \partial F / \partial H$ dies away continuously with heating

Famous exact results

- Critical temperature: $kT_{\mathrm{c}} = \dfrac{2}{\log(1+\sqrt{2})}$

L. Onsager, Phys. Rev. 65, 117 (1944)

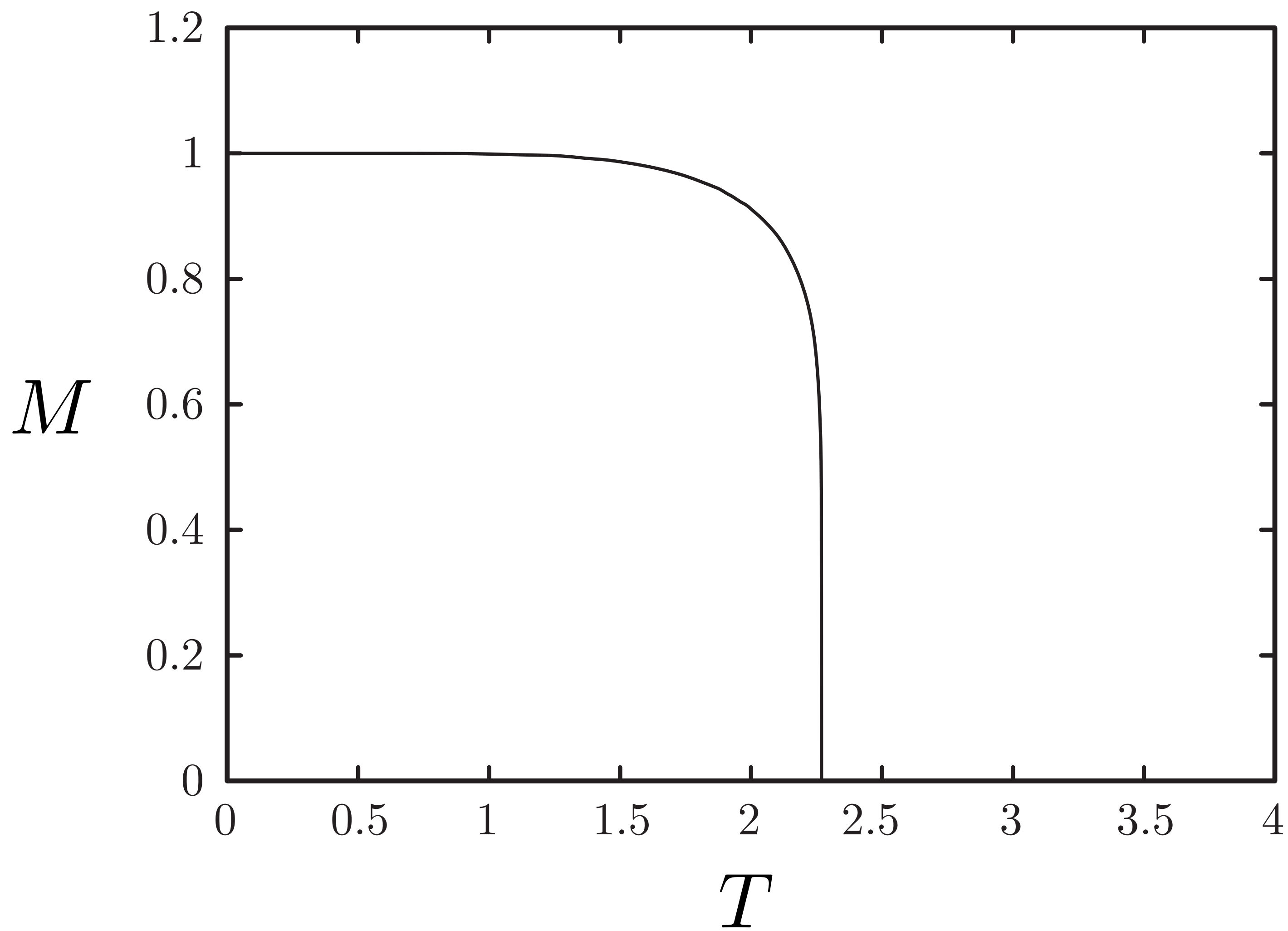
- Magnetization: $M = \left[\dfrac{1+x^2}{(1-x^2)^2} (1 - 6x^2 + x^4)^{1/2} \right]^{1/4}$

$$x = e^{-2/kT}$$

C.N. Yang, Phys. Rev. 85, 808 (1952)

Critical behaviour

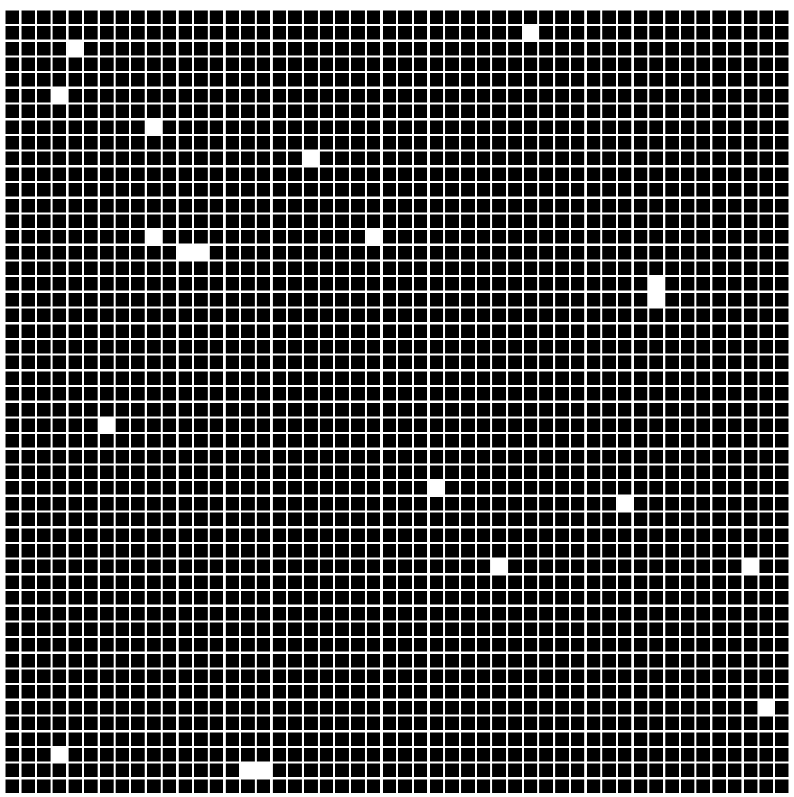
$$M \approx [4(\sqrt{2}+2)(x_c - x)]^{1/8} \sim (T_c - T)^{1/8}$$



$$\alpha = 0, \beta = \frac{1}{8},$$
$$\gamma = \frac{7}{4}, \delta = 15$$

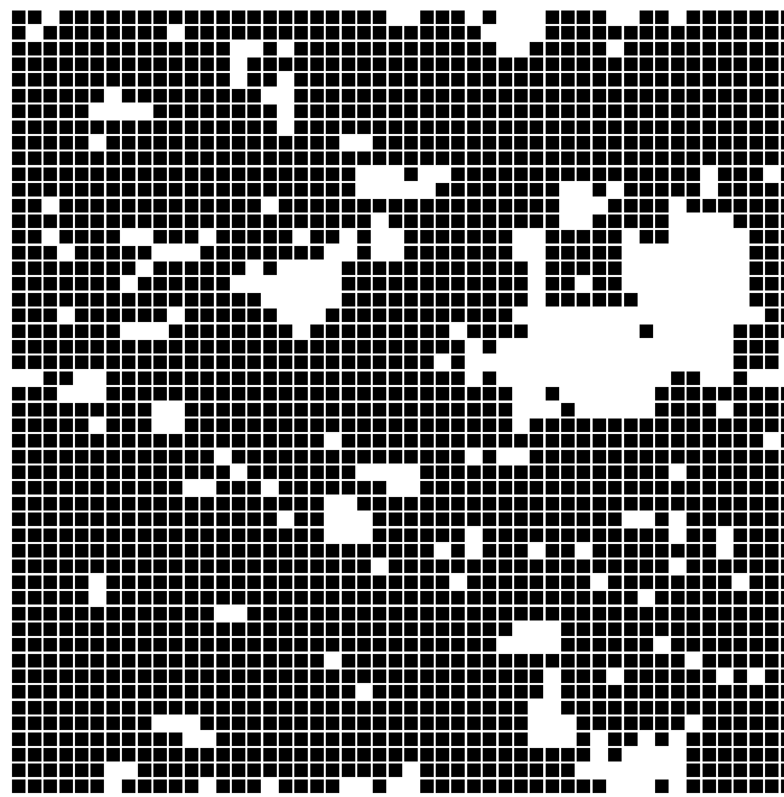
transition characterized by a set of critical exponents

Critical behaviour



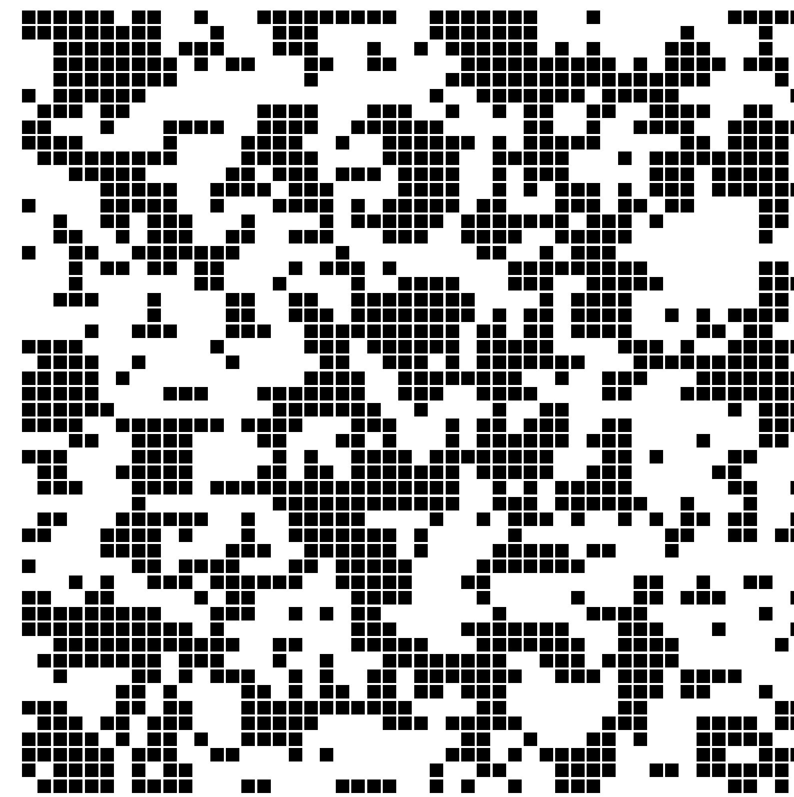
$T = \frac{2}{3} T_c$

dominant cluster



$T = T_c$

fractal clusters (cf. percolation)

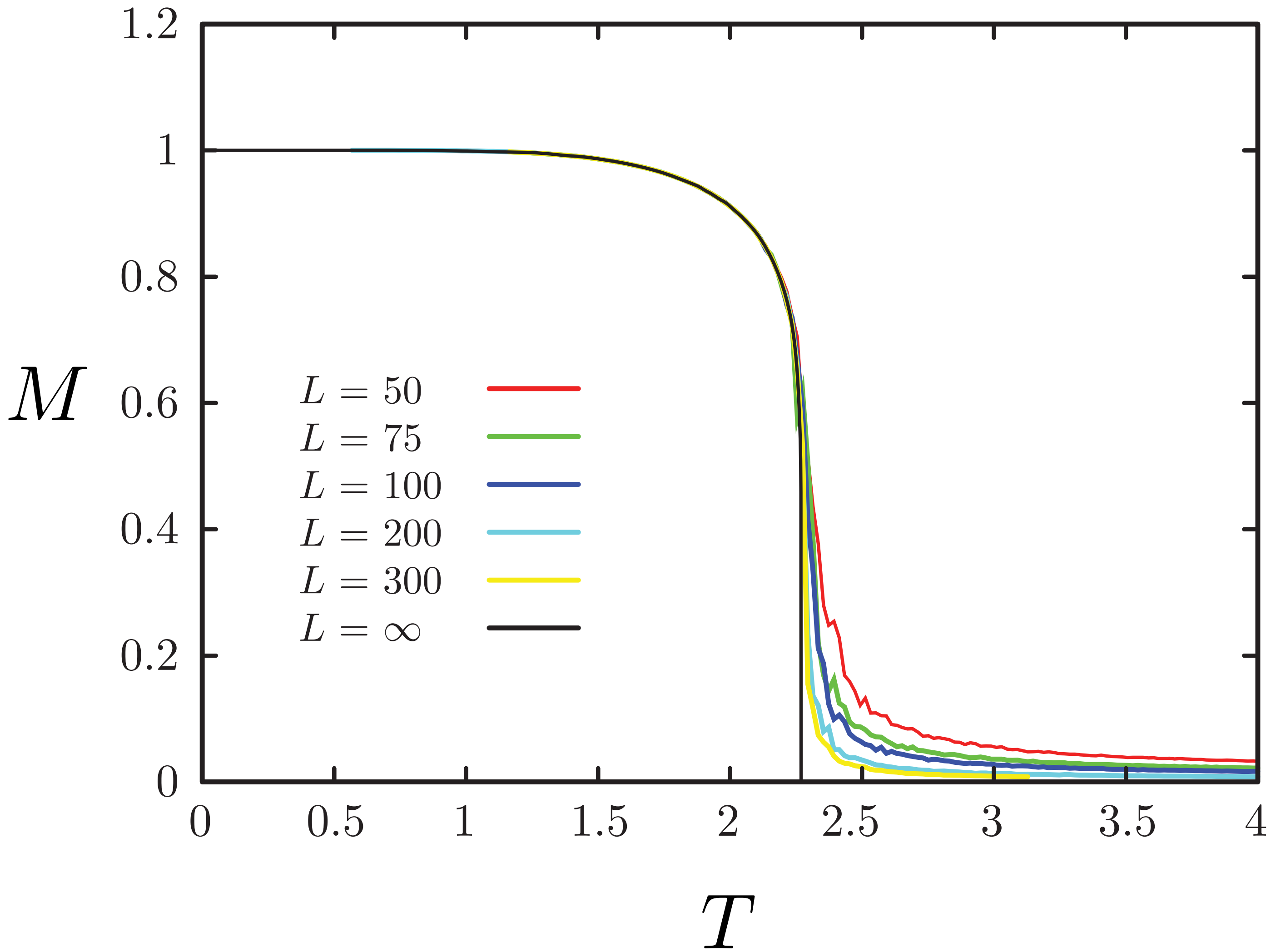


$T = \frac{3}{2} T_c$

thermally disordered

Finite-size scaling

- Simulations of increasing size approach the thermodynamic limit result



Finite-size scaling

- The magnetic correlation length diverges as $T \to T_c^+$

correlation length exponent

$$\xi(T) = \xi_0 t^{-\nu} \qquad t = \frac{T - T_c}{T_c}$$

reduced temperature

- The system becomes "scale invariant" at the critical point

$$\left(\frac{L}{\xi}\frac{\xi_0}{L_0}\right)^{1/\nu} = t\left(\frac{L}{L_0}\right)^{1/\nu}$$

- Implies that the free energy density has the form

$$f(L,T) = \frac{F}{L^d} = L^{-d}\mathbb{Y}(C_1 t L^{1/\nu})$$

"universal function"

Finite-size scaling

- All thermodynamic quantities (which are derivatives of the free energy) inherit a scaling form

$$M(L,T) = \mathbb{M}(tL^{1/\nu})L^{-\beta/\nu}$$
$$\chi(L,T) = \mathbb{X}(tL^{1/\nu})L^{\gamma/\nu}$$
$$C(L,T) = \mathbb{C}(tL^{1/\nu})L^{\alpha/\nu}$$

- Also leads to relationships amongst the exponents:

$$\alpha + 2\beta + \gamma = 2 \qquad \gamma = \beta(\delta - 1)$$

$$d = 2 - \alpha \qquad \gamma = \nu(2 - \eta)$$

Finite-size scaling

- Helpful to construct scaling-free quantities from combinations of measurements
- E.g., the moments $\langle m^2 \rangle \sim (L^d L^{-\beta/\nu})^2$
  and $\langle m^4 \rangle \sim (L^d L^{-\beta/\nu})^4$
- The ratio $\langle m^4 \rangle / \langle m^2 \rangle^2$ is order zero in L
- Data collapse for the "Binder cumulant" versus $x = tL^{1/\nu}$

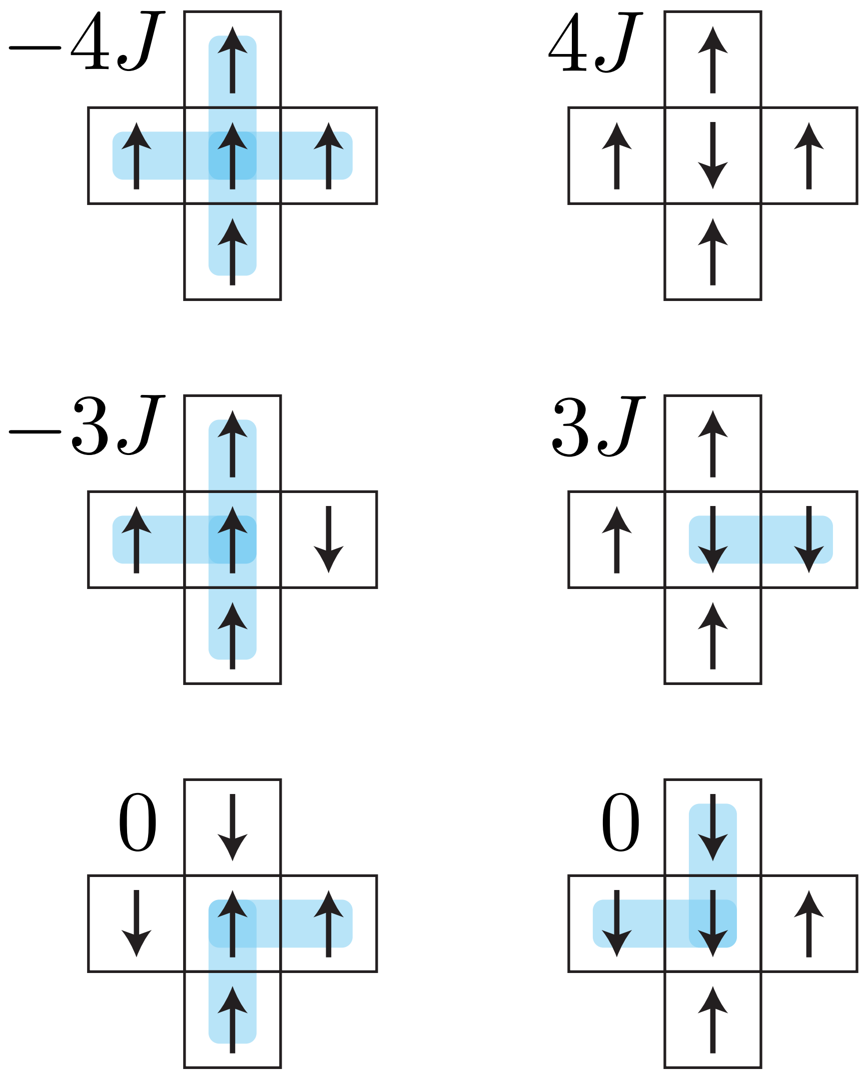
$$U = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2} = \mathbb{U}(tL^{1/\nu}) \qquad U \to \begin{cases} 2/3 & \text{if } T < T_\mathrm{c} \\ 0.61 & \text{if } T = T_\mathrm{c} \\ 0 & \text{if } T > T_\mathrm{c} \end{cases}$$

Metropolis updates

- How might we simulate this?
- Impose a fictitious Monte Carlo dynamics based on single spin flips $s_i \mapsto s_i' \equiv -s_i$
- Traversal of the phase space is ergodic but slow
- Accept move with probability $P = \min(1, e^{-\beta \Delta \mathcal{H}})$, where

$$\Delta \mathcal{H} = \mathcal{H}[\ldots, s_i', \ldots] - \mathcal{H}[\ldots, s_i, \ldots]$$

Metropolis updates



$$\Delta\mathcal{H} = 4J - (-4J) = 8J$$
$$P = e^{-8J/T}$$

$$\Delta\mathcal{H} = 6J$$
$$P = e^{-6J/T}$$

$$\Delta\mathcal{H} = 0$$
$$P = 1$$

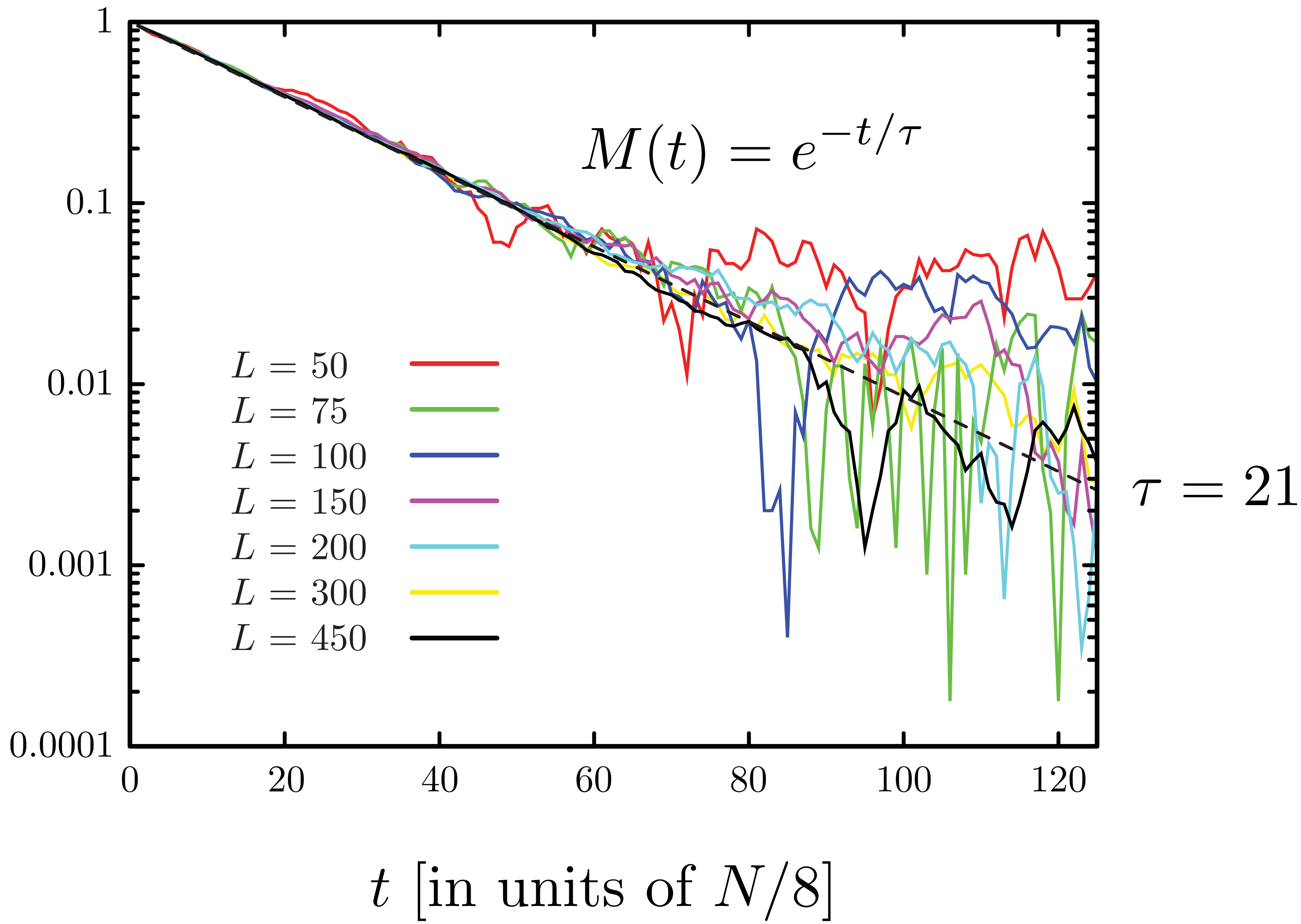
- **General rule:** $\Delta\mathcal{H} = -2s_i \times \sum_{j\in \mathrm{nn}(i)} s_j$

Equilibration process

starting from a perfectly ferromagnetic configuration

$T = 2T_c$

relaxing to disorder

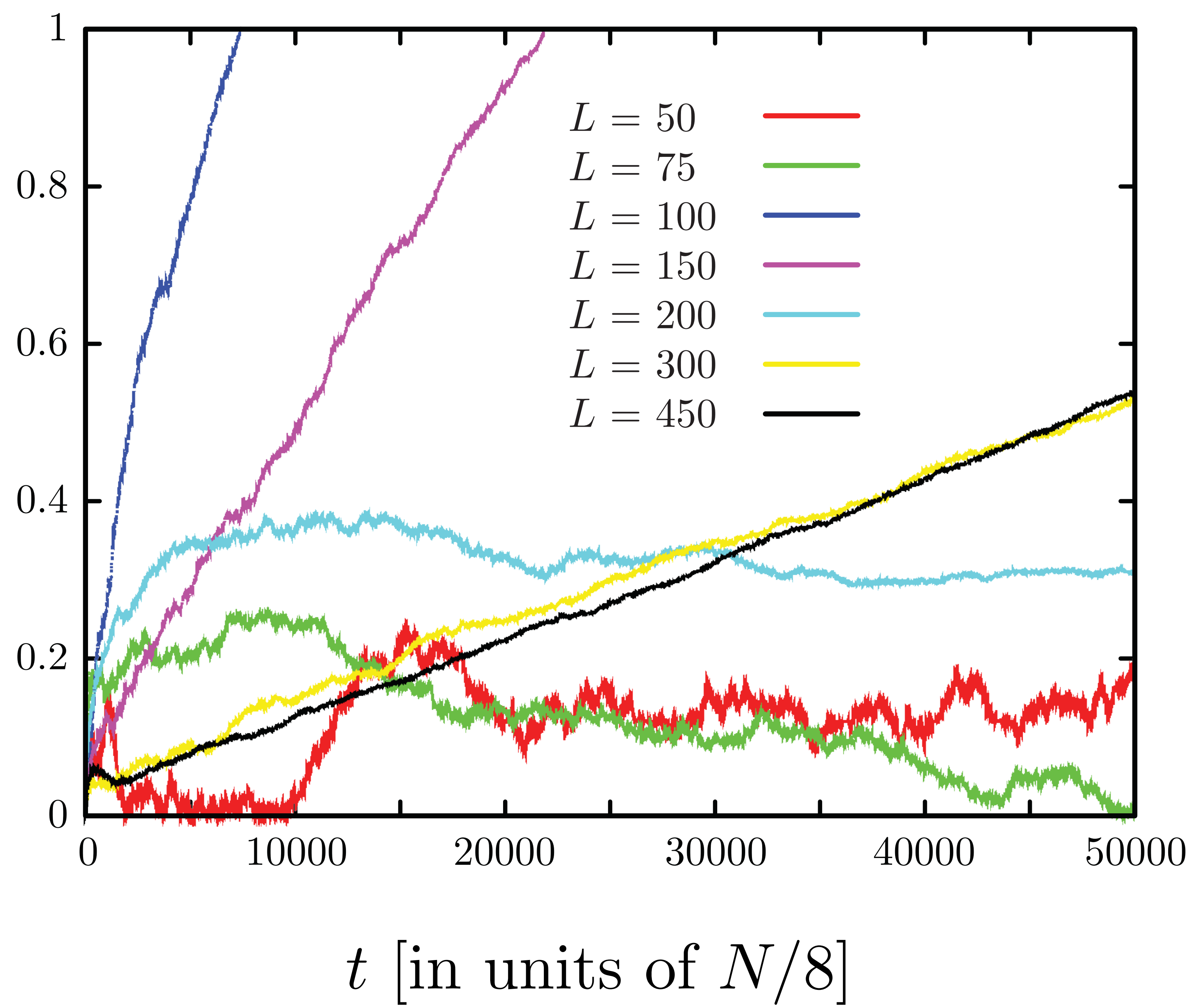


Equilibration process

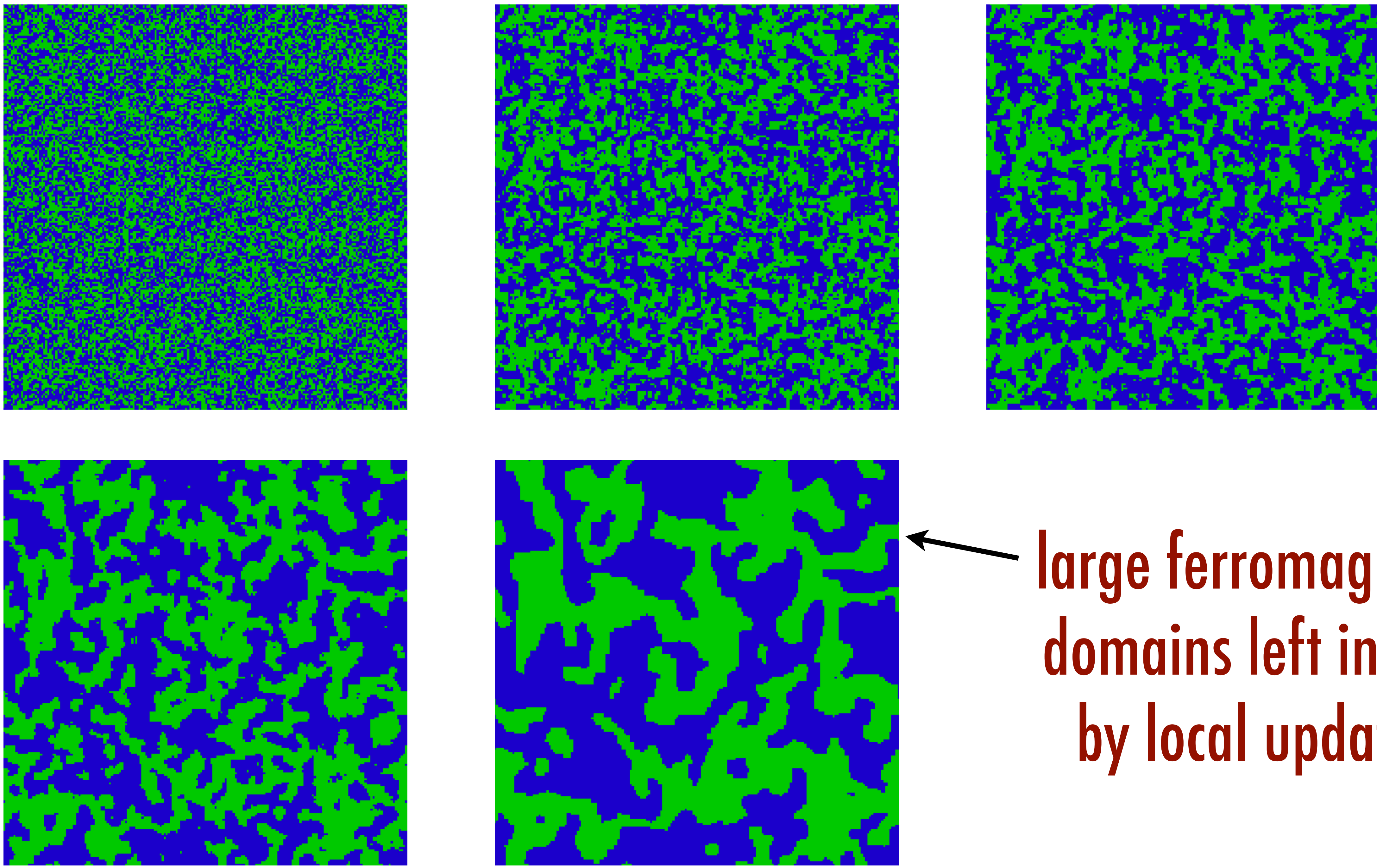
starting from a perfectly disordered configuration

$T = \frac{1}{2} T_c$

relaxing to magnetism

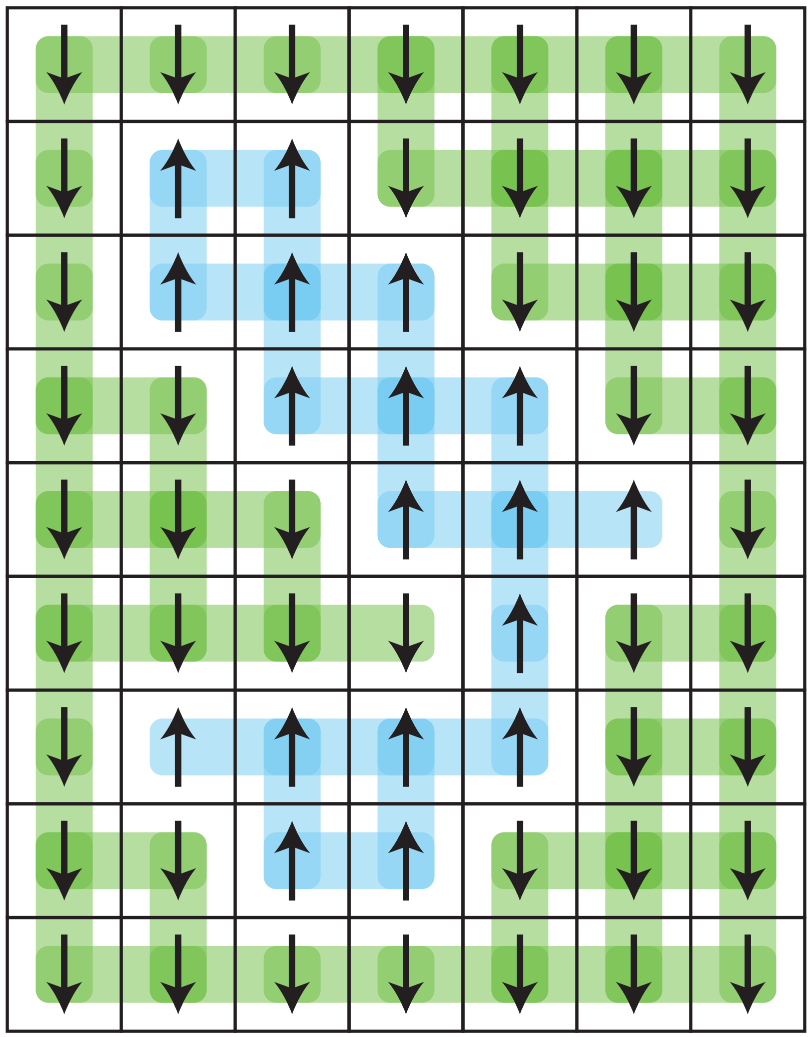


Rapid quenching



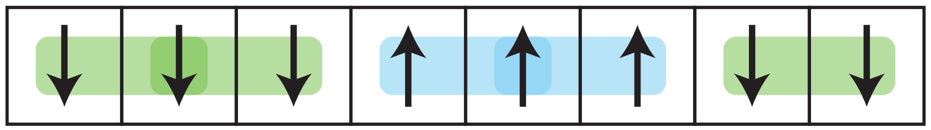
large ferromagnetic
domains left in tact
by local updates

Cluster updates



perimeter $\sim N_{\text{cl}}^{1/2}$

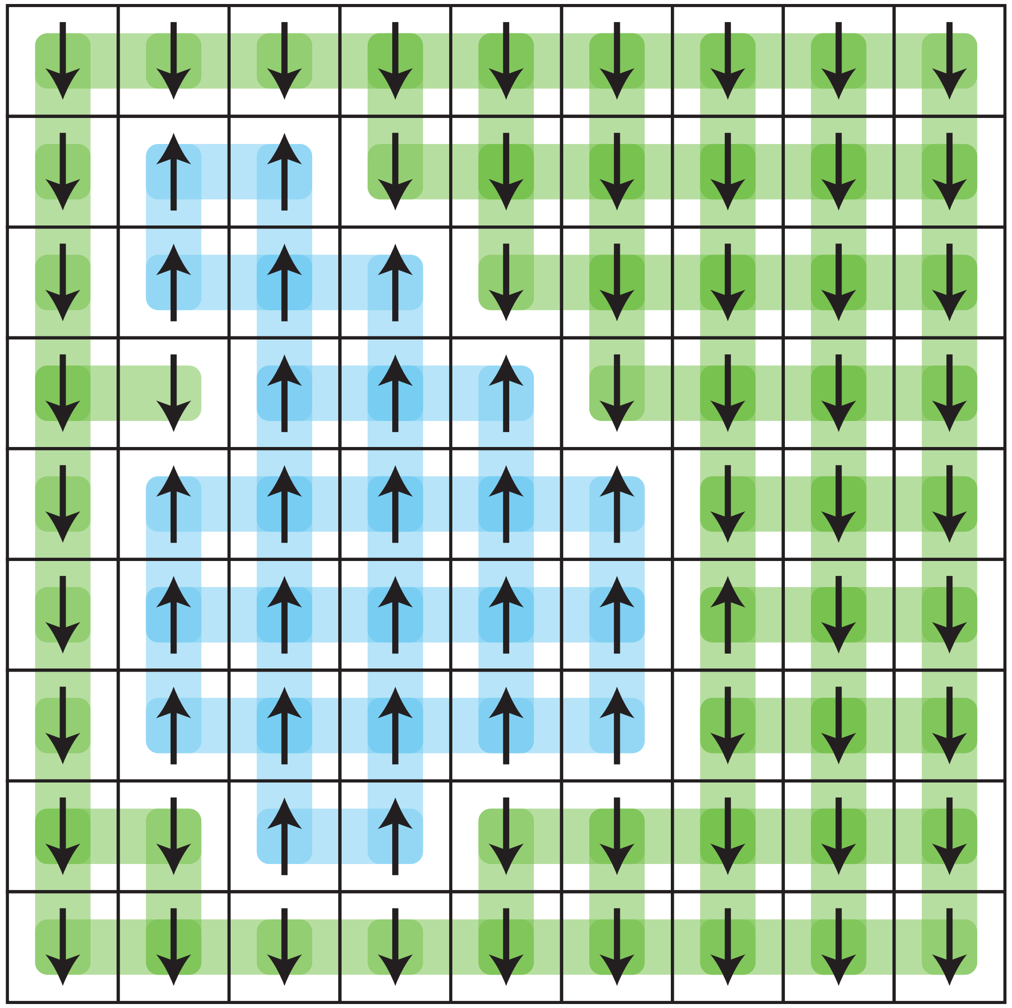
- More efficient to flip clusters of spins
- Swendson-Wang and Wolff algorithms eliminate the problem of critical slowing down



boundary $= 2$

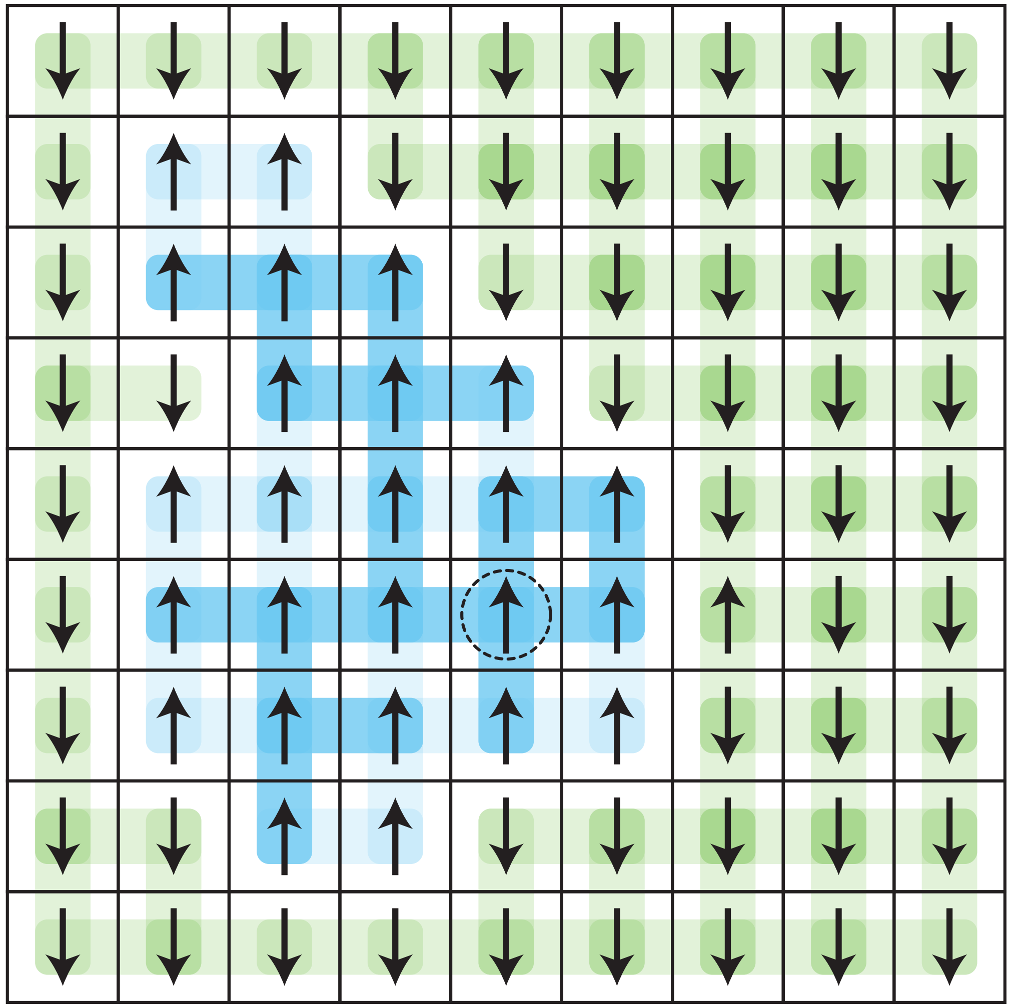
Wolff algorithm

- Focus on the set of links connecting sites that have the same spin



Wolff algorithm

- Focus on the set of links connecting sites that have the same spin
- Choose a site at random
- Grow cluster by activating set of adjacent links with probability $1 - e^{-2J/T}$



Wolff algorithm

- Focus on the set of links connecting sites that have the same spin
- Choose a site at random
- Grow cluster by activating set of adjacent links with probability $1 - e^{-2J/T}$
- Flip the entire cluster