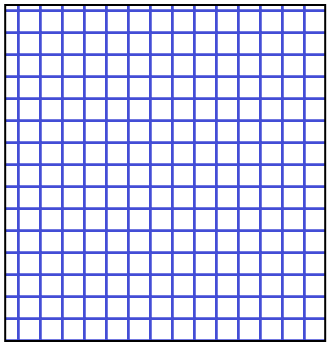
The Ising Model

Today we study one of the most studied models in statistical physics, the **Ising Model (1925).**

- Some applications:
  - Magnetism (the original application)
  - Liquid-gas transition
  - Binary alloys (can be generalized to multiple components)
- Onsager found the exact answer for the 2D square lattice (1944). (1D was done by Ising in 1925.)
- Used to develop *renormalization group theory* of phase transitions in 1970's.
- We'll discuss critical slowing down of Metropolis and a "cluster method".

Figures from Landau and Binder (LB), MC Simulations in Statistical Physics, 2000.

The Ising Model

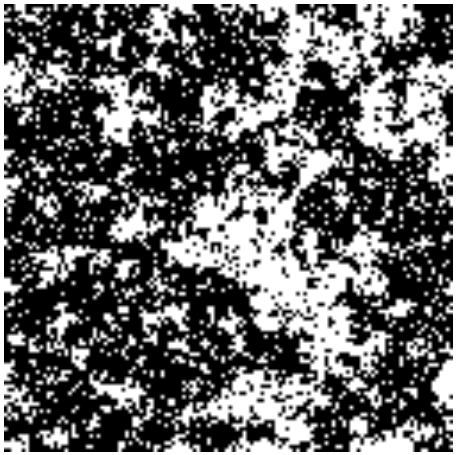


- Consider a lattice with L^2 sites and the connectivity of. a square lattice.
- Each lattice site has a single spin variable: $s_i = \pm 1$.
- With magnetic field **h**, the energy is:

$$H = -\sum_{(i,j)} J_{ij} s_i s_j - \sum_{i=1}^{N} h_i s_i \qquad and \qquad Z = \sum e^{-\beta H}$$

- J is the nearest neighbor (i,j) coupling:
  - J > 0 models a ferromagnet.
  - J < 0 models an antiferromagnet.

- Picture of spins at the critical temperature T_c. Note the connected (percolated) clusters.



Mapping a liquid-gas model to the Ising Model

- For ***liquid-gas*** transition let n(r) be the density at lattice site r which can have two values n(r)=(0,1).

$$E = \sum_{(i,j)} v_{ij} n_i n_j + \mu \sum_i n_i$$

- First term models an interatomic repulsion.
- Second term is the chemical potential.
- Let's map this into the Ising model spin variables:

$$s = 2n - 1 \quad \text{or} \quad n = \frac{1}{2}(s+1)$$

$$H = \frac{v}{4} \sum_{(i,j)} s_i s_j + \frac{(v+\mu)}{2} \sum_i s_i + c$$

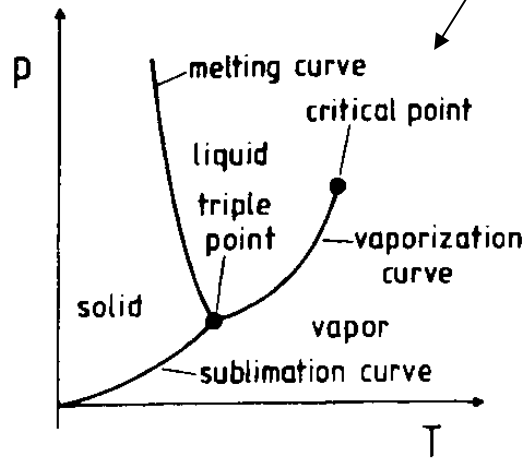
$$J = -v/4$$

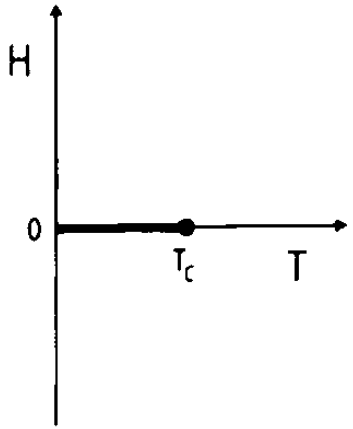
$$h = -(v+\mu)/2$$

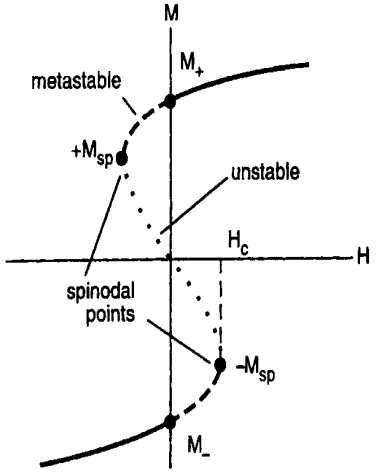
$$M = \frac{1}{N} \sum_i s_i \qquad \langle \mathrm{n} \rangle = \frac{1}{N} \sum_i n_i = \frac{1}{2}(M+1)$$

Phase Diagram (J>0)

- **High-T phase:** spins are random (uncorrelated).
- **T > T_c phase near T_c:** spins are random but correlated: magnetic short-range (local) order.
- **Low-T (T~0) phase:** spins are aligned (fully correlated).
- A ***first-order transition*** (where there is a discontinuous jump in **M**) occurs as H passes through zero for $T<T_c$.
- Similar to **liquid-gas phase diagram**. Magnetic field=pressure.







Critical point

- Concepts and understanding are universal.

  They apply to all phase transitions of a similar type.
- Order parameter is the *average* magnetization: $\langle s(r)\rangle = m(r)$.
- Look at correlation function: $\chi(r-r') = \langle s(r)s(r')\rangle - \langle s(r)\rangle\langle s(r')\rangle$.
- Magnetic susceptibility is: $dm(r)/dh(r')|_{h\to 0} = \beta\chi(r-r')$
- In ordered phase, spins are correlated over long distances.
- At the critical point, fluctuations at all length scales.

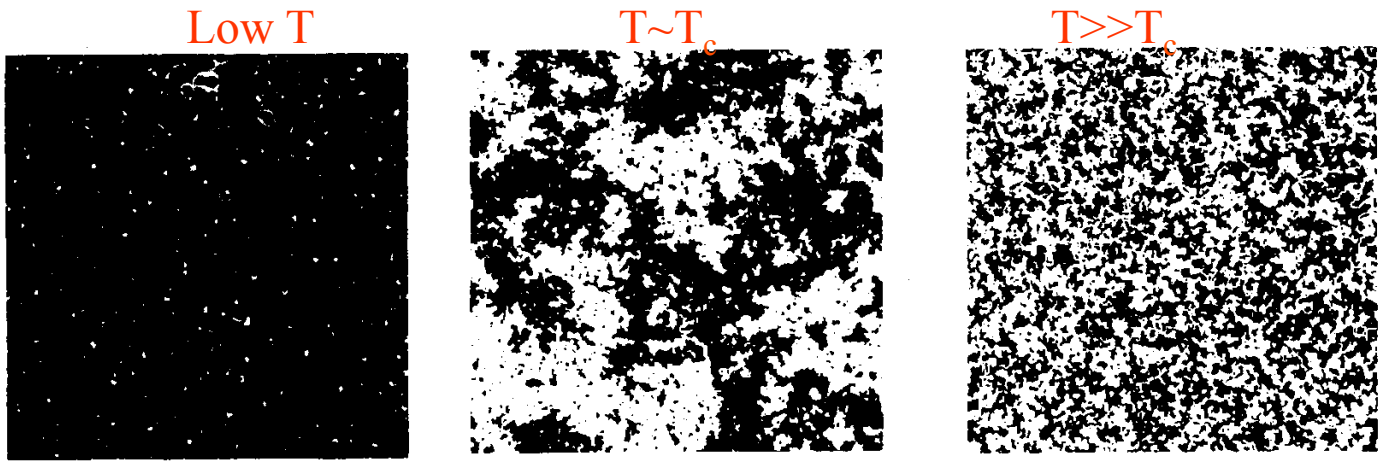
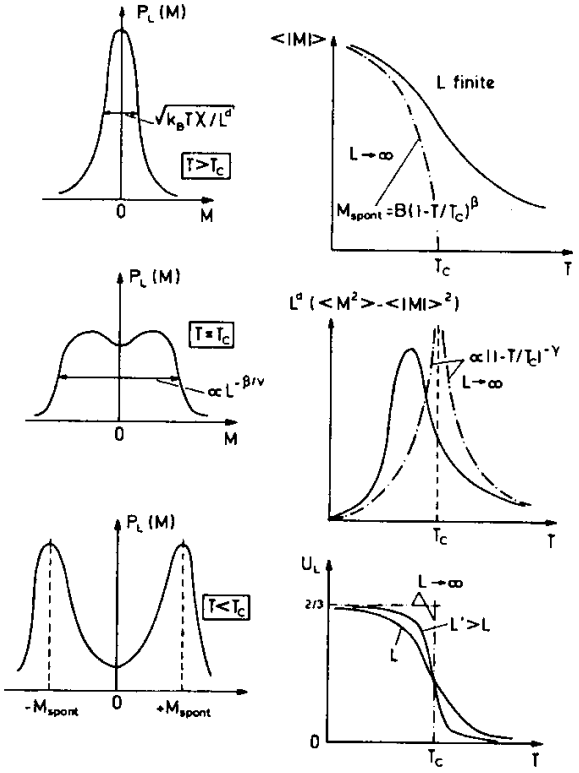


Fig. 4.1 Typical spin configurations for the two-dimensional Ising square lattice: (left) $T \ll T_c$; (center) $T \sim T_c$; (right)

Magnetization probability

- How does magnetization vary across transition?
- And with the system size?
- In ordered phase, broken symmetry and barrier to flipping.



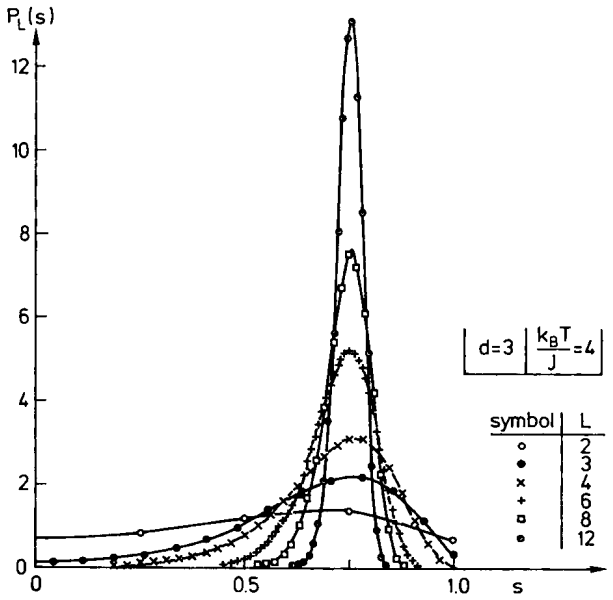


Figure 2. Probability distribution $P_L(s)$ of the magnetization s per spin of $L \times L \times L$ subsystems of a simple cubic Ising lattice with $N = 24^3$ spins and periodic boundary conditions for zero magnetic field and temperature $k_B T/J = 4.0$ (note that the critical temperature occurs at about $k_B T_c/J \approx 4.51$[26].

Figure 3. Schematic variation of the probability distribution $P_L(m)$ to magnetization m in a finite system of linear dimension L from $T > T_c$ to (left part) and the associated temperature variation of the average order pa $< |m| >$, "susceptibility" $k_B T\chi' = L^d(< m^2 > - < |m| >^2)$ and reduced order cumulant $U_L = 1 - < m^4 > / \left[3 < m^2 >^2\right]$ (right part).

- If we quench too fast we will end in a two phase region.
- The larger the system the sharper the phase transition.

Phase Diagram: T vs. M

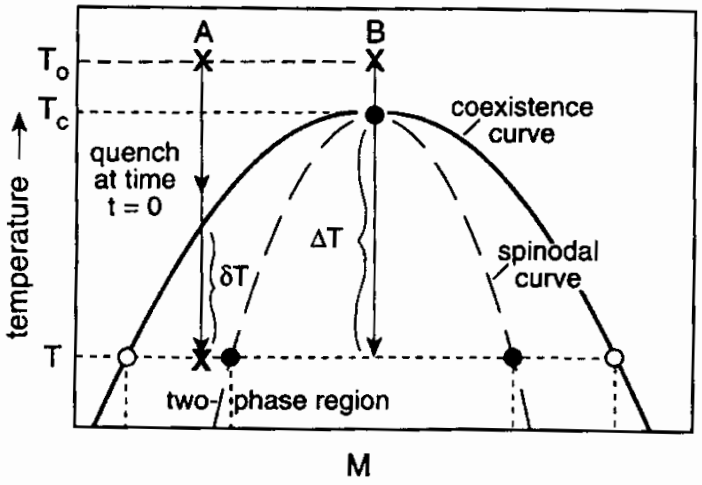
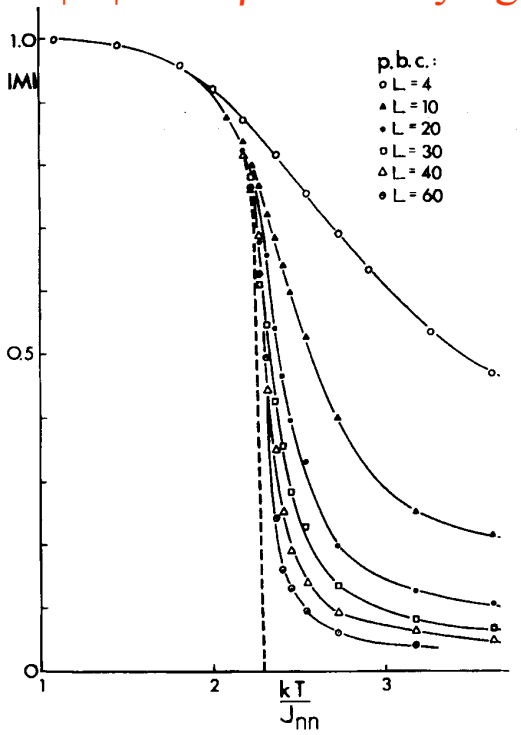


Fig. 2.11 Schematic phase coexistence diagram showing the 'spinodal' line. Paths (A) and (B) represent quenches into the nucleation regime and the spinodal decomposition regime, respectively.

|M| vs. 1/βJ for varying L



Magnetization Scaling depends on T:

$M \sim (T_c - T)^{\beta}$ for $T < T_c$

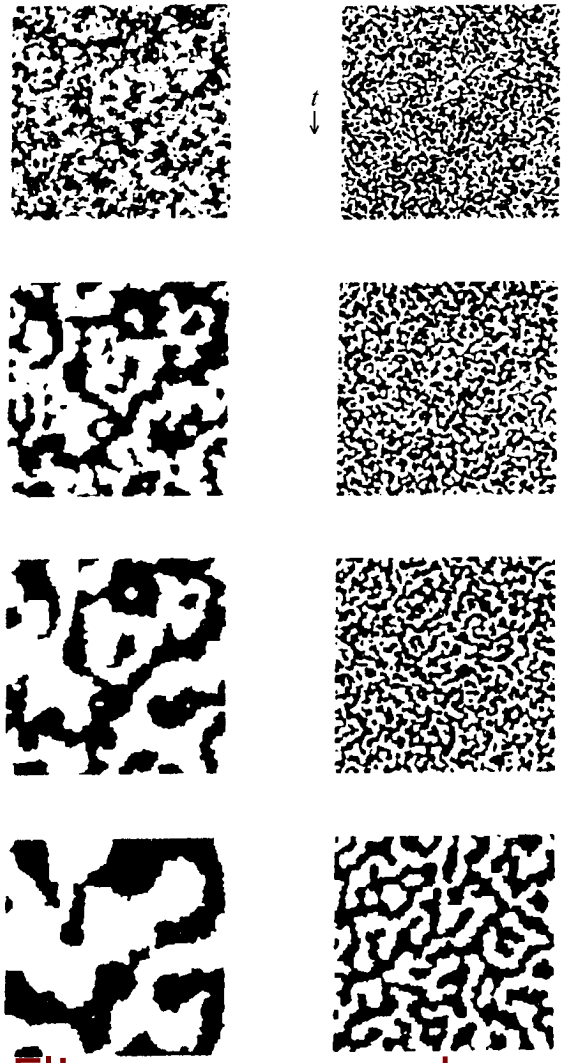
$\beta = 0.125$ for D=2.

$\beta = 0.325$ for D=3.

Spinoidal decomposition

Suppose only local spin flips.

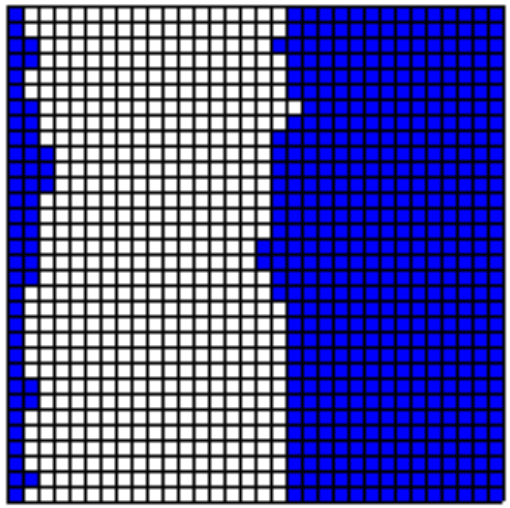
- Model for phase separation such as a binary “alloy” (or oil and vinegar).
- Dynamics depends on whether the spin is conserved
  - Spin flip (left)
  - Spin exchange (right) conserves particle number.
- Transition appears through a coarsening of the separation.
- Becomes slower and slower as the transition proceeds: Critical Slowing down.



$T=0.6T_c$

Surfaces/Boundary Conditions

- By quenching quickly we may catch a “trapped” surface.
- Topological excitation.
- You can see steps, etc.
- Can use *twisted boundary conditions* to study a liquid-gas surface without worrying about it disappearing.
- Just put -J along one plane (side): i.e. antiferromagnetic interaction along one plane.

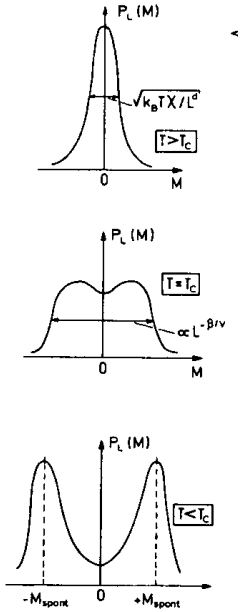


$$H = -\sum_{(i,j)} J_{ij} s_i s_j$$

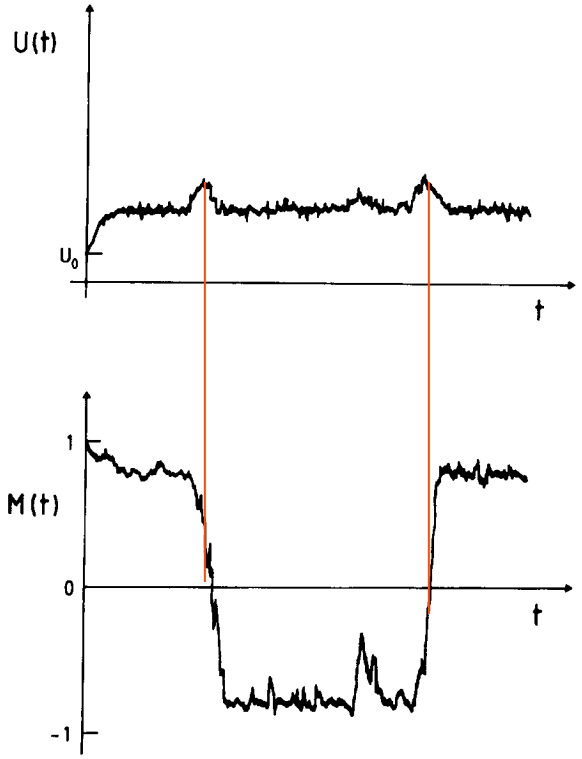
$$J_{ij} = \begin{cases} J & i \neq 0 \\ -J & i = 0 \end{cases}$$

Critical slowing down

- Near the transition dynamics gets very slow if you use any local update method.
- The larger the system th less likely it is that the system can flip over.



Monte Carlo of a zero-field Ising Lattice
U vs. time and M vs. time.



Simple Metropolis algorithm

- Simplest Metropolis:
  - Lots of tricks to make it run faster.
  - Tabulate exp(-E/kT)
  - Do several flips each cycle by packing bits into a word
  - But critical slowing down near Tc.
  - At low T accepted flips are rare--can speed up by sampling ***acceptance time***.
  - At high T all flips are accepted--ergodic problem.

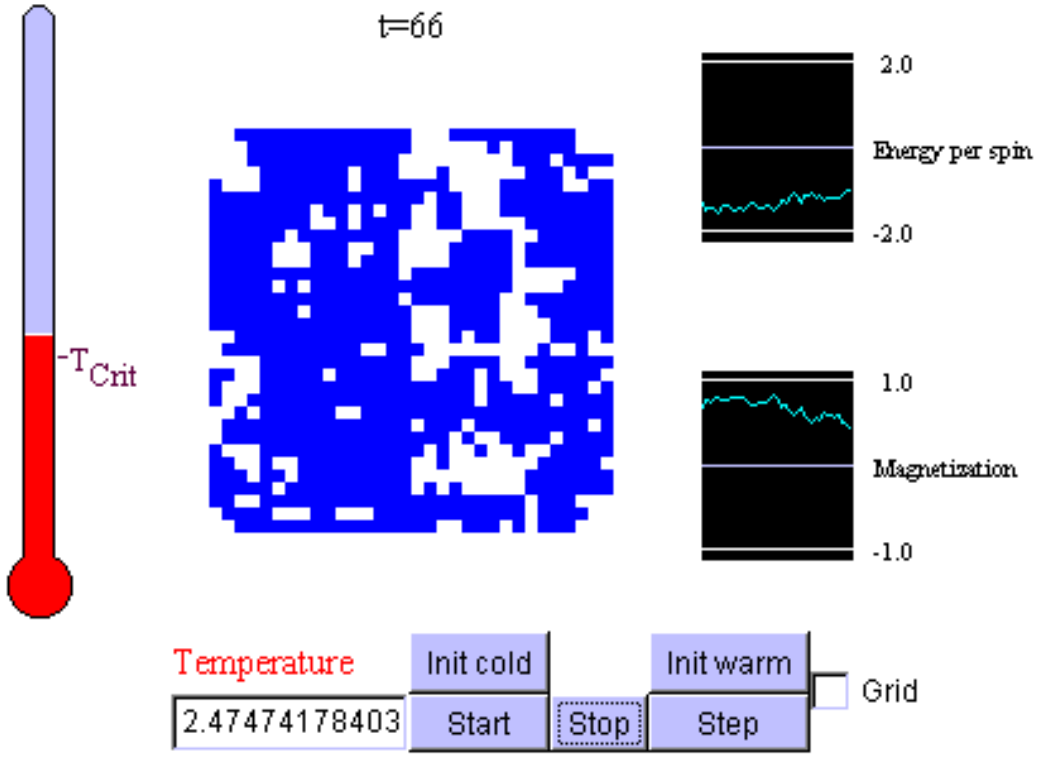
Metropolis importance sampling Monte Carlo scheme

(1) Choose an initial state
(2) Choose a site i
(3) Calculate the energy change ΔE which results if the spin at site i is overturned
(4) Generate a random number r such that $0 < r < 1$
(5) If $r < \exp(-\Delta E/k_B T)$, flip the spin
(6) Go the next site and go to (3)

JAVA Ising applet

http://physics.weber.edu/schroeder/software/demos/IsingModel.html

Dynamically runs using the heat bath algorithm.



Glauber and Kawasaki dynamics

- **Heat bath or Glauber:**
  - Pick a spin and flip with probability
  - Will have lower flipping rate but no high T problem.

$$p^i = \frac{\pi_i}{\pi_i + \pi_j} = \frac{1}{1 + e^{-\beta \Delta E}}$$

- **N-fold way:**
  - Look at all the sites, choose the site "i" according to:
  - The normalization determines how time advances.
  - Discuss this later with kinetic MC

$$T^i = \frac{\pi_i}{\sum_j \pi_j}$$

- **Kawasaki dynamics**
  - Exchange spins and accept or reject
  - Spin is constant as in spinoidal decomposition.
- ALL THESE ARE LOCAL hence suffer from slowdown.