Final Project and Reports

- grading:
  - (i) a collective grade for a project proposal and its presentation in class,
  - (ii) a collective grade for the final report,
    (iii) a collective grade for the presentation of the final results
  - For your project proposal and final report we will use peer review, which will also be part of your grade

  - **Scientific Research.** Each project should be research oriented, something concerning new developments in classical or quantum simulations and with a scientific component.
  - **Algorithm development.** This could involve an optimization of an existing code or algorithm, a new implementation, some interesting science, the use of new computer architectures, or databases.
  - **Presentation.** We expect a written report from each team that explains your project. This should include graphics, literature links, and potentially web references.

Final Project and Reports

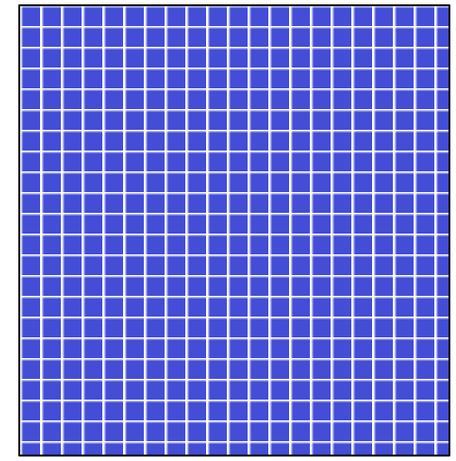
- **Friday Nov. 10** Project proposal drafts due (for comment)
- **Thursday Nov. 16** Project proposals in class
- **Friday Nov. 17** Peer reviews due (for redistribution)
- **Wednesday Dec. 6** Final reports due
- **Friday Dec. 8** In class presentations; slides due *by 10:00am*
- **Thursday Dec. 14** Peer reviews due

Phase transitions and finite-size scaling

- Critical slowing down and “cluster methods”.
- Theory of phase transitions/ “Renormalization Group”
- Finite-size scaling

Detailed treatment: “Lectures on Phase Transitions and the Renormalization Group” Nigel Goldenfeld (UIUC).

The Ising Model

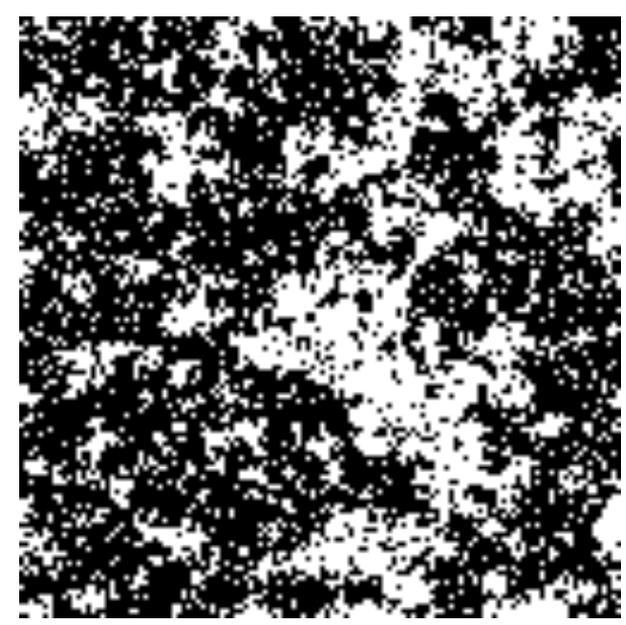


- Suppose we have a lattice, with L^2 lattice sites and connections between them. (e.g. a square lattice).
- On each lattice site, is a single spin variable: $s_i = \pm 1$.
- With mag. field h, energy is:

$$H = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$$

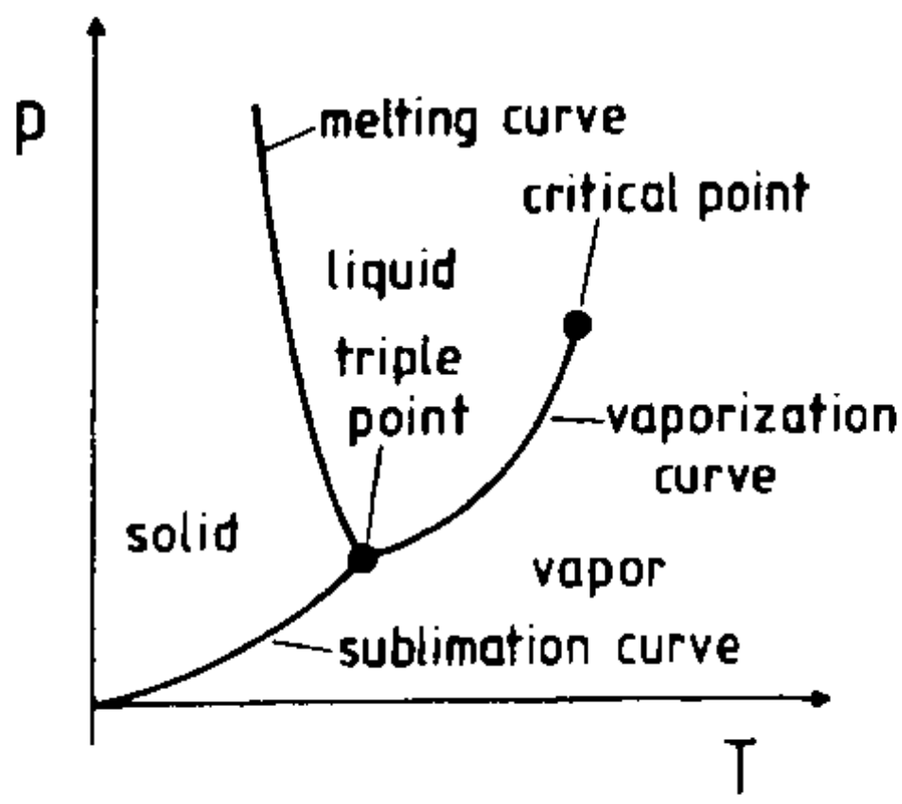
- J is the coupling between nearest neighbors (i,j)
  - J>0 ferromagnetic
  - J<0 antiferromagnetic.

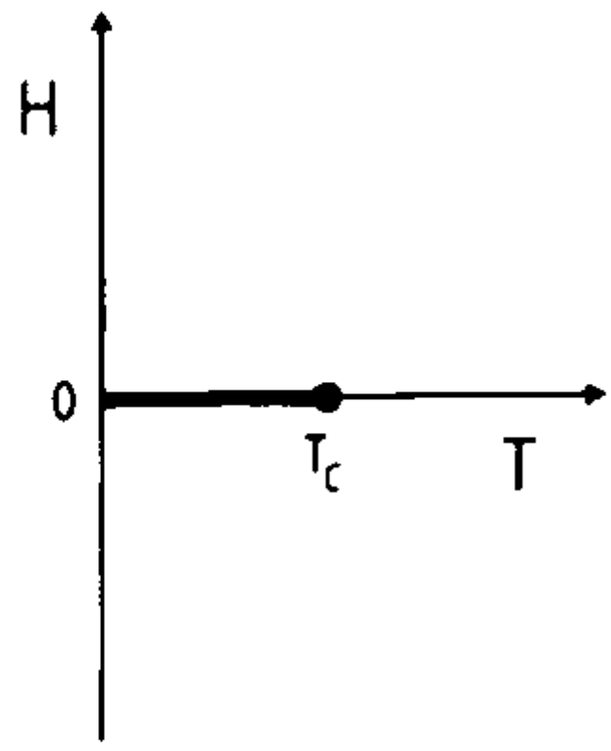
$$Z = \sum_{s_i = \pm 1} e^{-\beta H}$$



Phase Diagram

- **High temperature phase:** spins are random
- **Low temperature phase:** spins are aligned
- A first-order transition occurs as H passes through zero for $T<T_c$.
- Similar to LJ phase diagram. (Magnetic field=pressure).





Local algorithms

- Simplest Metropolis:
  - Tricks make it run faster.
  - Tabulate exp(-E/kT)
  - Do several flips each cycle by packing bits into a word.

But,

- Critical slowing down ~ T_c.
- At low T, accepted flips are rare
  --can speed up by sampling acceptance time.
- At high T all flips are accepted
  --quasi-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)

Critical slowing down

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

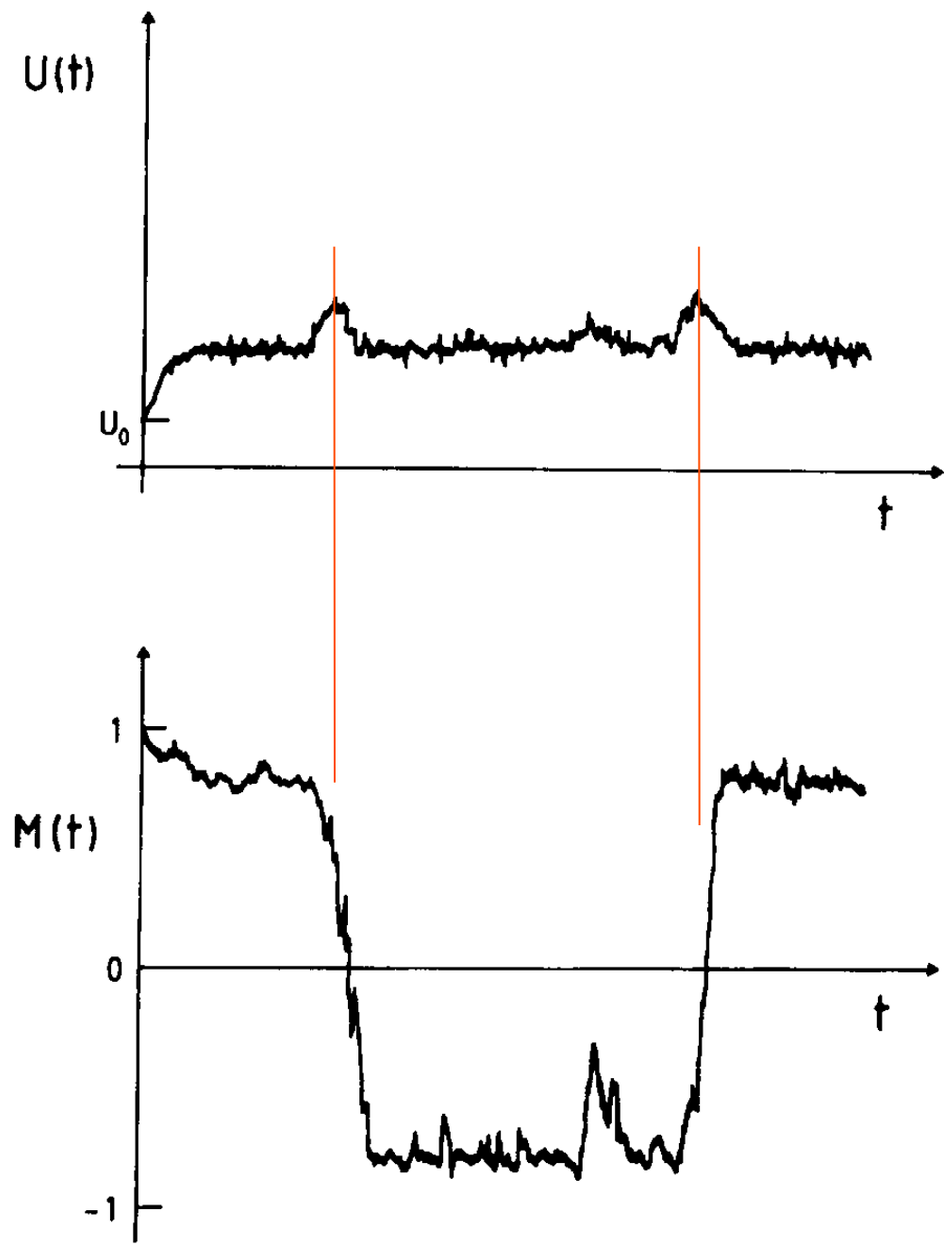


Fig. 4.2 Schematic variation of internal energy and spontaneous magnetization with time for a Monte Carlo simulation of an Ising square lattice in zero field.

Dynamical Exponent

Monte Carlo <u>efficiency</u> is governed by a critical dynamical exponent Z.

with τ_0 = correlation time

and ξ = correlation length

$$\text{Efficiency} = \zeta = 1/vT$$

v = error^2 of mean and T = total CPU time

$$\zeta = (\mathrm{var}(O)\tau_0 \text{ time/step})^{-1}$$

$$\tau_0 \propto \xi^2/D$$

$$\text{near } T_c: \ \xi \to L \ \& \ \tau \to L^2$$

$$\tau \propto L^z$$

Non-local updates reduce the Exponent, allowing exploration of The "critical region."

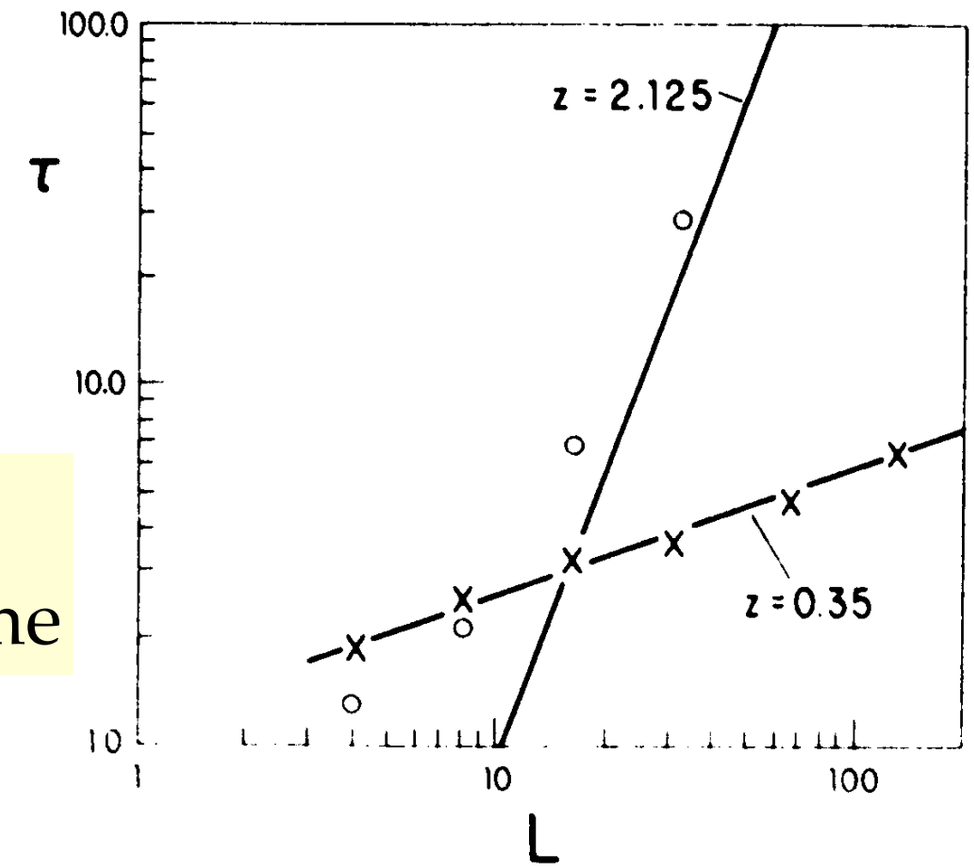


FIG. 1. Log-log plots of correlation times for Monte Carlo simulations of the two-dimensional Ising model at the critical temperature as a function of the linear dimension L. The circles show data for a standard Monte Carlo simulation, and the line marked "$z = 2.125$" gives the expected asymptotic slope (Ref. 4). The crosses show data for the new method, with a least-squares fit labeled with its slope of "$z = 0.35$."

Swendsen and Wang, PRL **58**, 86 (1987)

Swendsen-Wang algorithm

Phys. Rev. Letts 58, 86 (1987).

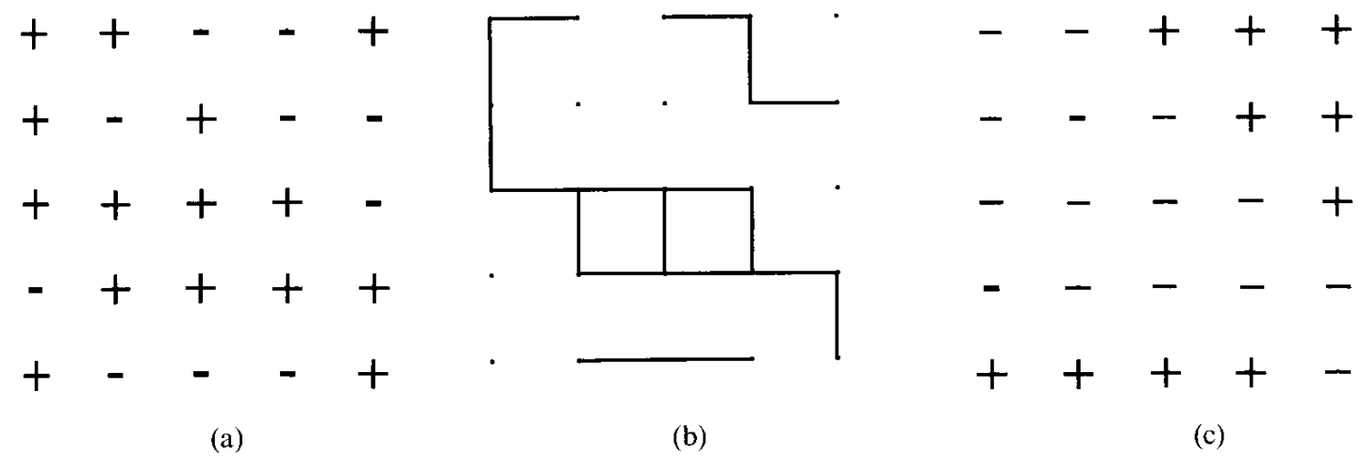


Fig. 5.1 Schematic view of the Swendsen–Wang algorithm for an Ising model: (a) original spin configuration; (b) clusters formed; (c) 'decorated' clusters.

Wolff cluster flipping method for the Ising model

(1) Randomly choose a site
(2) Draw bonds to all nearest neighbors with probability $p = 1 - e^{-K\delta_{\sigma_i\sigma_j}}$
(3) If bonds have been drawn to any nearest neighbor site j, draw bonds to all nearest neighbors k of site j with probability $p = 1 - e^{-K\delta_{\sigma_j\sigma_k}}$
(4) Repeat step (3) until no more new bonds are created
(5) Flip all spins in the cluster
(6) Go to (1)

Swendsen–Wang algorithm for a q-state Potts model

(1) Choose a spin
(2) Calculate $p = 1 - e^{-K\delta_{\sigma_i\sigma_j}}$ for each nearest neighbor
(3) If $p < 1$, generate a random number $0 < rng < 1$;
If $rng < p$ place a bond between sites i and j
(4) Choose the next spin and go to (2) until all bonds have been considered
(5) Apply the Hoshen–Kopelman algorithm to identify all clusters
(6) Choose a cluster
(7) Generate a random integer $1 \leq R_i \leq q$
(8) Assign $\sigma_i = R_i$ to all spins in the cluster
(9) Choose another cluster and go to (7)
(10) When all clusters have been considered, go to (1)

Little critical slowing down at the critical point.

Non-local algorithm.

Wolff, PRL **62**, 361 (1989)

Correctness of cluster algorithm

- Cluster algorithm:
  - Transform from spin space to bond space n_{ij}

    (Fortuin-Kasteleyn transform of Potts model)
  - Identify clusters: draw bond between

    only like spins and those with p=1-exp(-2J/kT)
  - Flip some of the clusters.
  - Determine the new spins

  Example of embedding method: solve dynamics problem by enlarging the state space (spins and bonds).
- Two points to prove:
  - Detailed balance

    joint probability:
  - Ergodicity: we can go anywhere

$$\Pi(\sigma, n) = \frac{1}{Z} \prod_{\langle ij \rangle} \left[(1-p)\delta_{n_{ij},0} + p\delta_{\sigma_i,\sigma_j}\delta_{n_{ij},1} \right]$$

$$p \equiv 1 - e^{-2J/k_{\mathrm{B}}T}$$

How can we extend to other models?

$$\mathrm{Tr}_n \{\Pi(\sigma, n)\} = \frac{1}{Z} \exp\left[K \sum_{\langle ij \rangle} \left(\delta_{\sigma_i,\sigma_j} - 1 \right) \right]$$

RNG Theory of phase transitions

K. G. Wilson 1971

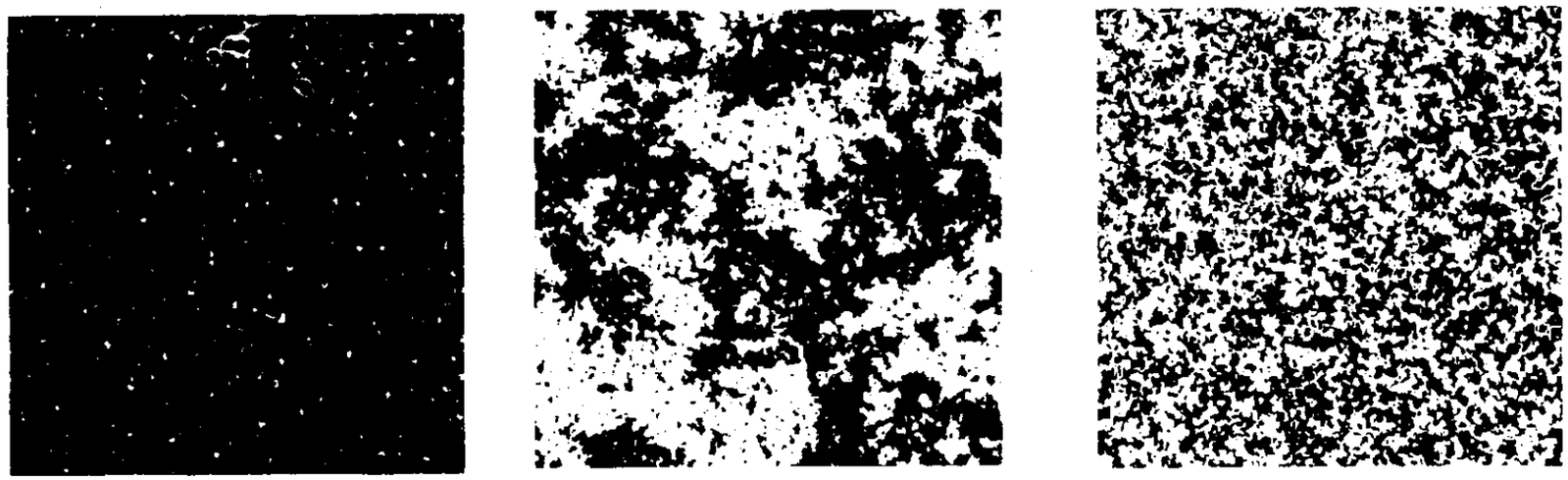


Fig. 4.1 Typical spin configurations for the two-dimensional Ising square lattice: (left) $T \ll T_c$; (center) $T \sim T_c$; (right) $T \gg T_c$.

- Near to critical point the spin is correlated over long distance; fluctuations of all scales
- Near T_c the system forgets most microscopic details. Only remaining details are dimensionality of space and the type of order parameter.
- Concepts and understanding are universal. Apply to all phase transitions of similar type.
- Concepts: Order parameter, correlation length, scaling.

Observations

What does experiment "see"?

- Critical points are temperatures (T), densities (ρ), etc., above which a parameter that describes long-range order, vanishes.
  - e.g., spontaneous magnetization, M(T), of a ferromagnet is zero above T_c.
  - The evidence for such increased correlations was manifest in critical opalescence observed in CO_2 over a hundred years ago by Andrews.

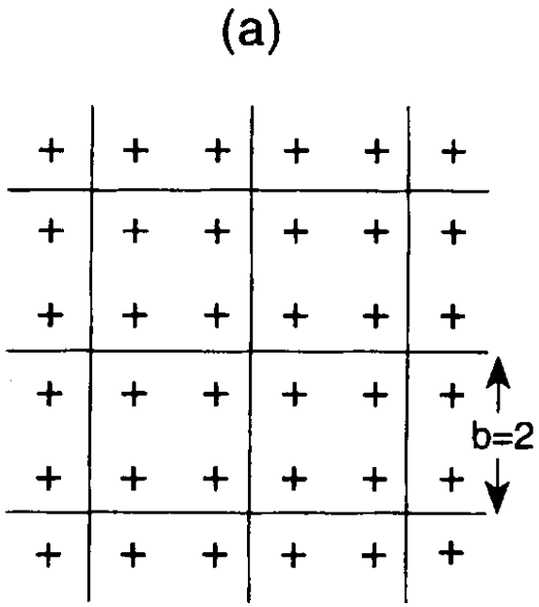
    As the critical point is approached from above, droplets of fluid acquire a size on the order of the wavelength of light, hence scattering light that can be seen with the naked eye!
- Define: Order Parameters that are non-zero below T_c and zero above it.
  - e.g., M(T), of a ferromagnet or $\rho_L - \rho_G$ for a liquid-gas transition.
- Correlation Length ξ is distance over which state variables are correlated.

Near a phase transition you observe:

- Increase density fluctuations, compressibility, and correlations (density-density, spin-spin, etc.).
- Bump in specific heat, caused by fluctuations in the energy

$$C = \left\langle (V - \bar{V})^2 \right\rangle$$

Blocking transformation



$$H_{\text{new}} = \sum_{\alpha} K_\alpha S_\alpha$$

$$S_1 = \sum_{\langle ij \rangle = \text{nn}} \sigma_i \sigma_j$$

$$S_2 = \sum_{\langle ij \rangle = \text{nnn}} \sigma_i \sigma_j$$

- Add 4 spins together and make into one superspin flipping a coin to break ties.
- This maps H into a new H (with more long-ranged interactions)
- $R(H^n)=H^{n+1}$

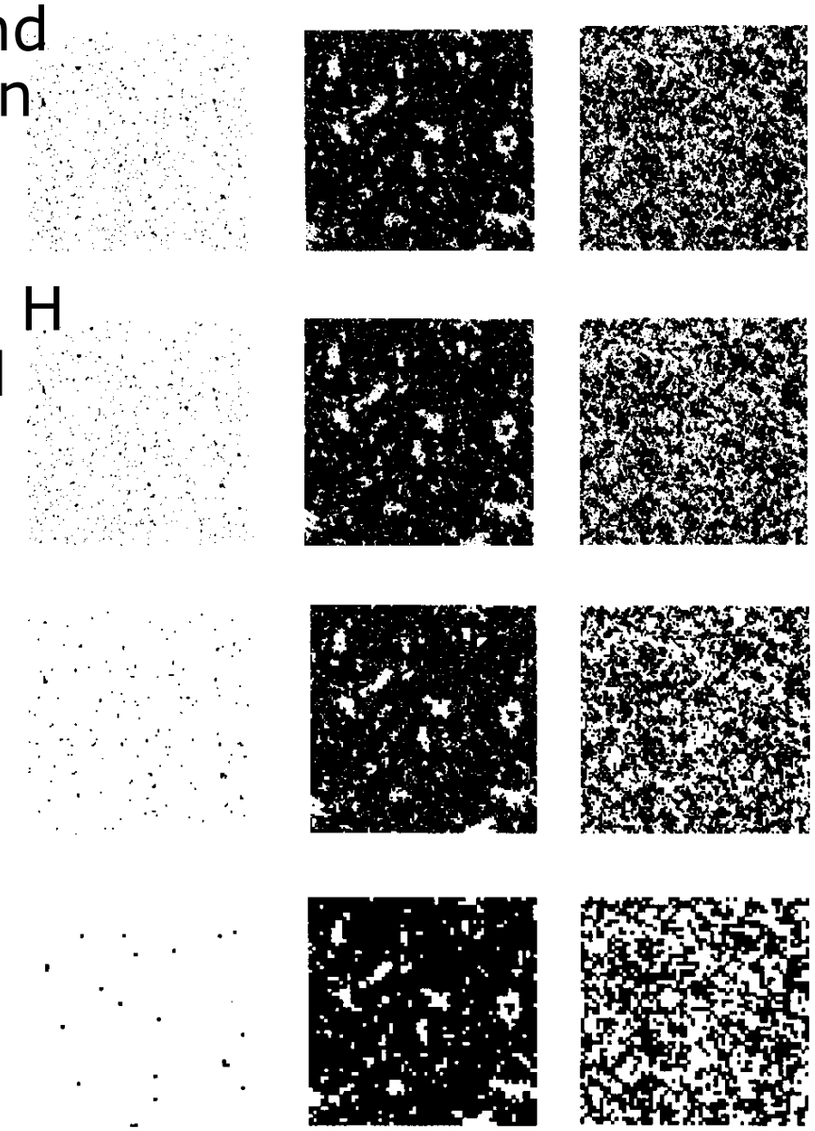


Figure 11. "Snapshots" of the 2-dim Ising model at: (a) $T = 0.9T_c$; (b) $T = T_c$, (c) $T = 1.1T_c$. The upper row shows Monte Carlo generated configurations on a 480×480 lattice with periodic boundaries. Successive rows show the configurations after 2×2 blockspin transformations have been applied and the lattices rescaled to their original size.

- Critical points are fixed points. $R(H^*)=H^*$.
- At a fixed point, pictures look the same!

Renormalization Flow

- Hence there is a flow in H space.
- The fixed points are the critical points.
- Trivial fixed points are at T=0 and T=∞.
- Critical point is a non-trivial unstable fixed point.
- Derivatives of Hamiltonian near fixed point give exponents.

See online notes for simple example of RNG equations for blocking the 2D Ising model

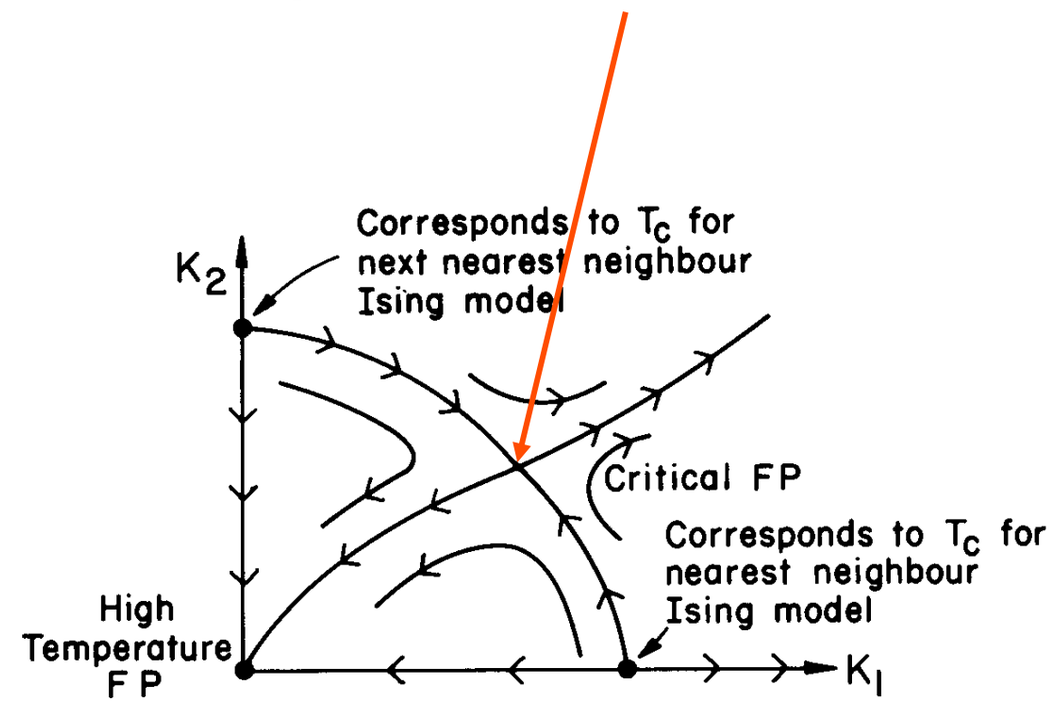


Figure 9.3 Flow diagram for an Ising model with nearest and next nearest neighbour interactions.

Universality

- Hamiltonians fall into a few general classes according to their dimensionality and the symmetry (or dimensionality) of the order parameter.
- Near the critical point, an Ising model behaves *exactly* the same as a classical liquid-gas. It forgets the original H, but only remembers conserved things.
- Exponents, scaling functions are universal
- T_c P_c, … are not (they are dimension-full).
- Pick the most convenient model to calculate exponents
- The blocking rule doesn't matter.
- MCRG: Find temperature such that correlation functions, blocked n and n+1 times are the same. This will determine T_c and exponents.

G. S. Pawley et al., Phys. Rev. B 29, 4030 (1984).

Scaling is a common feature of phase transitions

In fluids,

- A single (universal) curve is found plotting T/T_c vs. ρ/ρ_c .
- A fit to curve reveals that $\rho_c \sim |t|^{\beta}$ (β=0.33).
  - with reduced temperature $|t| = |(T-T_c)/T_c|$
  - For percolation phenomena, $|t| \rightarrow |p| = |(p-p_c)/p_c|$
- Generally, $0.33 \leq \beta \leq 0.37$, e.g., for liquid Helium $\beta = 0.354$.

A similar feature is found for other quantities, e.g., in magnetism:

- Magnetization: $M(T) \sim |t|^{\beta}$ with $0.33 \leq \beta \leq 0.37$.
- Magnetic Susceptibility: $\chi(T) \sim |t|^{-\gamma}$ with $1.3 \leq \gamma \leq 1.4$.
- Correlation Length: $\xi(T) \sim |t|^{-\nu}$ where ν depends on dimension.
- Specific Heat (zero-field): $C(T) \sim |t|^{-\alpha}$ where $\alpha \sim 0.1$

β, γ, ν, and α are called critical exponents.

Exponents

Table 3.1 CRITICAL EXPONENTS FOR THE ISING UNIVERSALITY CLASS

Exponent	Mean Field	Experiment	Ising ($d = 2$)	Ising ($d = 3$)
α	0 (disc.)	0.110 – 0.116	0 (log)	0.110(5)
β	1/2	0.316 – 0.327	1/8	0.325±0.0015
γ	1	1.23 – 1.25	7/4	1.2405±0.0015
δ	3	4.6 – 4.9	15	4.82(4)
ν	1/2	0.625±0.010	1	0.630(2)
η	0	0.016 – 0.06	1/4	0.032±0.003

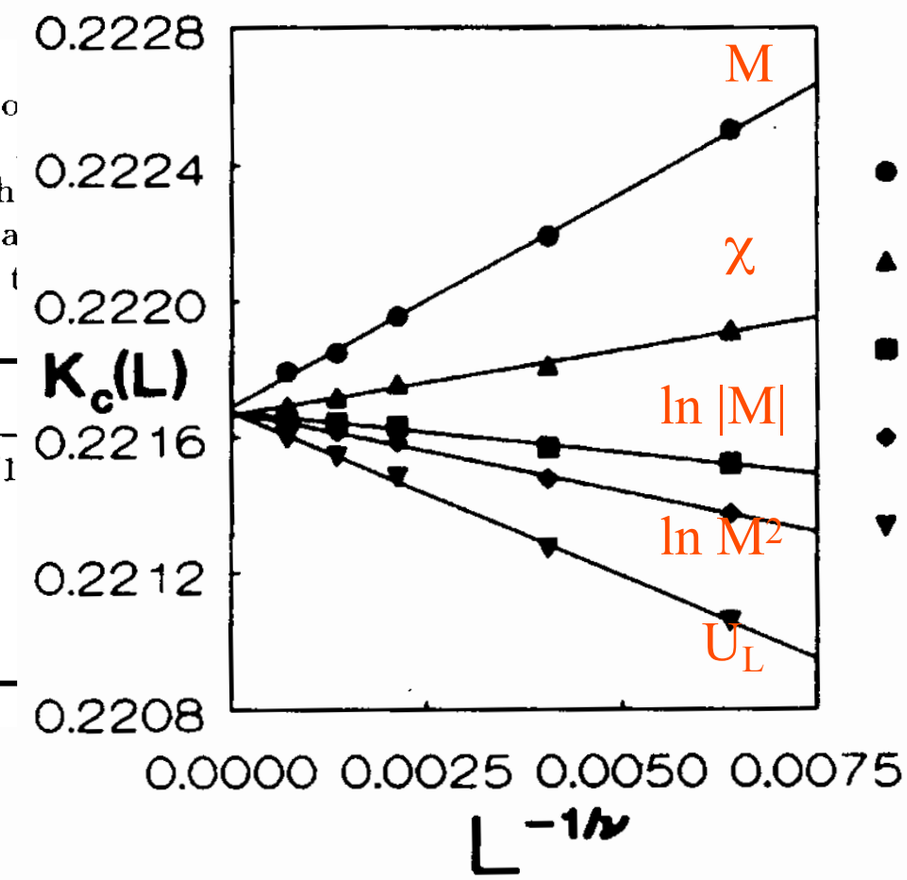
$$\xi = t^{-\nu} \qquad M = t^{\beta}$$

$$\chi = t^{-\gamma} \qquad C = t^{-\alpha}$$

$$t \equiv \left| \frac{T}{T_c} - 1 \right|$$

Table 1. Critical parameters for the n–vector model in $d = 3$ spatial dimensio estimated by recent high–accuracy MC simulations, where $K_c = J/(k_B T_c)$. simulations were performed on the simple cubic lattice except for the last entry wh was done on the body–centered cubic lattice. The second entry has used MCRG a determined $\eta = 0.0262 \pm 0.003$, from which β and γ have been calculated via t scaling laws. Similarly, for the third entry the paper gives $\gamma/\nu = 1.976 \pm 0.006$.

n	Ref.	$L \leq$	K_c	ν	β	γ
1	[40]	96	0.2216595 ± 0.0000026	0.6289 ± 0.0008	0.3258 ± 0.0044	1.2390 ± 0.0071
1	[41]	128	0.221652 ± 0.000004	0.624 ± 0.002	0.320 ± 0.001	1.232 ± 0.006
2	[42]	112	0.45420 ± 0.00002	0.662 ± 0.007	0.339 ± 0.006	1.31 ± 0.02
3	[43]	40	0.693035 ± 0.000037	0.7048 ± 0.003	0.3639 ± 0.0035	1.3873 ± 0.085
3	[43]	40	0.486798 ± 0.000012	(same)	(same)	(same)



Primer for Finite-Size Scaling: Homogeneous Functions

- Function f(r) "scales" if for all values of λ, $f(\lambda r) = g(\lambda) f(r)$

$$f(r) = Br^2 \rightarrow f(\lambda r) = \lambda^2 f(r) \rightarrow g(\lambda) = \lambda^2$$

If we know function at $f(r=r_0)$, then we know it everywhere!

- The scaling function is not arbitrary; it must be $g(\lambda)=\lambda^P$, p=degree of homogeneity.

- A generalized homogeneous function is given by (since you can always rescale by λ^{-P} with a'=a/P and b'=b/P)

$$f(\lambda^a x, \lambda^b y) = \lambda f(x,y)$$

The static scaling hypothesis asserts that G(t,H), the Gibbs free energy, is a homogeneous function.

- Critical exponents are obtained by differentiation, e.g. M=-dG/dH

$$\lambda^{a_H} M(\lambda^{a_t} t, \lambda^{a_H} H) = \lambda M(t,H) \quad at \quad H = 0, \quad M(t,0) = \lambda^{a_H - 1} M(\lambda^{a_t} t, 0)$$

Finite-Size Scaling

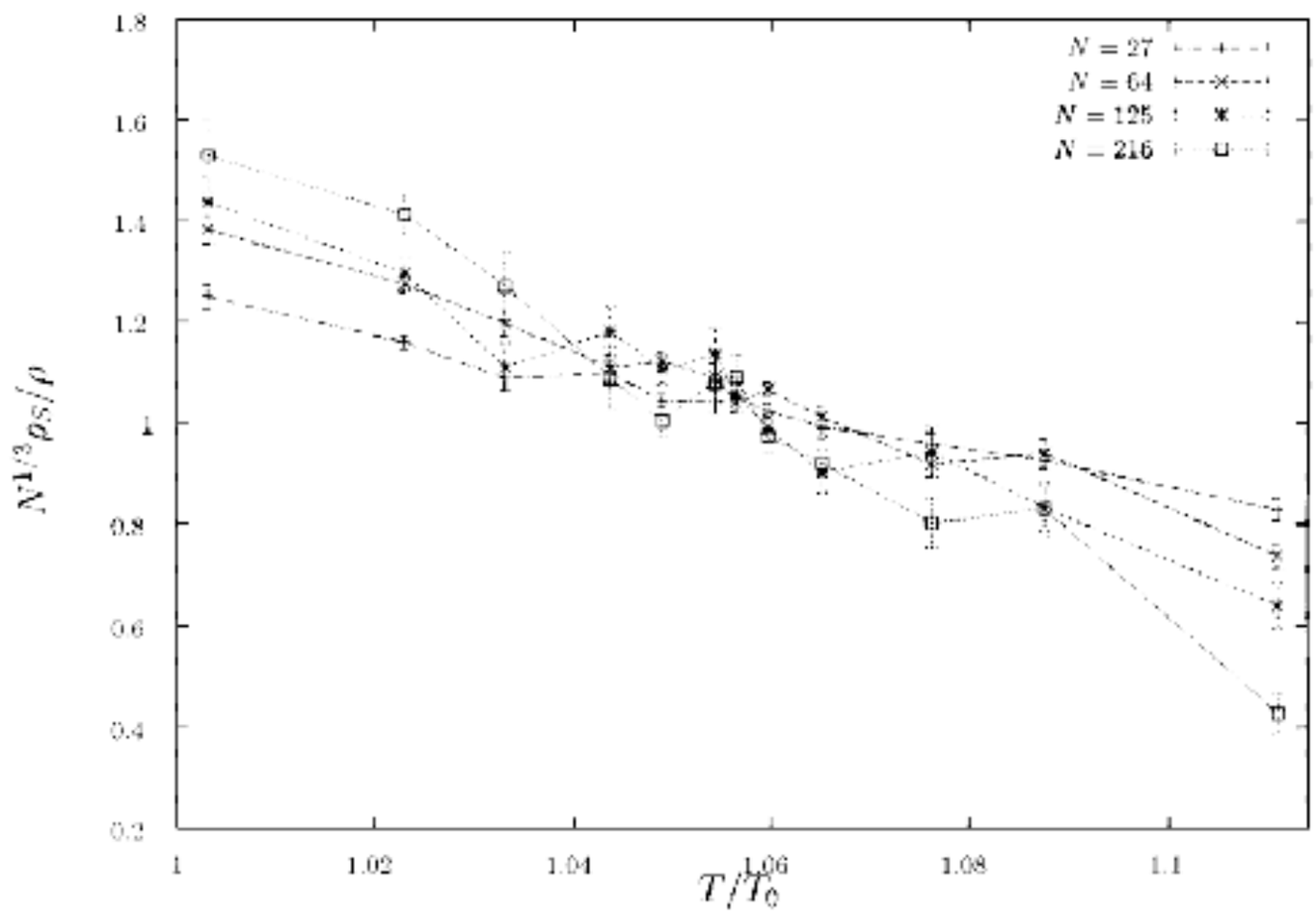
- General technique-not just for the Ising model, but for other continuous transitions.
- Used to:
  - prove existence of phase transition
  - Find exponents
  - Determine T_c etc.
- Assume free energy can be written as a function of correlation length and box size. (dimensional analysis).

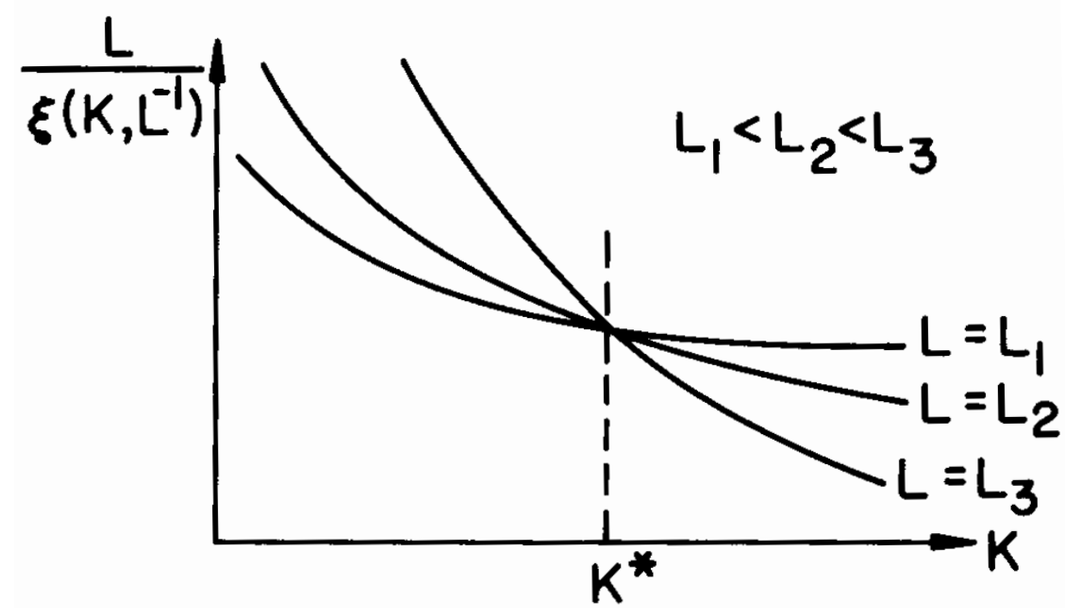
$$F_N = L^{\gamma} f\left(t\, L^{1/\nu}, H\, L^{\beta\delta/\nu}\right),\ t \equiv |1 - T/T_c|$$

- By differentiating we can find scaling of all other quantities
- Do runs in the neighborhood of T_c with a *range of system sizes*.
- **Exploit finite-size effects - don't ignore them.**
- Using scaled variables, put correlation functions on a common graph.
- How to scale the variables (exponent) depends on the transition in question. Do we assume we know the exponent or do we calculate it?

Correlation Length

- Near a phase transition a single length characterizes the correlations
- The length diverges at the transition but is cutoff by the size of the simulation cell.
- All curves will cross at T_c; we use to determine T_c.

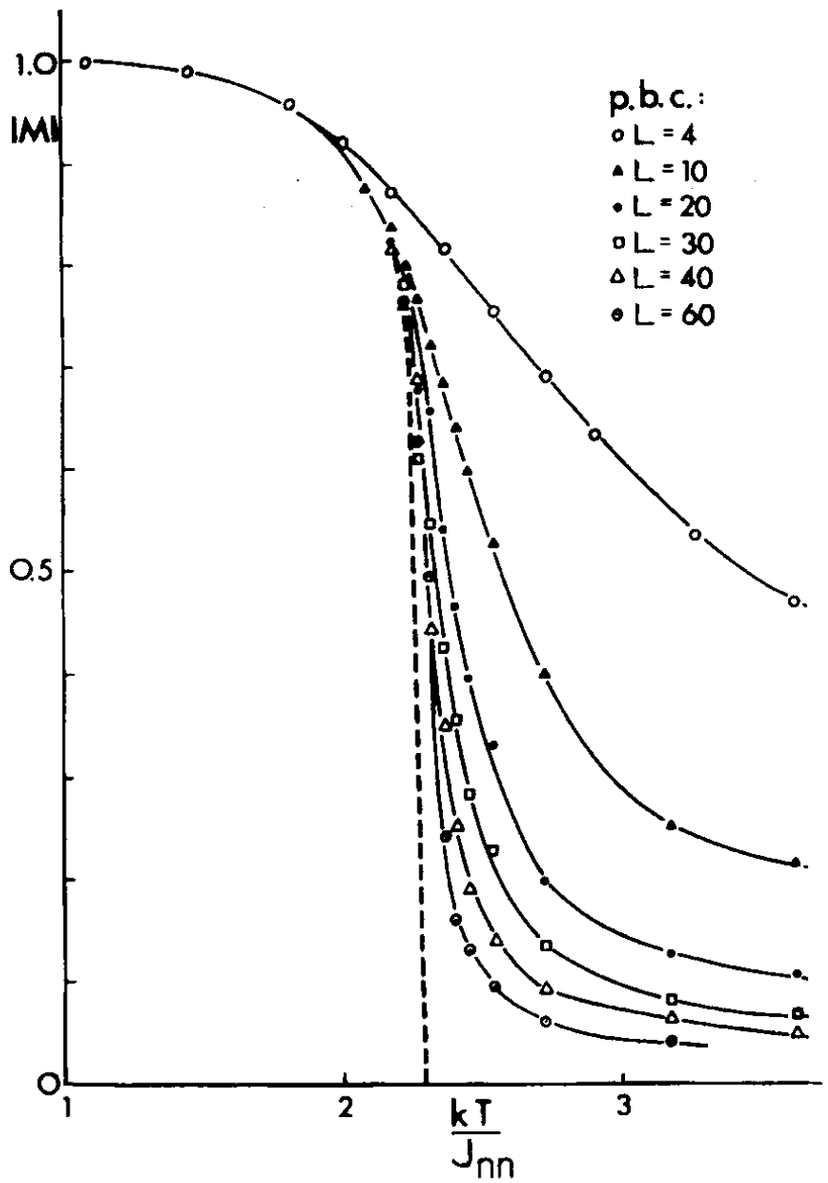


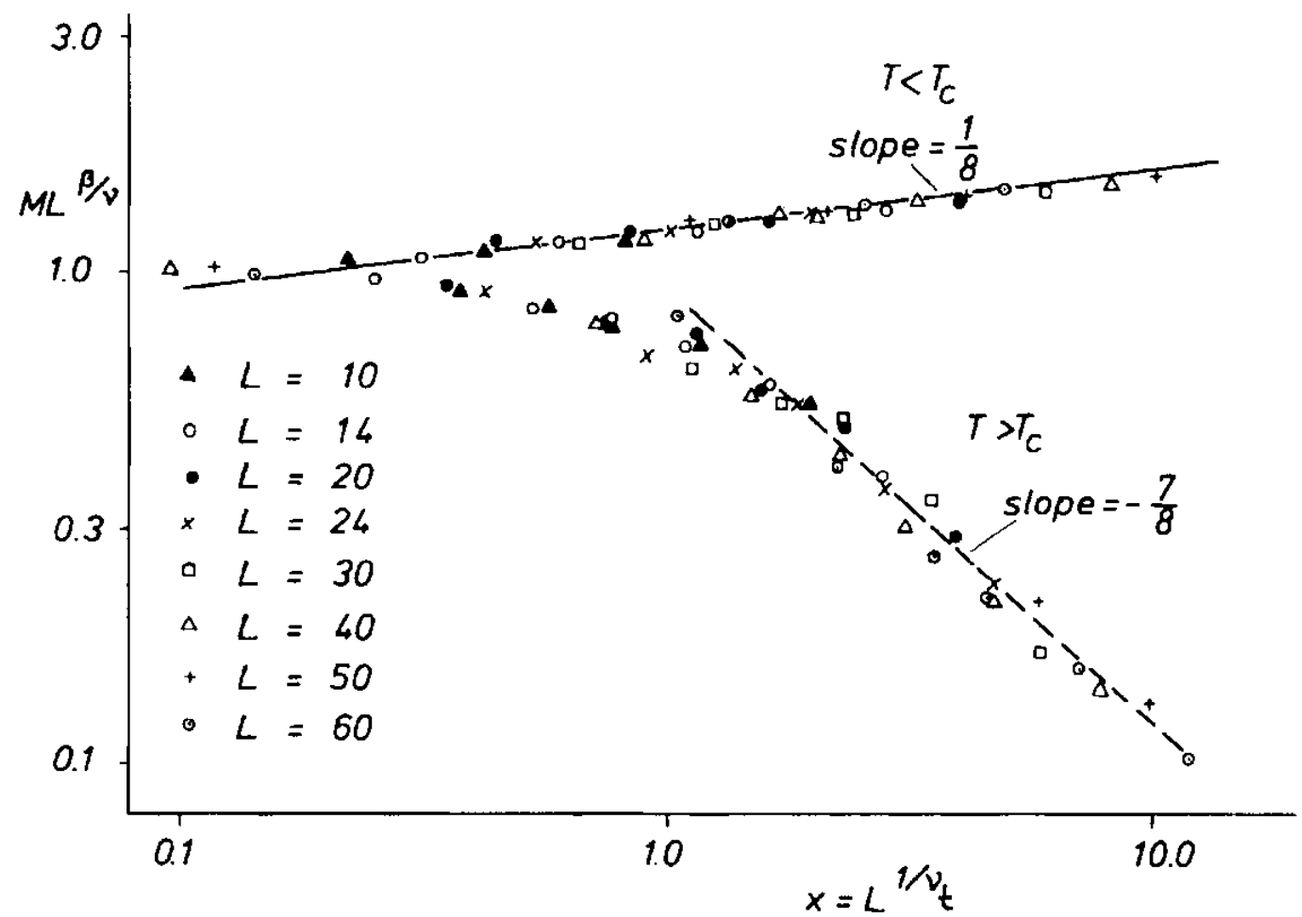


Finite size scaling of the correlation length.

Scaling example

- Magnetization of 2D Ising model
- After scaling *data falls onto two curves*
  - above T_c and below T_c.





Magnetization probability

- How does magnetization vary across transition?
- And with the system size?

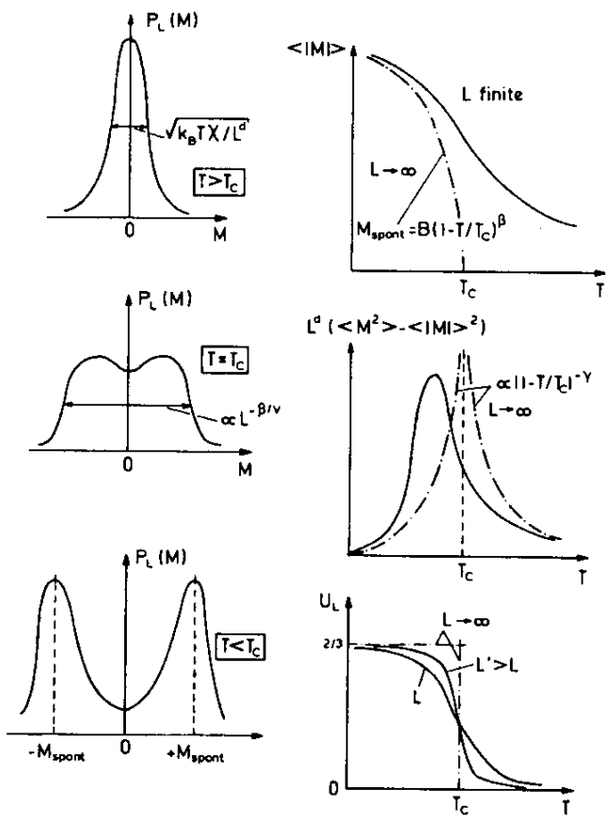


Figure 3. Schematic variation of the probability distribution $P_L(m)$ to find a magnetization m in a finite system of linear dimension L from $T > T_c$ to $T < T_c$ (left part) and the associated temperature variation of the average order parameter $< |m| >$, "susceptibility" $k_B T\chi' = L^d(< m^2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

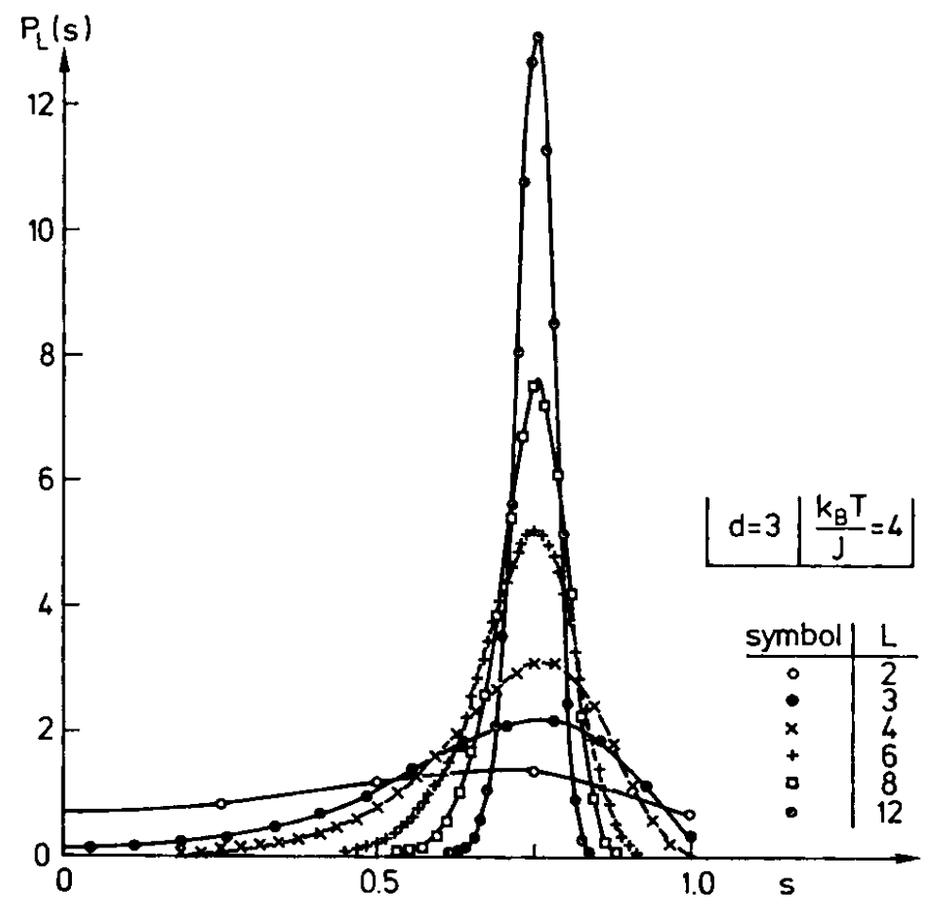


Figure 2. Probability distribution $P_L(s)$ of the magnetization s per spin of $L \times L \times L$ subsystems of a simple cubic Ising lattice with $N = 24^3$ spins and periodic boundary conditions for zero magnetic field and temperature $k_B T/J = 4.0$ (note that the critical temperature occurs at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

Fourth-order moment

- Look at cumulants of the magnetization distribution
- Fourth order moment is the kurtosis (or bulging)
- When they change scaling that is determination of T_c.
- A Gaussian distribution has $U_4=0$. what about the central limit theorem?

Binder 4th-order Cumulant

$$U_4 = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$$

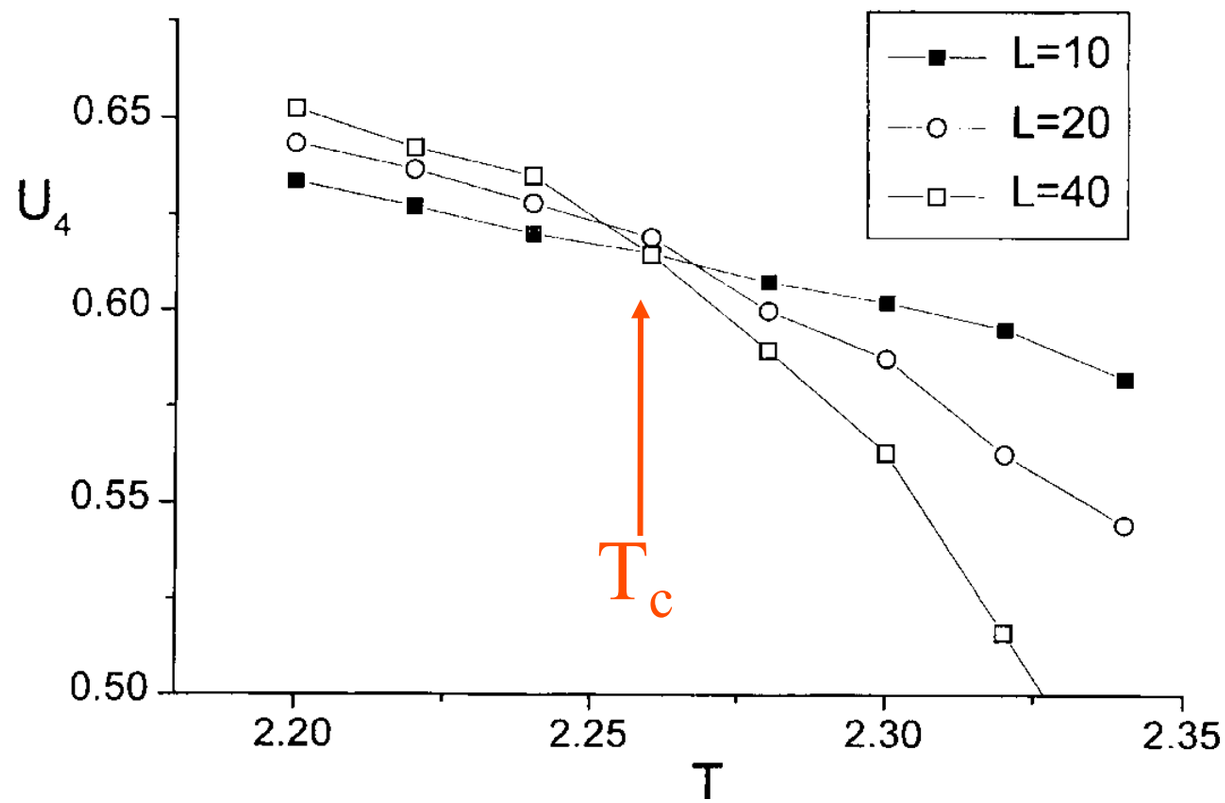


Fig. 4.5 Temperature dependence of the fourth order cumulant for $L \times L$ Ising square lattices with periodic boundary conditions.

First-order transitions

- Previous theory was for *second-order transitions*
- **For first-order, there is no divergence but hysteresis**.

  EXAMPLE: Change H in the Ising model.
- **Surface effects dominate** (boundaries between the two phases) and nucleation times (metastablity).

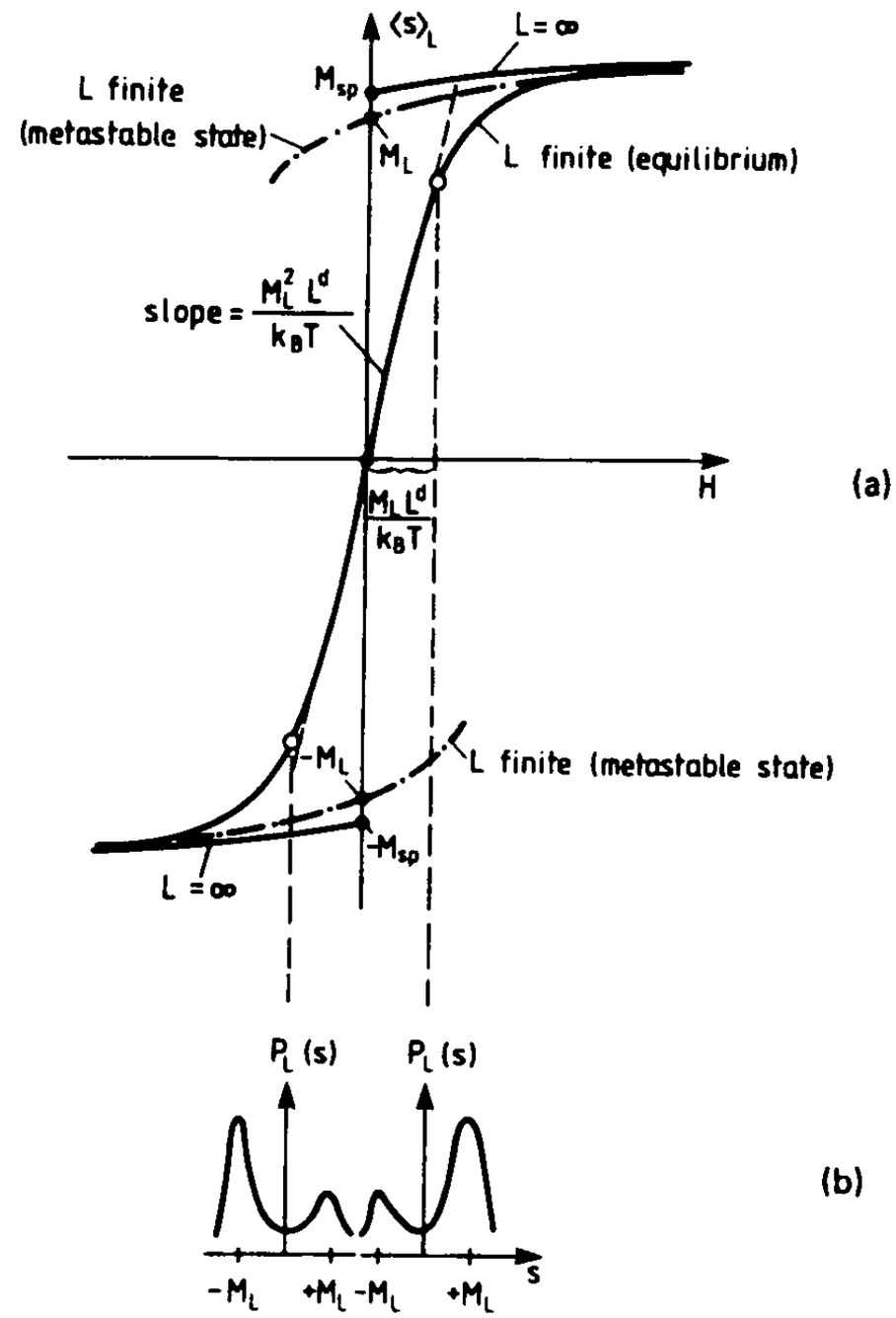


Fig. 4.6 Variation of the magnetization in a finite ferromagnet with magnetic field H. The curves include the infinite lattice behavior, the equilibrium behavior for a finite lattice, and the behavior when the system is only given enough time to relax to a metastable state. From Binder and Landau (1984).