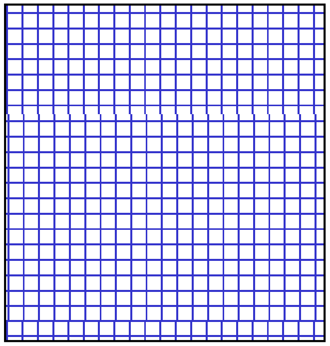
# Phase transitions and finite-size scaling

- 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

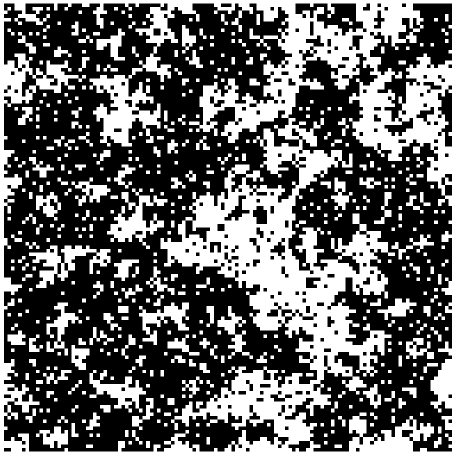


- Suppose we have a lattice, with $L^2$ lattice sites and connections between them. (e.g. a square lattice).
- On each lattice site, is a single spin variable: $s_i = \pm 1$.
- With mag. field h, energy is:

$$H = -\sum_{i=1}^{N} h s_i - \sum_{(i,j)} J s_i s_j$$

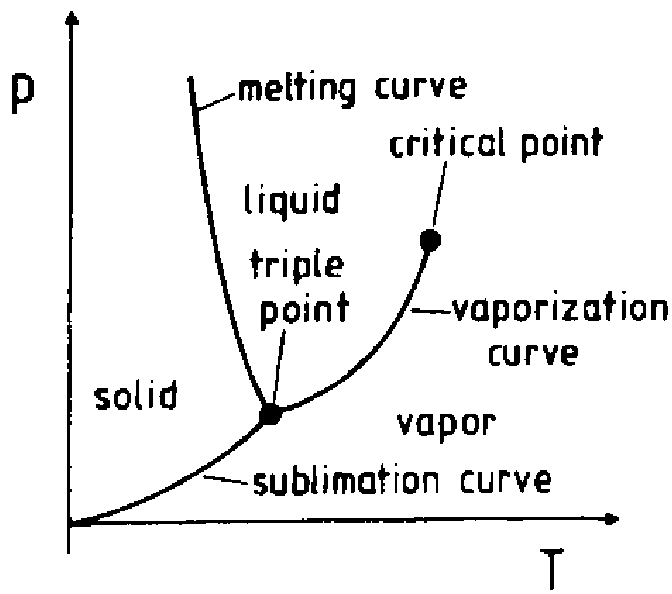
$$Z = \sum_{s_i = \pm 1} e^{-\beta H}$$

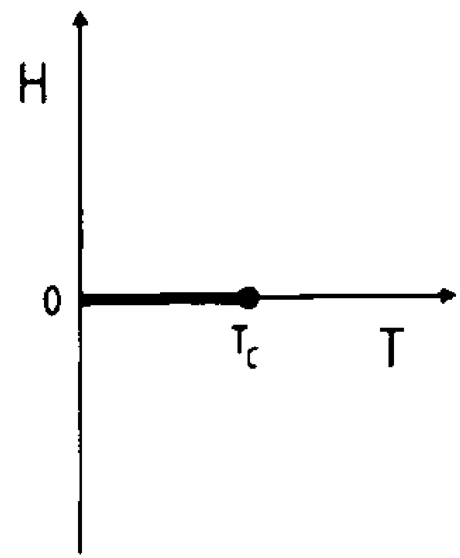
- J is the coupling between nearest neighbors (i,j)
  - J>0 ferromagnetic
  - J<0 antiferromagnetic.



# 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 $\Delta E$ 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

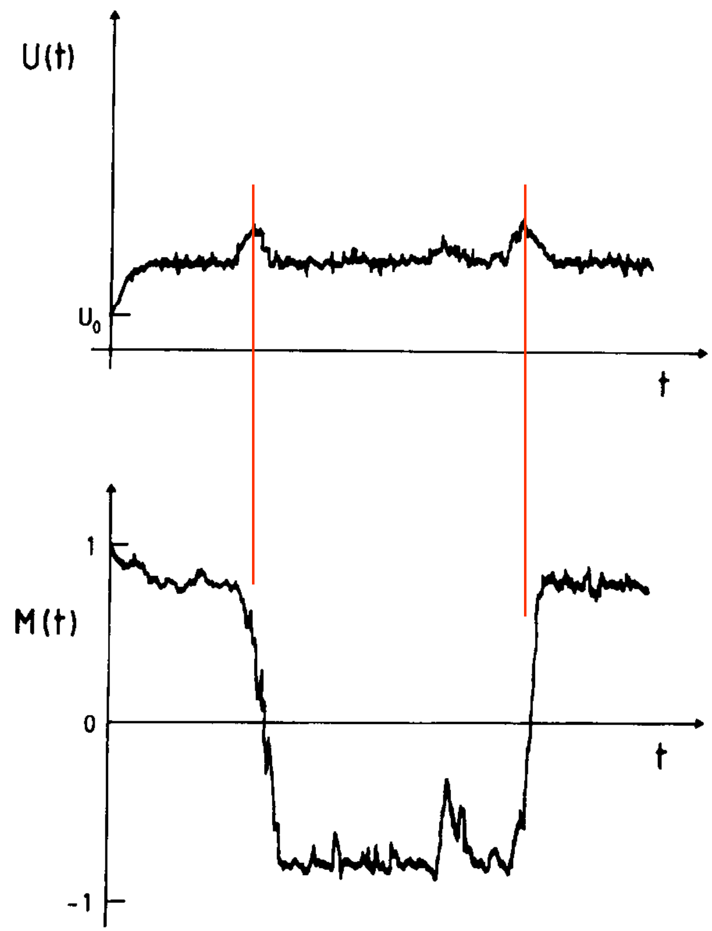



Fig. 4.2 Schematic variation of internal energy and spontaneous magnetization with time for a Monte Carlo simulation of an Ising square lattice in zero field.

# Dynamical Exponent

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

$$\textit{With} \quad \tau_O = \text{correlation time}$$
$$\textit{and} \quad \xi = \text{correlation length}$$

$$\zeta = \left(\mathrm{var}(O)\tau_O \,\text{time/step}\right)^{-1}$$
$$\tau_O \propto \xi^2 / D$$
$$\text{near } T_c \quad \xi \to \mathrm{L} \quad \Rightarrow \quad \tau \to L^2$$
$$\tau \propto L^z$$

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

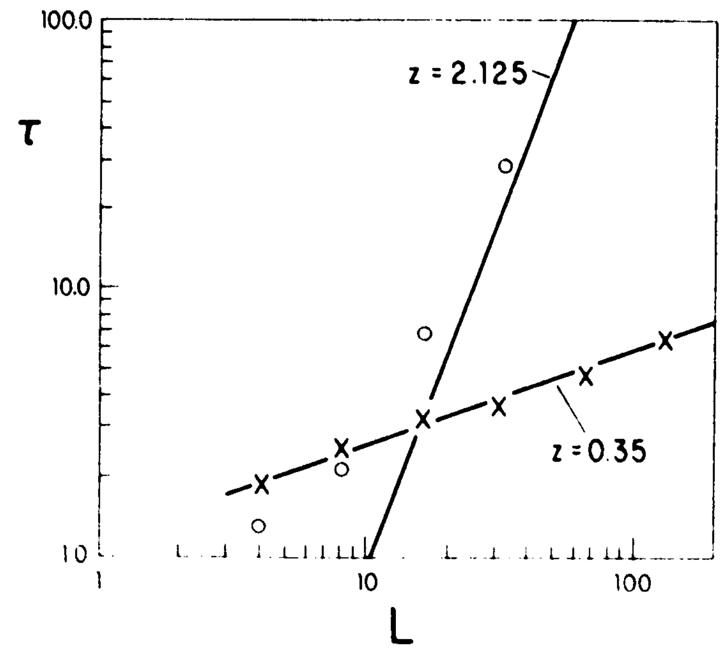



FIG. 1. Log-log plots of correlation times for Monte Carlo simulations of the two-dimensional Ising model at the critical temperature as a function of the linear dimension $L$. The circles show data for a standard Monte Carlo simulation, and the line marked “$z = 2.125$” gives the expected asymptotic 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-Wang algorithm

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

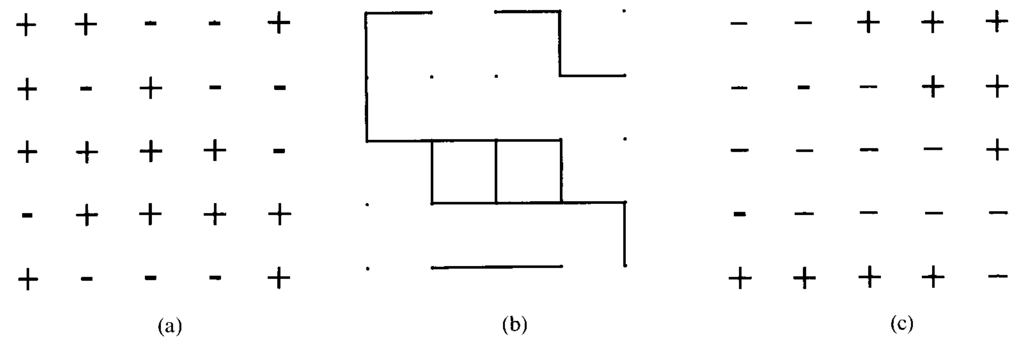



Fig. 5.1 Schematic view of the Swendsen–Wang algorithm for an Ising model: (a) original spin configuration; (b) clusters formed; (c) 'decorated' clusters.

**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)

**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)

Little critical slowing down at the critical point.

Non-local algorithm.

# 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

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

$$p \equiv 1 - e^{-2J/kT}$$

*How can we extend to other models?*

$$Tr_n\left\{\Pi(\sigma,n)\right\} = \frac{1}{Z}e^{K\sum_{\langle i,j\rangle}\left(\delta_{\sigma_i-\sigma_j}-1\right)}$$

# RNG Theory of phase transitions

K. G. Wilson 1971

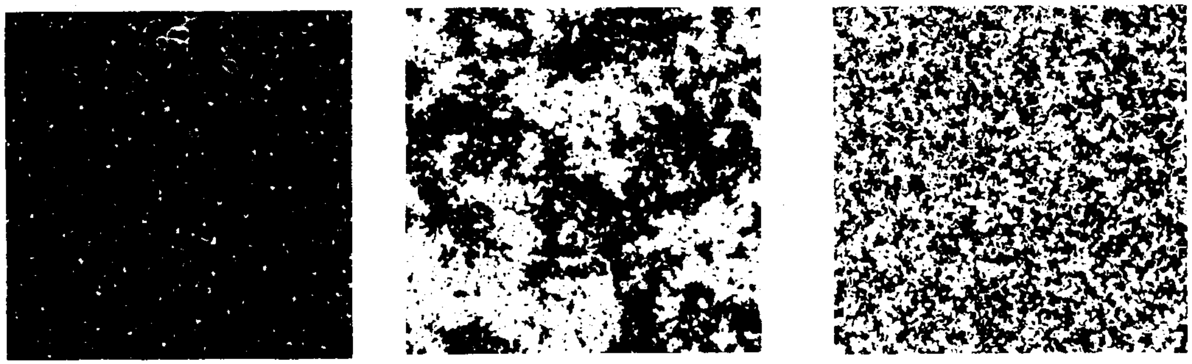


Fig. 4.1 Typical spin configurations for the two-dimensional Ising square lattice: (left) $T \ll T_c$; (center) $T \sim T_c$; (right) $T \gg T_c$.

- 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"?

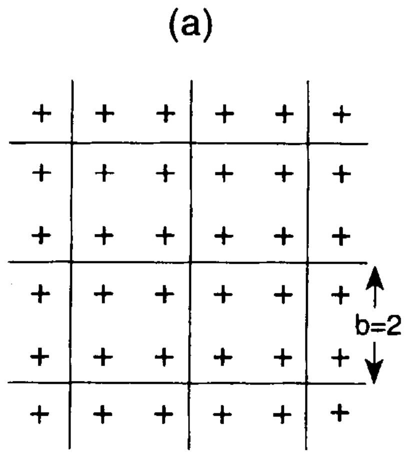
- **Critical points** are temperatures (T), densities (ρ), etc., above which a parameter that describes *long-range order*, vanishes.
  - e.g., spontaneous magnetization, M(T), of a ferromagnet is zero above $T_c$.
  - The evidence for such increased *correlations* was manifest in *critical opalescence* 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 $C = \left\langle \left(V - \bar{V}\right)^2 \right\rangle$

# Blocking transformation




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

$$S_1 = \sum_{\langle i,j \rangle = nn} \sigma_i \sigma_j$$

$$S_2 = \sum_{\langle i,j \rangle = nnn} \sigma_i \sigma_j$$

- 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)
- $R(H^n)=H^{n+1}$

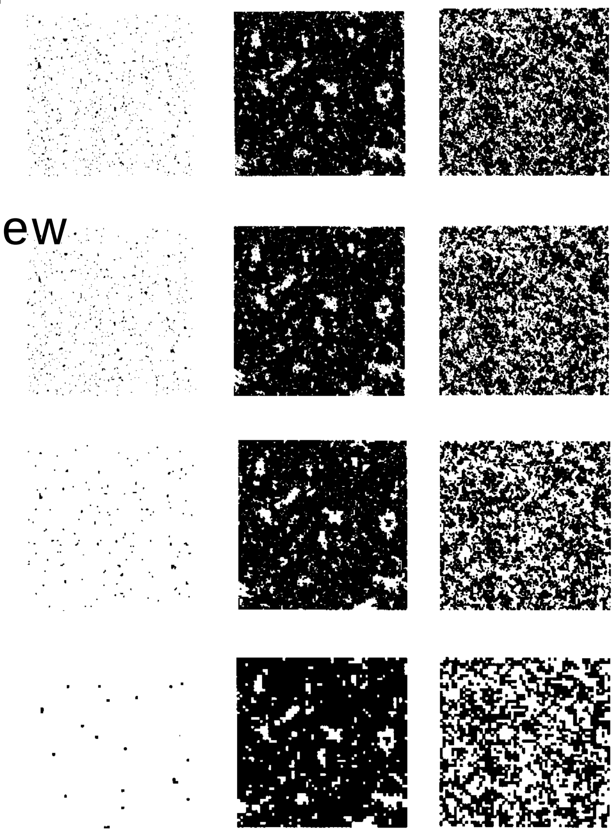


**Figure 11.** "Snapshots" of the 2-dim Ising model at: (a) $T = 0.9T_c$; (b) $T = T_c$, (c) $T = 1.1T_c$. The upper row shows Monte Carlo generated configurations on a $480 \times 480$ lattice with periodic boundaries. Successive rows show the configurations after $2 \times 2$ blockspin transformations 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

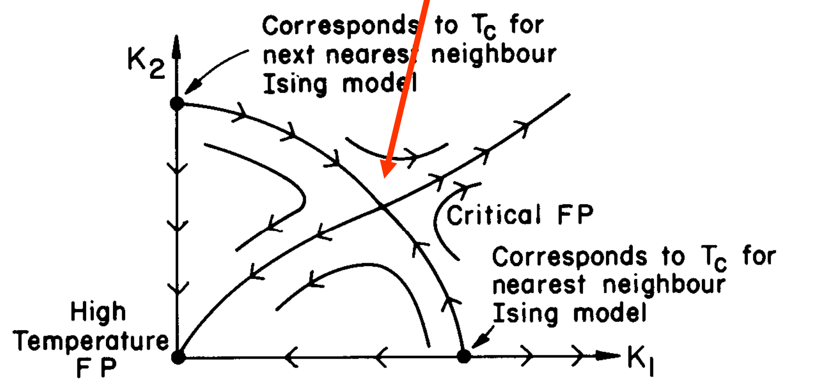



**Figure 9.3** Flow diagram for an Ising model with nearest and next nearest neighbour interactions.

# 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 an important feature of phase transitions

*In fluids,*

- A single (universal) curve is found plotting $T/T_c$ vs. $\rho/\rho_c$ .
- A fit to curve reveals that $\rho_c \sim |t|^\beta$ ($\beta$=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 $\nu$ depends on dimension.
- Specific Heat (zero-field): $C(T) \sim |t|^{-\alpha}$ where $\alpha \sim 0.1$

$\beta$, $\gamma$, $\nu$, and $\alpha$ are called critical exponents.

# Exponents

**Table 3.1 CRITICAL EXPONENTS FOR THE ISING UNIVERSALITY CLASS**

| Exponent | Mean Field | Experiment | Ising ($d = 2$) | Ising ($d = 3$) |
|---|---|---|---|---|
| $\alpha$ | 0 (disc.) | 0.110 – 0.116 | 0 (log) | 0.110(5) |
| $\beta$ | 1/2 | 0.316 – 0.327 | 1/8 | 0.325±0.0015 |
| $\gamma$ | 1 | 1.23 – 1.25 | 7/4 | 1.2405±0.0015 |
| $\delta$ | 3 | 4.6 – 4.9 | 15 | 4.82(4) |
| $\nu$ | 1/2 | 0.625±0.010 | 1 | 0.630(2) |
| $\eta$ | 0 | 0.016 – 0.06 | 1/4 | 0.032±0.003 |

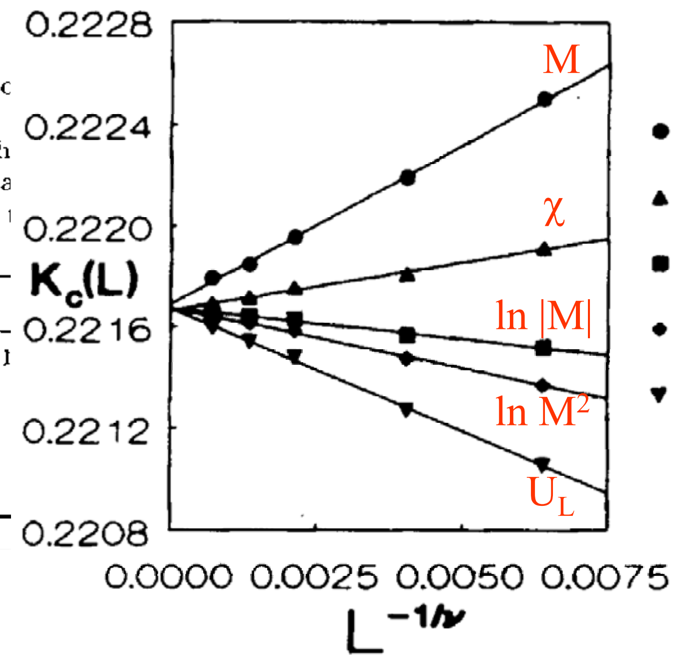
$$\xi = t^{-\nu} \qquad M = t^{\beta}$$

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

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

Table 1. Critical parameters for the $n$-vector model in $d = 3$ spatial dimensic 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 $\beta$ and $\gamma$ have been calculated via t scaling laws. Similarly, for the third entry the paper gives $\gamma/\nu = 1.976 \pm 0.006$.

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



# Primer for Finite-Size Scaling: Homogeneous Functions

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

$$e.g., \quad f(r) = Br^2 \rightarrow f(\lambda r) = \lambda^2 f(r) \rightarrow g(\lambda) = \lambda^2$$

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 $\lambda^{-P}$ 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).

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

- 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 exponent or calculate it?

# Heuristic Arguments for Scaling

**Scaling is revealed from the behavior of the correlation length.**

With reduced temperature $|t| = |(T-T_c)/T_c|$, **why does $\xi(T) \sim |t|^{-\nu}$ ?**

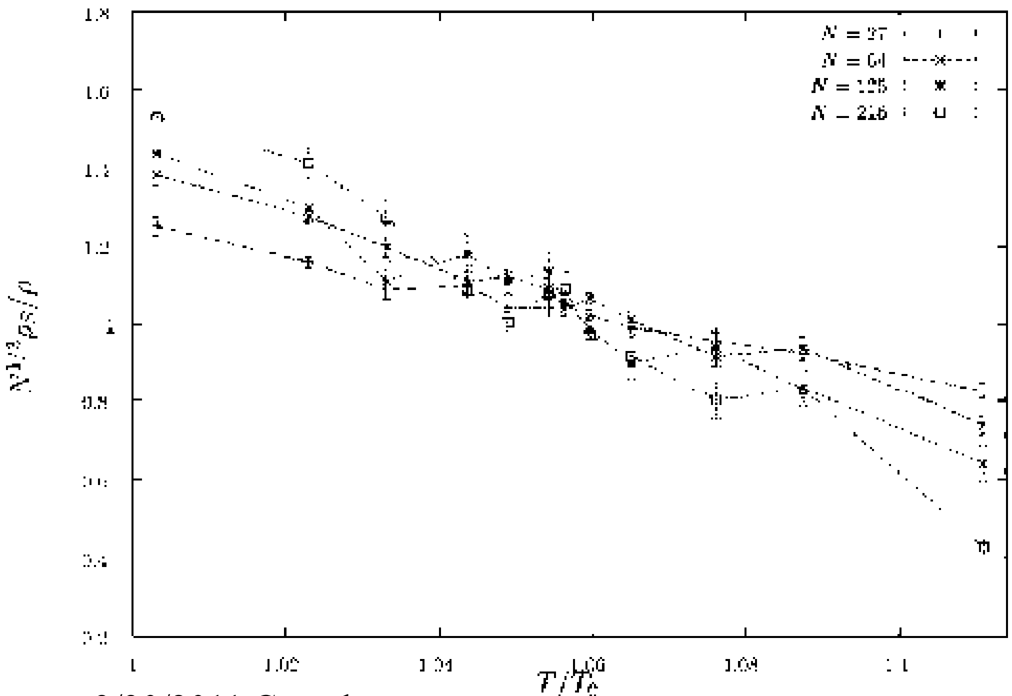
- If **$\xi(T) \ll L$, power law behavior** is expected because the correlations are local and do not exceed L.
- If **$\xi(T) \sim L$,** then $\xi$ **cannot change appreciable** and $M(T) \sim |t|^{\beta}$ is no longer expected. power law behavior.
- For **$\xi(T) \sim L \sim |t|^{-\nu}$**, a quantitative change occurs in the system.

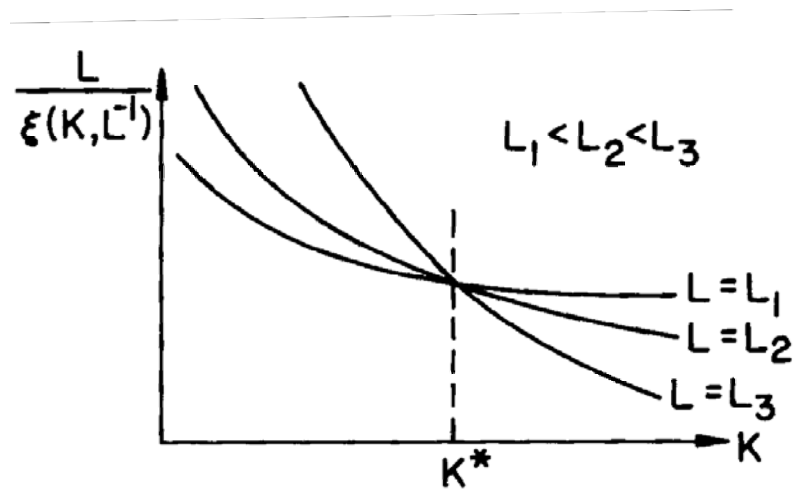
Thus, $|\mathbf{t}| \sim |\mathbf{T}-\mathbf{T_c}(\mathbf{L})| \sim \mathbf{L}^{-1/\nu}$, giving a scaling relation for $T_c$.

***For 2-D square lattice*, $\upsilon$=1. Thus, $T_c(L)$ should scale as 1/L!**
Extrapolating to $L=\infty$ the $T_c(L)$ obtained from the $C_v(T)$.

# 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 $T_c$.

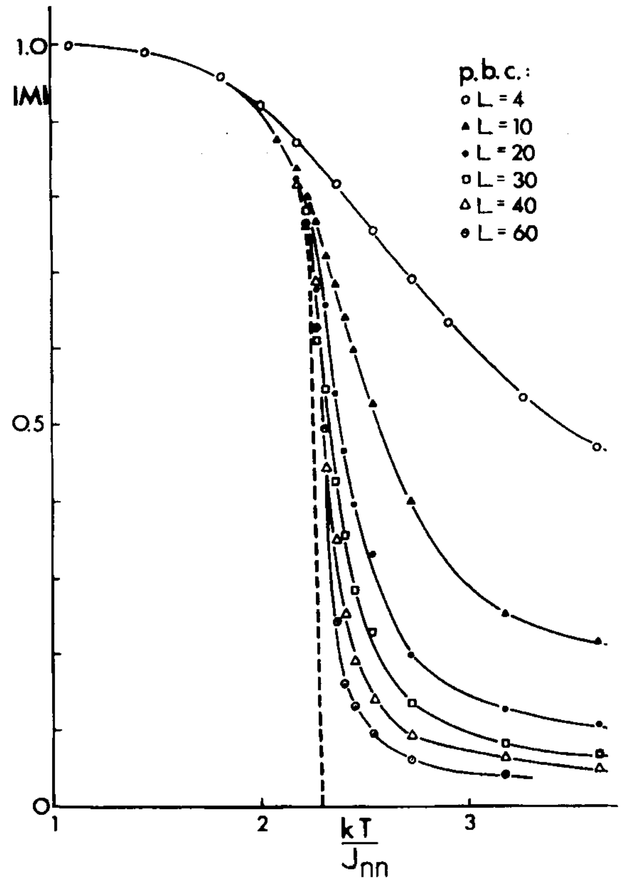


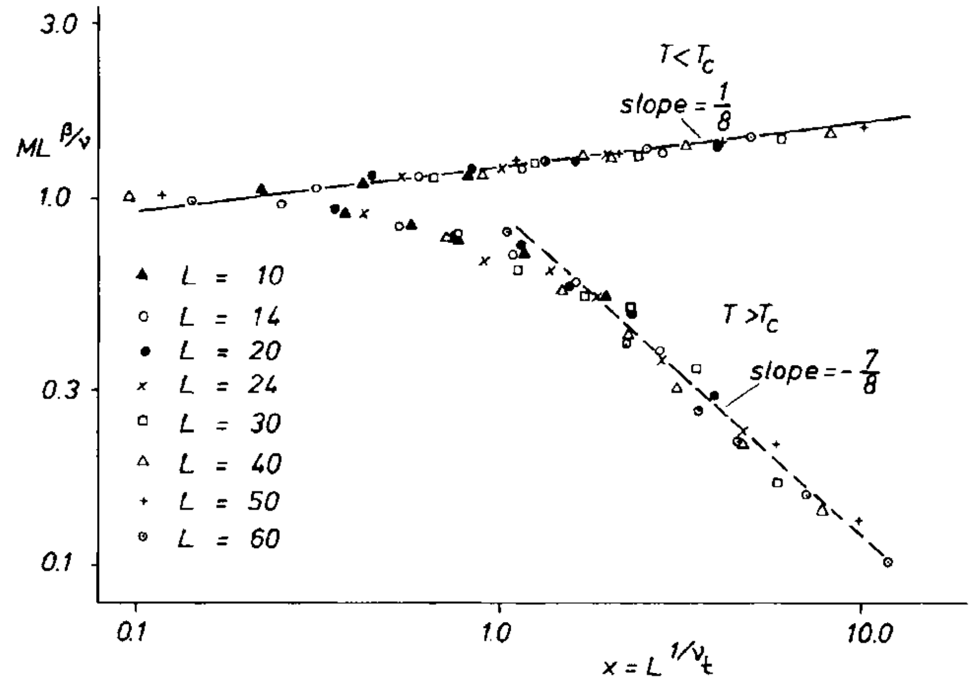




Finite size scaling of the correlation length.

# 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?

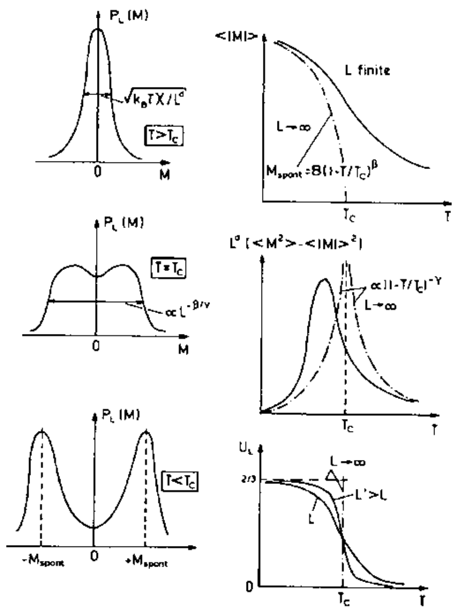


**Figure 3.** Schematic variation of the probability distribution $P_L(m)$ to find a magnetization $m$ in a finite system of linear dimension $L$ from $T > T_c$ to $T < T_c$ (left part) and the associated temperature variation of the average order parameter $< |m| >$, "susceptibility" $k_B T \chi' =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

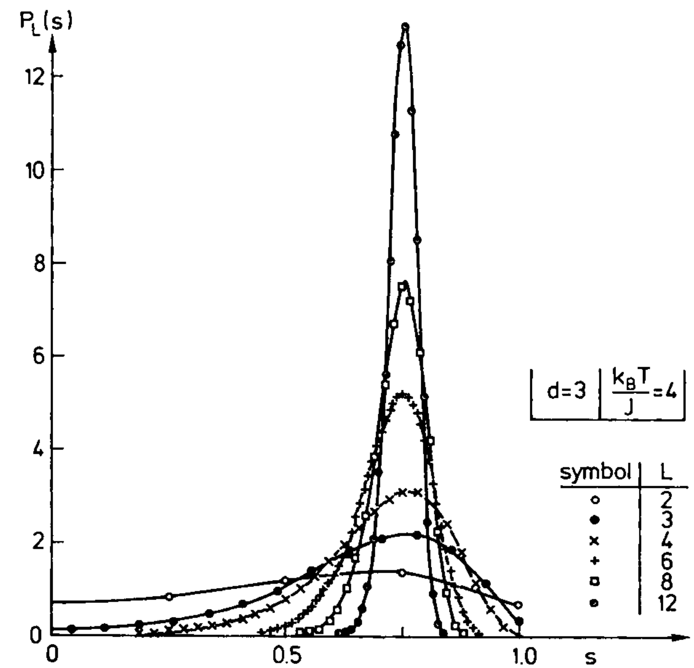



**Figure 2.** Probability distribution $P_L(s)$ of the magnetization $s$ per spin of $L \times L \times L$ subsystems of a simple cubic Ising lattice with $N = 24^3$ spins and periodic boundary conditions for zero magnetic field and temperature $k_B T/J = 4.0$ (note that the critical temperature occurs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

Binder 4th-order Cumulant

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

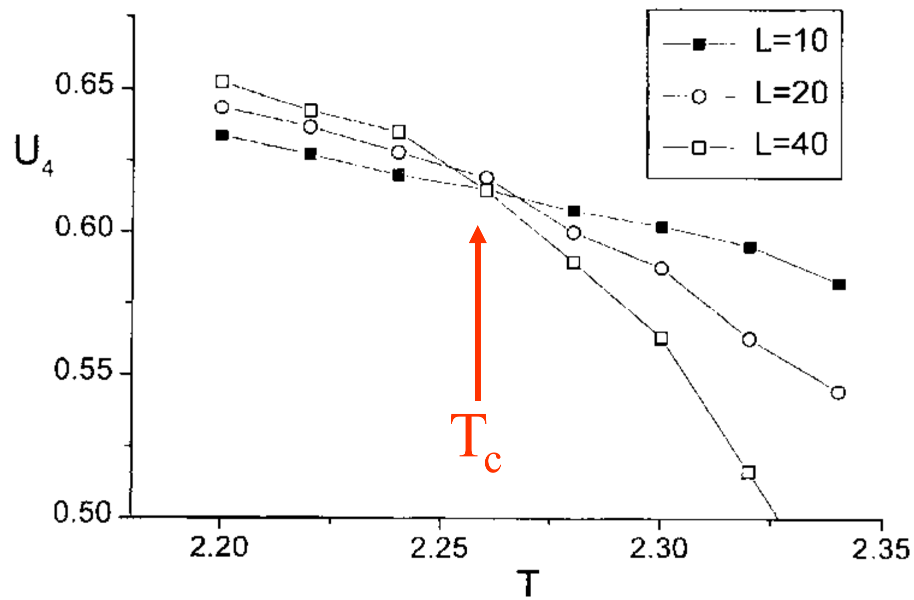



Fig. 4.5 Temperature dependence of the fourth order cumulant for $L \times L$ Ising square lattices with periodic boundary conditions.

# 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).

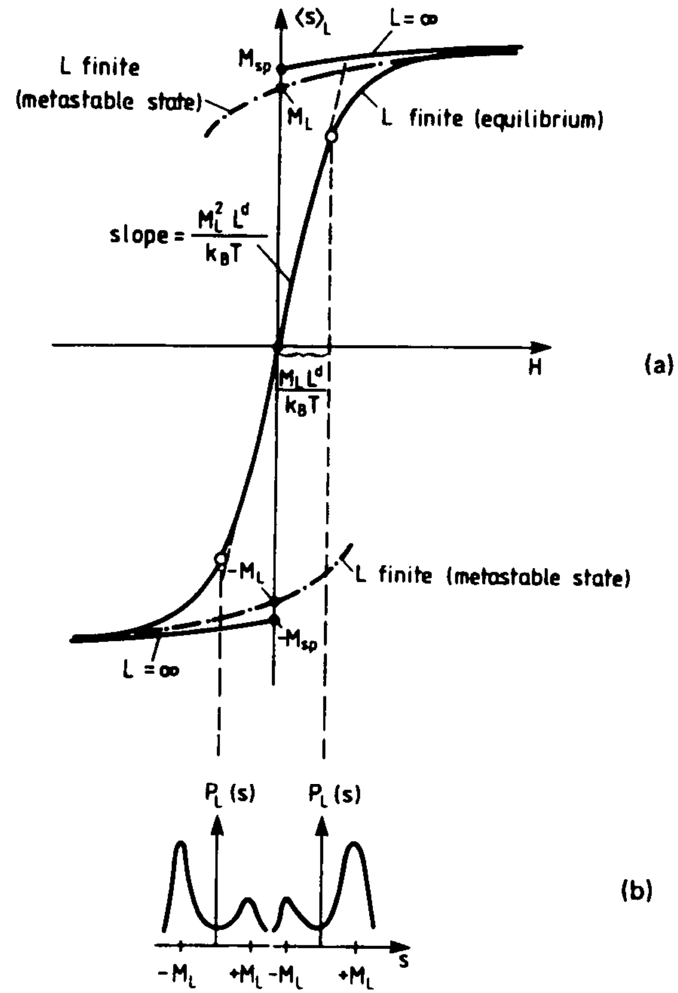



Fig. 4.6 Variation of the magnetization in a finite ferromagnet with magnetic field $H$. The curves include the infinite lattice behavior, the equilibrium behavior for a finite lattice, and the behavior when the system is only given enough time to relax to a metastable state. From Binder and Landau (1984).