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:

\[ H = -\sum_{i=1}^{N} hs_i - \sum_{(i,j)} J s_i s_j \]

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

• $J$ 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 $\sim T_c$.
- 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 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.
Monte Carlo efficiency is governed by a critical dynamical exponent $Z$.

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

$$\zeta = \left( \text{var}(O) \tau_O \text{time/step} \right)^{-1}$$

$$\tau_O \propto \frac{\xi^2}{D}$$

near $T_c$, $\xi \rightarrow L \Rightarrow \tau \rightarrow L^2$

$$\tau \propto L^z$$

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

3/30/2011 Ceperley
Swendsen-Wang algorithm

Little critical slowing down at the critical point.

Non-local algorithm.

3/30/2011 Ceperley
Correctness of cluster algorithm

- Cluster algorithm:
  - Transform from spin space to bond space $\Pi_{ij}$
    (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

How can we extend to other models?

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

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

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

3/30/2011 Ceperley
RNG Theory of phase transitions

K. G. Wilson 1971

- 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 ($\rho$), 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** $\xi$ 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 $C = \langle (V - \overline{V})^2 \rangle$
Blocking transformation

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

Critical points are fixed points.
$R(H^*) = H^*$.

At a fixed point, pictures look the same!

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.
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 $T=\infty$.
- 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.
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.

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

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

$\xi = t^{-\nu}$  \hspace{1cm} $M = t^\beta$

$\chi = t^{-\gamma}$  \hspace{1cm} $C = t^{-\alpha}$

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

Table 1. Critical parameters for the $\nu$-vector model in $d = 3$ spatial dimension 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 which was done on the body-centered cubic lattice. The second entry has used MCHG $\eta$ determined $\eta = 0.026\pm 0.003$, from which $\beta$ and $\gamma$ have been calculated via scaling laws. Similarly, for the third entry the paper gives $\gamma/\nu = 1.976 \pm 0.006$.

\begin{tabular}{cccccc}
\hline
$n$ & Ref. & $L \leq K_c$ & $\nu$ & $\beta$ & $\gamma$ \\
\hline
1 & [40] & 96 & 0.2216895 \pm 0.0000026 & 0.6289 \pm 0.0008 & 0.3258 \pm 0.0044 & 1.2989 \pm 0.0071 \\
1 & [41] & 128 & 0.221662 \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) \\
\hline
\end{tabular}

3/30/2011 Ceperley
Primer for Finite-Size Scaling: Homogeneous Functions

- Function $f(r)$ “scales” if for all values of $\lambda$, $f(\lambda r) = g(\lambda)f(r)$
  
  e.g., $f(r) = Br^2 \rightarrow f(\lambda r) = \lambda^2 f(r) \rightarrow g(\lambda) = \lambda^2$
  
  If we know function at $f(r=r_0)$, then we know it everywhere!

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

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

  $$f(\lambda^ax, \lambda^by) = \lambda f(x, y)$$

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. $M = -dG/dH$

  $$\lambda^a M(\lambda^at, \lambda^aH) = \lambda M(t, H) \text{ at } H = 0, \quad M(t, 0) = \lambda^{a_H-1}M(\lambda^a t, 0)$$
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).

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

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

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

3/30/2011 Ceperley
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 $T_c$.  

3/30/2011 Ceperley
Magnetization probability

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

**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 \( k_B T_c / J \approx 4.51 \) [20].

**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 \( \langle |m| \rangle \), "susceptibility" \( k_B T \chi' = L^4 \langle m^4 \rangle - \langle |m| \rangle^2 \) and reduced fourth order cumulant \( U_L = 1 - \langle m^4 \rangle / [3 \langle m^2 \rangle^2 ] \) (right part).
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 $T_c$.

Binder 4th-order Cumulant

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

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 (metastability).

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).