Ising model and phase transitions.

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This lecture follows D. Chandler: Introduction to modern statistical mechanics.

If you find a mistake, kindly report it to the author :-}
The Ising model

• Magnetic spins on a lattice, two states: $s = \pm 1$

• Total energy of state $\nu$:

$$E_{\nu} = - \sum_{j=1}^{N} H \mu s_j + J \sum_{i,j}^{'} s_i s_j$$

• Nearest neighbour interactions

• Coupling constant $J > 0$ \(\Rightarrow\) aligned configuration energetically favourable

• $\mu$ is the magnetic moment per spin

• $H$ is the magnetic field (not Hamiltonian!)

• Periodic boundary conditions (PBC)
Thermodynamic observables

Ground state energy at $H = 0$ in $D$ dimensions:

$$E_0 = -DNJ$$

- Simple cubic lattice: $2D$ nearest neighbours per spin

Magnetization (per spin):

$$M = \sum_{i=1}^{N} \mu s_i, \quad m = \frac{M}{N}$$

The partition function:

$$Q(\beta, N, H) = \sum_{\nu} e^{-\beta E_{\nu}}$$

$$= \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N=\pm 1} \exp \left( \beta \mu H \sum_{i=1}^{N} s_i + \beta J \sum_{ij}' s_i s_j \right)$$

- Prime indicates restricted summation over nearest neighbours

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Lecture 11: Ising and phase transitions.
Some features of the Ising model

- Order-disorder transition
- Entropy wins at high $T \to$ disorder
- Interactions win at low $T \to$ order
- Spontaneous magnetization ($H = 0$) below the critical (Curie) temperature
- One-to-one correspondence with solid-liquid phase transition
- Cooperative effect of short-ranged interactions
- Analytically tractable in 1 and 2 dimensions
- Very precise simulation results for 3 dimensions
- Can be extended beyond 2 states (Potts), and beyond nearest neighbours (Heisenberg)
Classification of phase transitions

First-Order Transition

Second-Order Transition

Figure from W. Janke: Statistical Analysis of Simulations: Data Correlation and Error Estimation

Ising model in 1 dimension

- Nearest-neighbour interaction energy can be rewritten as

\[ E_{\text{int}} = -J \sum_{i=1}^{N} s_i s_{i+1} \]

where \( s_{N+1} \equiv s_1 \) due to PBC.

- The partition function can be evaluated analytically (we omit the derivation)

\[ Q(N, \beta, 0) = \left[ 2 \cosh(\beta J) \right]^N, \quad T_c \approx \frac{J}{Nk_B} \to 0 \text{ for } N \to \infty \]

- No order-disorder transitions in 1 dimension
- But there is an order-disorder transition in 2 dimensions
- Full derivation is involved, we give a qualitative argument instead
Energy of order-disorder transition

Transition barrier to cross from fully ordered to a disordered state: flip N/2 spins in one half of the lattice*

One dimension:
\[ \Delta E = +4J \sim O(1) \]
\[ T_c \sim J/Nk_B \to 0 \text{ for } N \to \infty \]

Two dimensions:
\[ \Delta E = +2N^{1/2}J \sim O(N^{1/2}) \]

*Scaling argument: the exponent is independent of which spins we actually flip, only the numerical prefactor depends on this.
Ising model in 2 dimensions

- Partition function evaluated analytically by Lars Onsager (1940s):

\[ Q(N, \beta, 0) = \left[2 \cosh(\beta J)e^I\right]^N \]

where

\[
I = \frac{1}{2\pi} \int_0^\pi \ln \left\{ \frac{1}{2} \left[ 1 + \left( 1 - \kappa^2 \sin^2 \phi \right)^{1/2} \right] \right\} d\phi,
\]

\[ \kappa = \frac{2 \sinh(2\beta J)}{\cosh^2(2\beta J)} \]

- Spontaneous magnetization below critical temperature

\[ T_c = 2.269 \frac{J}{k_B} \quad \text{←} \quad \sinh(2J/k_BT_c) = 1 \]

- Heat capacity and magnetization diverge near \( T_c \):

\[
\frac{C}{N} \sim \frac{8k_B}{\pi} (\beta J)^2 \ln \left| \frac{1}{T - T_c} \right|; \quad \frac{M}{N} \sim (\text{const.})(T_c - T)^{\beta'} \quad \text{for} \quad T < T_c
\]

- Critical exponent \( \beta' = 1/8 \)
Ising model in 3 dimensions

- Analytical solution not available (yet?)
- Extensive simulation results available
- Heat capacity and magnetization diverge near $T_c$:
  \[ \frac{C}{N} \propto |T - T_c|^{\alpha}; \quad \frac{M}{N} \propto (T_c - T)^{\beta'} \text{ for } T < T_c \]
- Critical exponents:
  \[ \alpha \approx 0.125, \quad \beta' \approx 0.313 \]
Analogy between Ising model and lattice gas

Lattice gas
- One particle per site
- Occupation numbers: $n_i = 0, 1$
- Nearest-neighbour interaction:
  $$E_{\text{int}} = -\varepsilon \sum_{ij} n_i n_j$$

Ising
- One spin per site
- Spin states: $s_i = \pm 1$
- Nearest-neighbour interaction:
  $$E_{\text{int}} = -J \sum_{ij} s_i s_j$$

$s_j = 2n_j - 1$

$J = \varepsilon/4$
Analogy between Ising model and lattice gas

Grandcanonical partition function of the lattice gas:
($\mu$ is chemical potential)

$$\Xi(\beta, N, \mu) = \sum_{n_1} \sum_{n_2} \cdots \sum_{n_N=0,1} \exp \left( \beta \mu \sum_{i=1}^{N} n_i + \beta \varepsilon \sum_{ij}^\prime n_i n_j \right)$$

Canonical partition function of the Ising model:
($\mu$ is magnetic moment per spin)

$$Q(\beta, N, H) = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N=\pm 1} \exp \left( \beta \mu H \sum_{i=1}^{N} s_i + \beta J \sum_{ij}^\prime s_i s_j \right)$$

Substitution:

$$s_i = 2n_i - 1, \quad J = \varepsilon / 4$$

- Phase transitions in a lattice gas follow the same equations as the Ising model
Broken symmetry

- At $H = 0$ the Ising model is symmetric: for each state with magnetization $M$ there is an equally probable state with magnetization $-M$.

- We should obtain $\langle M \rangle = 0$ for all temperatures from:

$$\langle M \rangle = Q^{-1} \sum_* \left( \sum_{1=1}^{N} \mu_s i \right) e^{-\beta \nu} \quad \text{where} \quad M = \sum_{1=1}^{N} \mu_s i$$

- For finite (small) $H$, define $\Delta(M - M_\nu) = 1$ if $M = M_\nu$, 0 otherwise:

$$\bar{Q}(M) = \sum_{\nu} \Delta(M - M_\nu) e^{-\beta E_\nu}$$

$$Q = \sum_{M} \bar{Q}(M), \quad P_M = \bar{Q}(M)/Q$$

- Reversible work to change $M$:

$$-k_B T \ln \bar{Q}(M) = \tilde{A}(M)$$

Fig. 5.4. Reversible work function for the magnetization.
Broken symmetry

- Flipping the magnetization requires energy $E^*$. 
- In 2 dimensions, $E^* \sim N^{1/2}$ 
- Vanishingly small field breaks the symmetry for $N \to \infty$ 
- Probability of spontaneous fluctuation $> E^*$ vanishes as $N \to \infty$ 
- Below $T_c$ spontaneous fluctuations do not suffice to destroy the broken symmetry (enthalpy wins :-). 
- At $N \to \infty$ the field due to a single spin suffices to break the symmetry 
- $\langle M \rangle$ is the order parameter for the order-disorder transition

Fig. 5.4. Reversible work function for the magnetization.
Range of correlations and PBC

Range of correlations $R$, lattice size, $L$

- If $R \ll L$, the range is microscopic
- Lattice can be divided to mutually uncorrelated cells of size $> R$
- Then $\langle M \rangle = 0$

- If $R \gtrsim L$, the range is macroscopic
- Then $\langle M \rangle \neq 0$ can exist

Pair correlation function:

$$c_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$$

$$\sum_{j=2}^{N} c_{1j} = \text{number of spins correlated to } 1$$

Fig. 5.5. Partitioning with different lengths on a lattice.
Correlations and susceptibility

- Magnetic susceptibility

\[ \chi(\beta, H) = \frac{1}{N} \left( \frac{\partial \langle M \rangle}{\partial \beta H} \right)_\beta = \frac{1}{N} \langle (\delta M)^2 \rangle \]

where

\[ \delta M = M - \langle M \rangle = \mu \sum_{i=1}^{N} (s_i - \langle s_i \rangle) \]

\[ \langle \delta M^2 \rangle = \langle (M - \langle M \rangle)^2 \rangle = \langle M^2 \rangle - 2 \langle M \rangle \langle M \rangle + \langle M \rangle^2 = \langle M^2 \rangle - \langle M \rangle^2 \]

- We can rewrite \( \chi \) in terms of the correlation function

\[ \chi(\beta, H) = \langle M^2 \rangle - \langle M \rangle^2 = \frac{\mu^2}{N} \sum_{i,j=1}^{N} (\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle) = \mu^2 \sum_{j=2}^{N} c_{1j} \]

- Divergence of \( \chi \) is related to long-range correlations
Correlations and susceptibility

- For $H \to 0^+$, $N \to \infty$ and $T < T_c$: $\langle M \rangle = N m_0 \mu$ where $m_0$ is the spontaneous magnetization per spin (at zero field)
- For $H \to 0^-$, $N \to \infty$ and $T < T_c$: $\langle M \rangle = -N m_0 \mu$
- For $N \to \infty$, $\langle M \rangle$ is a discontinuous function of $H$
- The derivative $\partial \langle M \rangle / \partial \beta H$ diverges at $H = 0$
- Due to symmetry $\langle s_i \rangle = 0$
- Each spin biases its neighbourhood to its own orientation, therefore
  \[ \sum_{j=1}^{N} \langle s_1 s_j \rangle = +N m_0 \]
  independent of the value of $s_1$.

\[ \chi = N m_0 \mu^2 \text{ for } N \to \infty, \ T < T_c \]
Macroscopic correlations

- Divergence only for $N \to \infty$, for finite $N$ the transition is smooth
- For spontaneous magnetization, correlations span the whole system
- Analogy: coalescence of droplets in a gravitational field
- Near $T_c$ divergence for different reasons
- Distinction between phases disappears
- Surface (line) tension vanishes
- Macroscopic fluctuation range
- For a lattice gas at $T \to T_c$

$$\left( \frac{\partial \beta \mu}{\partial \rho} \right)_T = \frac{1}{\rho} \left( \frac{\partial \beta \rho}{\partial \rho} \right)_{\beta} = 0$$
The mean field (MF) approximation

- Consider one selected spin
- Interaction with other spins through an average mean field
- Ubiquitous in physics of many-body systems

![Diagram](Fig. 5.8. Schematic view of mean field theory.)
The mean field (MF) approximation

- Write the full interaction energy as

\[ E_\nu = -\mu H \sum_i s_i - \frac{1}{2} \sum_{ij} J_{ij} s_i s_j \]

\( J_{ij} = 1 \) if \( i, j \) are nearest neighbours, \( J_{ij} = 0 \) otherwise

- Mean force due to neighbouring spins (\( z \) neighbours):

\[ -\frac{\partial E_\nu}{\partial s_i} = \mu H + \sum_j J_{ij} s_j = \mu H + z J \langle s_j \rangle \]

- Mean field acting on spin \( i \) (cf. potential of mean force):

\[ \mu H_i = \mu H + \sum_j J_{ij} s_j, \quad \langle H_i \rangle = H + \sum_j J_{ij} \langle s_j \rangle / \mu = H + z J \langle s_i \rangle / \mu \]

where \( z \) is the number of neighbours and we used \( \langle s_i \rangle = \langle s_j \rangle \)

- In the mean field we neglect fluctuations of \( H_i \) from \( \langle H_i \rangle \)
The mean field (MF) approximation

- Many-body problem reduced to two-body problem (spin+field):
  \[
  \langle s_1 \rangle = \frac{\sum_{s_1=\pm 1} s_1 \exp(\beta \mu (H + \Delta H) s_1)}{\sum_{s_1=\pm 1} \exp(\beta \mu (H + \Delta H) s_1)}, \quad \Delta H = \frac{J_z \langle s_1 \rangle}{\mu} = \frac{J z m}{\mu}
  \]

- Evaluation of the sum yields:
  \[
  m = \tanh(\beta \mu H + \beta z J m)
  \]
  \[
  m = \langle M \rangle \frac{1}{N \mu} = \frac{1}{N \mu} \left\langle \sum_{i=1}^{N} \mu s_i \right\rangle
  \]
  \[
  m = \langle s_i \rangle = \langle s_1 \rangle
  \]

- Non-zero solution for \( m \) at \( H = 0 \)
- From MF \( T_c = 2DJ/k_B \) (exact: \( 2.269J/k_B \) for \( D=2 \))
- Systematic improvements to MF: explicitly consider more than one spin
Variational treatment of the mean field

- Variational principle for first order perturbation theory
- Full partition function

\[ Q = \sum_{s_1,s_2,\ldots,s_N} \exp(-\beta E(s_1, \ldots, s_N)), \quad E = -\frac{1}{2} \sum_{i,j} J_{ij} s_i s_j - \mu H \sum_i s_i \]

- Consider the mean field interaction as an extra contribution to \( H \):

\[ E_{MF} = -\mu (H + \Delta H) \sum_i s_i \]

\[ Q_{MF} = \sum_{s=\pm1} \prod_{j=1}^{N} \exp(\beta \mu (H + \Delta H)) = \left( 2 \cosh(\beta \mu (H + \Delta H)) \right)^N \]

- What is the optimum choice for \( \Delta H \)?
- Define \( \Delta E \) as

\[ \Delta E = E - E_{MF} \quad \rightarrow \quad Q = \sum_{s=\pm1} \exp(-\beta (E_{MF} + \Delta E)) \]
Variational treatment of the mean field

- Rearrange the expression for $Q$

\[
Q = \sum_{s=\pm 1} \exp(-\beta(E_{MF} + \Delta E)) = \sum_{s=\pm 1} \exp(-\beta E_{MF}) \exp(-\beta \Delta E)
\]

\[
= Q_{MF} \sum_{s=\pm 1} \exp(-\beta E_{MF}) \exp(-\beta \Delta E) = Q_{MF} \langle \exp(-\beta \Delta E) \rangle_{MF}
\]

- This is the perturbation expression with MF as a reference system

- Expand the exponential

\[
\langle \exp(-\beta \Delta E) \rangle_{MF} = \langle 1 - \beta \Delta E + \cdots \rangle_{MF} = 1 - \beta \langle \Delta E \rangle_{MF} + \cdots
\]

\[
= \exp(-\beta \langle \Delta E \rangle_{MF}) + \cdots
\]

\[
Q = Q_{MF} \langle \exp(-\beta \Delta E) \rangle_{MF} \approx Q_{MF} \exp(-\beta \langle E - E_{MF} \rangle_{MF})
\]
Variational treatment of the mean field

- Consider the inequality \( e^x \geq 1 + x \):
  \[
  \langle e^f \rangle = e^{\langle f \rangle} \langle e^{(f - \langle f \rangle)} \rangle \geq e^{\langle f \rangle} \langle 1 + f - \langle f \rangle \rangle = e^{\langle f \rangle}
  \]

- The above implies the **Gibbs-Bogoliubov-Feynmann bound**
  \[
  Q = Q_{\text{MF}} \langle \exp(-\beta \Delta E) \rangle_{\text{MF}} \geq Q_{\text{MF}} \exp(-\beta \langle E - E_{\text{MF}} \rangle_{\text{MF}})
  \]

- Mean field yields an upper bound to the true free energy!

- Determine optimum \( \Delta H \) by solving
  \[
  0 = \frac{\partial}{\partial H} Q_{\text{MF}} \exp(-\beta \langle E - E_{\text{MF}} \rangle_{\text{MF}})
  \]

- The differentiation yields
  \[
  zJ \langle s_1 \rangle_{\text{MF}} = \mu \Delta H
  \]

- Our choice based on physical arguments was the optimum for MF.
Renormalization group (RG) theory

- Accounts for long-range fluctuations
- Key idea: rewrite the partition function, explicitly summing over some degrees of freedom in order to reduce the number of DOF.

Example: 1D Ising with $K = J/k_BT$

$$Q(K, N) = \sum_{s_1, s_2, s_3, ..., s_N} \exp \left[ K \left( s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_5 + \cdots \right) \right]$$

$$= \sum_{s_1, s_2, s_3, ..., s_N} \exp \left[ K \left( s_1 s_2 + s_2 s_3 \right) \right] \exp \left[ K \left( s_3 s_4 + s_4 s_5 \right) \right] \cdots$$

Explicitly sum over even spins:

$$Q(K, N) = \sum_{s_1, s_3, s_5, ...} \left\{ \exp \left[ K \left( s_1 + s_3 \right) \right] + \exp \left[ -K \left( s_1 + s_3 \right) \right] \right\} \cdot \left\{ \exp \left[ K \left( s_3 + s_5 \right) \right] + \exp \left[ -K \left( s_3 + s_5 \right) \right] \right\} \cdots$$
Renormalization group (RG) theory

• Seek a recursive relation to express $Q$ as a function of $N/2$ and a different constant $K'$:

$$e^{K(s+s')} + e^{-K(s+s')} = f(K)e^{K's's'}$$

$$Q(K, N) = \sum_{s_1, s_3, s_5, \ldots} f(K) \exp(K's_1s_3) \cdot f(K) \exp(K's_3s_5) \cdot \ldots$$

$$= [f(K)]^{N/2} Q(K', N/2)$$

• The above is called the Kadanoff transformation

• Two cases:

$$s = s' \rightarrow e^{2K} + e^{-2K} = f(K)e^{K'}, \quad s = -s' \rightarrow f(K) = 2e^K$$

• Eliminating $K'$ and $f(K)$, we obtain $K'$ and $f(K)$ in terms of $K$:

$$K' = (1/2) \ln \cosh(2K), \quad f(K) = 2 \cosh^{1/2}(2K)$$
Renormalization group (RG) theory

• Seek a function $g(K)$ such that
  \[ Q = [g(K)]^N \rightarrow \ln Q = Ng(K) \]

• Combine it with
  \[ \ln Q(K, N) = (N/2) \ln f(K) + \ln Q(K', N/2) \]

  to obtain
  \[ g(K) = \frac{1}{2} \ln f(K) + \frac{1}{2} g(K') \]

  \[ g(K') = 2g(K) - \ln \left[ 2\sqrt{\cosh(2K)} \right] \]

• Provided that we know or can well approximate $Q(K, N)$ (and hence $g(K)$) for a certain value of $K$, we can recursively obtain it for $K'$.

• Similarly in the opposite direction
Renormalization group (RG) theory

- The recursive application of the RG equations can be represented as a flow diagram.
- Its fixed points represent phase transitions.
- 1D Ising: trivial fixed points $K = 0$ and $K = \infty$.
- 2D Ising: additional non-trivial fixed point at the phase transition $K_c$. 

![Diagram of RG flow for 1D and 2D Ising models](http://www.natur.cuni.cz/chemie/fyzchem)