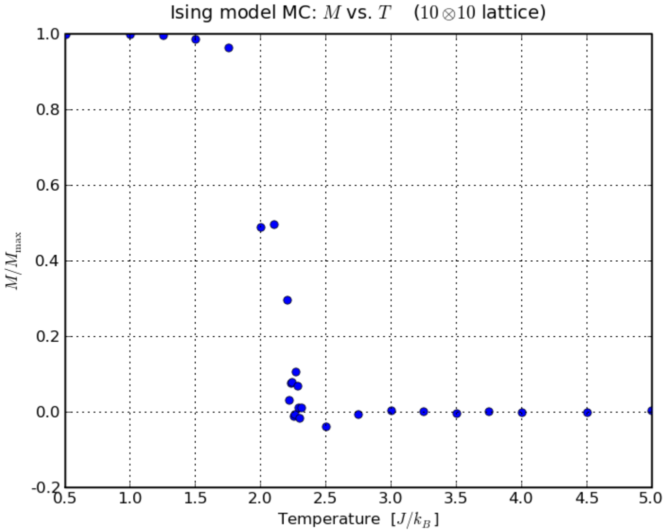
Lecture 9: Phase transitions

Introduction

- Discussed the Ising model in the last lecture
- Model exhibits a 2nd order phase transition at $T_c \approx 2.27$
- Use spontaneous magnetisation as order parameter: $M \sim |T - T_c|^{\beta}$, $\beta = 1/8$
- Mean field approximation yields $T_c = 4$, $\beta = 1/2$

Spontaneous magnetisation vs. temperature

- Consider a 10×10 lattice



More observables

- Up to now only spontaneous magnetisation, extend to more observables:

1. Energy: Calculate through

$$\langle E \rangle = -J \sum_{\langle ij \rangle} s_i s_j$$

$\Longrightarrow \langle E(T=0) \rangle = -NJj/2$ with $j = 4$, $N =$ number of spins, and factor $1/2$ due pairs

$\Longrightarrow \langle E(T \to \infty) \rangle \to 0$, because of random orientation of spins

2. Specific heat: $C = \mathrm{d}\langle E \rangle / \mathrm{d}T$

$C \approx \frac{1}{|T - T_c|^\alpha}$, exhibits divergence at T_c due to inflection point in energy.

According to fluctuation-dissipation theorem:

$$C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T},$$

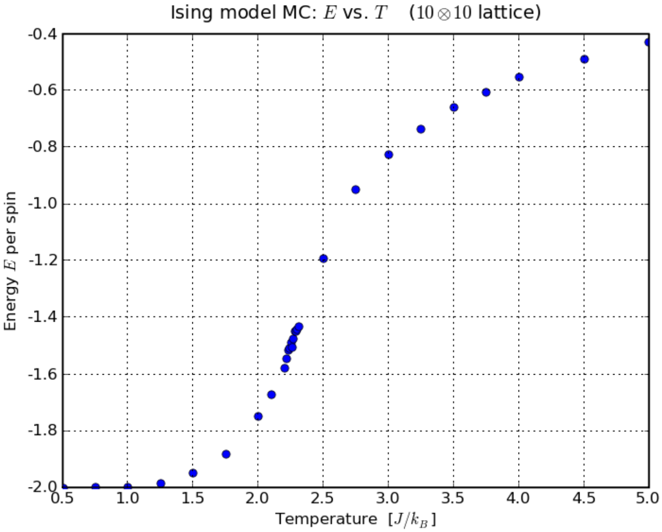
with $\langle E^m \rangle$ from sampling E^m during lattice sweeps.

More observables (cont'd)

3. Susceptibility: $\chi = \mathrm{d}\langle M \rangle / \mathrm{d}H$
   this measures how much magnetisation $\langle M \rangle$ is induced by a magnetic field H.
   Again, according to fluctuation-dissipation theorem:
   $$\chi = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T},$$
   with $\langle M^m \rangle$ from sampling M^m during lattice sweeps.
   χ diverges for $T \to T_c$, another power law with critical exponent γ.
   Note: This allows to investigate the system would react to an external field without ever applying one!
   The power of the fluctuation-dissipation theorem!

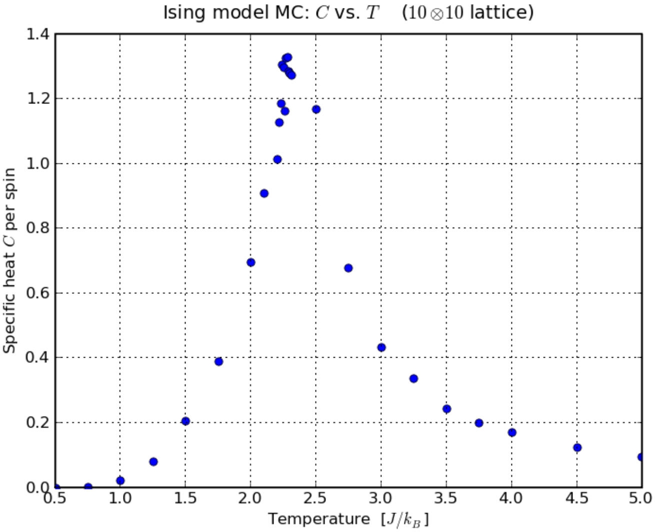
Energy

- Results from a 10×10 lattice



Specific Heat

- Results from a 10×10 lattice

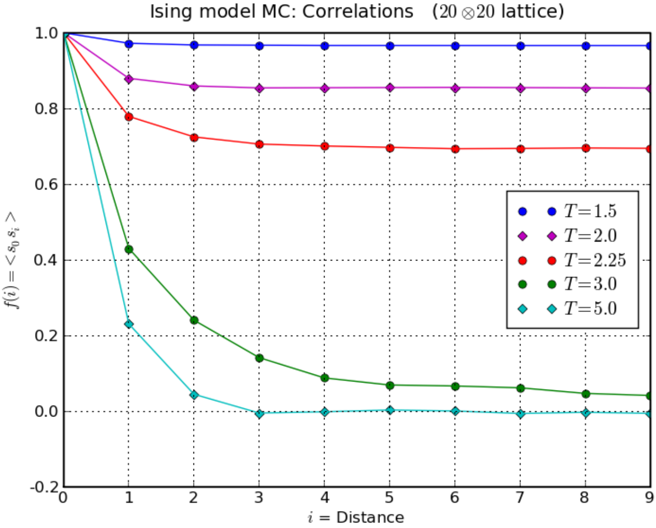


Correlations

- Consider again variation of energy with temperature
- Results suggest that even at $T \gg T_c$ there is some residual alignment of spins $\Longrightarrow$ correlations!
- Interpretation: disordering effect of temperature not strong enough to induce a truly random alignment among neighbouring spins.
- Quantifying it:
  - Pick a random spin s_0.
  - Calculate $f(i) = \langle s_0 s_i \rangle$ where s_i is i lattice sites away from s_0 (a.k.a. Manhattan distance)
  - $f(i)$ is called correlation function.
  - Realisation in MC: Use every spin as s_0 - go over all pairs of spins and form suitable averages.

Correlations

- Results from a 20×20 lattice



Discussion of correlations

- Strong & long-range correlations at low temperatures: $f(i) \approx 1$ for $T \approx 0$, nearly independent of distance. Spins quite well aligned over large distances.
- Around $T = T_c$: alignment significantly stronger at smaller than at larger distances, correlations decrease with distance, but remain visible.
- At $T > T_c$: Correlations only over small distances, die out quickly after a few lattice sites.
- Parametrise this as $f(i) = C_1 + C_2 \exp(-r_i \xi)$, where ξ is known as correlation length. For distance $r_i \to \infty$, the spins decouple and therefore $f(i) \to \langle s_0 \rangle \langle s_i \rangle = \langle s \rangle^2 = C_1$
- This allows to identify $f(i) - C_1 = (s_0 - \langle s \rangle)(s_i - \langle s \rangle) \sim C_2 \exp(-r_i/\xi)$

Discussion of correlations (cont'd)

- Therefore ξ measure the range over which the correlations of spin-fluctuations $(s - langles\rangle)$ approach zero.
- From the results we see that $\xi = \xi(T)$.
- In the limit of large lattices, $\xi \sim \dfrac{1}{|T - T_c|^\nu}$, where ν is yet another critical exponent.
- At the critical point, $\xi(T_c) = \infty$ for infinitely large lattices, and the exponential is replaced by a power law for the correlations.
- This implies that

  at T_c spins become correlated all over the lattice.

  Such a huge sensitivity is typical for phase transitions.
- Mean field approximation ignores such fluctuations, explaining why it fails to describe the phase transition quantitatively.

First-order phase transitions

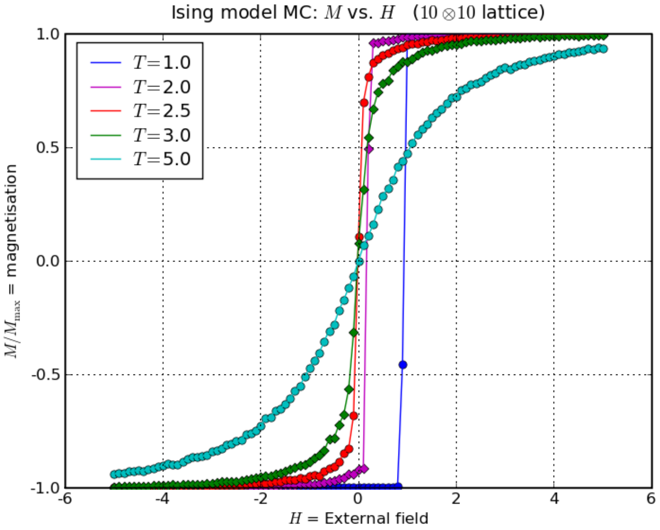
- Up to now: Two-dimensional Ising model around its critical point without external field.
  Order parameter: Spontaneous magnetisation, exhibits a 2nd order phase transition.
- Logical question(s): What is a 1st order phase transition? Can we convince the model to have one?

1st order phase transitions quite common in nature, e.g., water to ice!

- Have a 1st order phase transition in the Ising model with an external field switched on. Simple to include into simulation: Just add a term $\sim \mu H$ to the spin-flip probability.
- Now: two independent external parameters T and H $\Longrightarrow$ larger phase diagram to explore.

Magnetisation M vs. external field H at different T

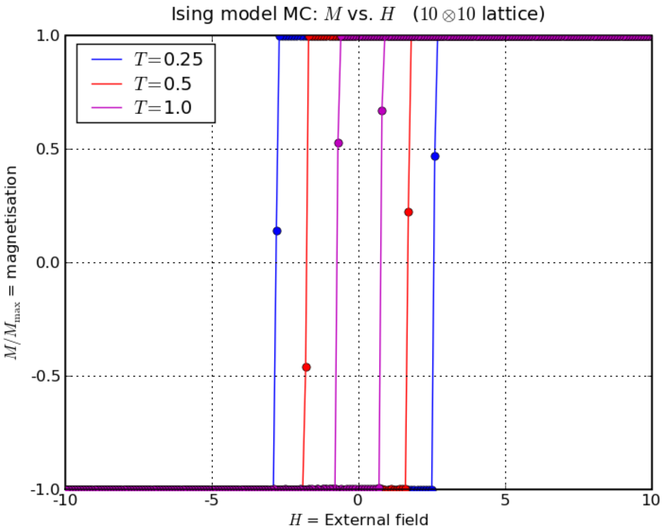
- Consider a 10×10 lattice



Discussion of results

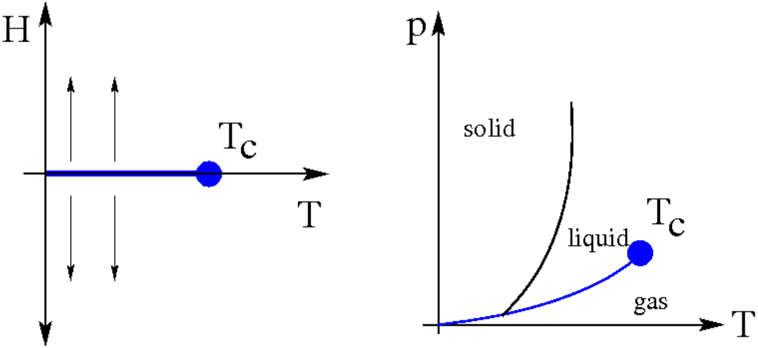
- Start with maximal negative H and ramp up the field.
- At low temperatures ($T = 1$) spins perfectly align with H, abrupt change ($M = -1 \rightarrow M = 1$) when H flips sign. discontinuous "jump": 1st order phase transition.
- But: hysteresis at $T = 1$ for H around 0. Reason: small field, meta-stable state of the system ($M < 0$, $H > 0$)
- Above T_c no more spontaneous magnetisation, therefore no more competition with $H \implies$ smooth transitions
- Size of jump below T_c: twice the spontaneous magnetisation from the simulation with $H = 0$.
- Suggest close relation between 1st order phase transition as function of H and 2nd order as a function of T.
- Difference: "Explosion" of correlation lengths in 2nd order, very abrupt in 1st order (no prior "warning").

Hysteresis loops



Phase diagrams

- Compare Ising model and water: critical points
- Can go from one phase to another "around" critical point
  $\Longrightarrow$ difference between phases vanishes
  $\Longrightarrow$ line of 1st order phase transition terminates



Scaling

- Assumption:

  Critical exponents and behaviour are universal.

- Can we prove this? We should elaborate.
- Key concept there: Scaling

  Idea: Can suitably normalise observables etc.: $h = \mu H/J$, $t = T/T_c - 1$ etc. and write equations in terms of these scaled objects. Then we can relate factors in one to factors in others in a natural way.

  Will discuss this with the example of the Ising model.

Scaling in mean field approximation

- Go back to implicit equation for $\langle s \rangle$:
$$\langle s \rangle = \tanh\left[\frac{zJ\langle s \rangle + \mu H}{k_B T}\right] \approx \frac{zJ\langle s \rangle + \mu H}{k_B T} - \frac{1}{3}\left(\frac{zJ\langle s \rangle}{k_B T}\right)^3$$
- Rewrite this dimensionless as equation of state (E.o.S.)
$$h = btm + um^3$$
with $h = \frac{\mu H}{zJ}$, $m = \langle s \rangle$ and $t = 1 - \frac{k_B T}{J} = 1 - \frac{T}{T_c}$.
(b and u just positive constants).
- Realise that this can be cast into
$$m(\lambda^{1/2} t,\, \lambda^{3/4} h) = \lambda^{1/4} m(t,\, h)$$
- Example: choose $\lambda = 16$ and plug into E.o.S.:
$$\lambda^{3/4} h = 8h = 8btm + 8um^3 = b\lambda^{1/2} t \lambda^{1/4} m + u(\lambda^{1/4} m)^3$$

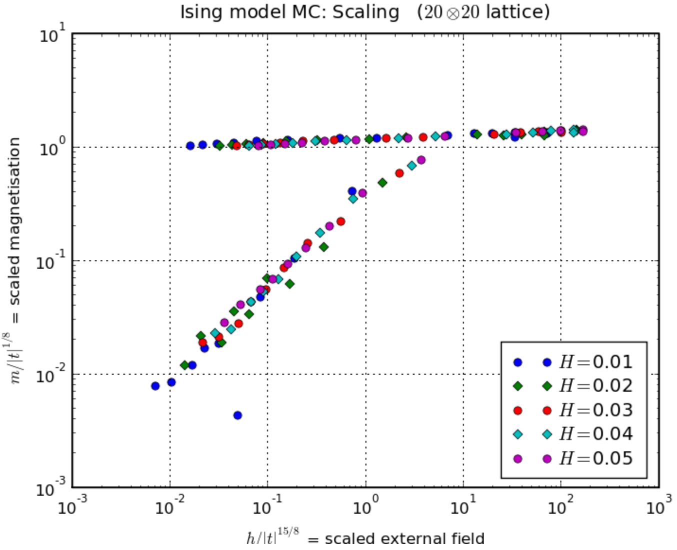
Scaling in mean field approximation (cont'd)

- Function of two parameters like the kind encountered before in $m(t,\, h)$, which exhibit this scaling property can be expressed by a single variable:
$$m(t,\, h) = |t|^{1/2} m\left(\pm 1,\, \frac{h}{|t|^{3/2}}\right) = |t|^{1/2} f_\pm\left(\frac{h}{|t|^{3/2}}\right)$$
- In the equation above $f_\pm$ refer to temperatures $t > 0$ and $t < 0$, i.e. $T > T_c$ and $T < T_c$, respectively.
- But we already know that mean field theory is not correct around the critical point, so we use a more general form, namely
$$m(t,\, h) = |t|^{\beta} f_\pm\left(\frac{h}{|t|^{\beta\delta}}\right)$$
with $\beta = 1/2$ and $\delta = 3$ in mean field theory.

Scaling: An appraisal

- Scaling provides an interesting and insightful way of describing the behaviour of systems around critical points and the corresponding critical exponents of the power laws.
- Equation like the one above connect different such laws and their exponents.
- This was not fully understood for some time, by now, the concept of the renormalisation group has shed light onto this issue. The renormalisation group describes how systems behave under general scale transformations.

Results


Ising model MC: Scaling (20⊗20 lattice)
$m/|t|^{1/8}$ = scaled magnetisation
$h/|t|^{15/8}$ = scaled external field
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{2}
10^{3}
$H=0.01$
$H=0.02$
$H=0.03$
$H=0.04$
$H=0.05$

Summary

- Continued discussion of phase transitions
- More observables
- Included a 1st order phase transition in the 2D Ising model by adding an external field
- Phase diagrams and critical points
- Fascinating property: Scaling