Monte Carlo methods

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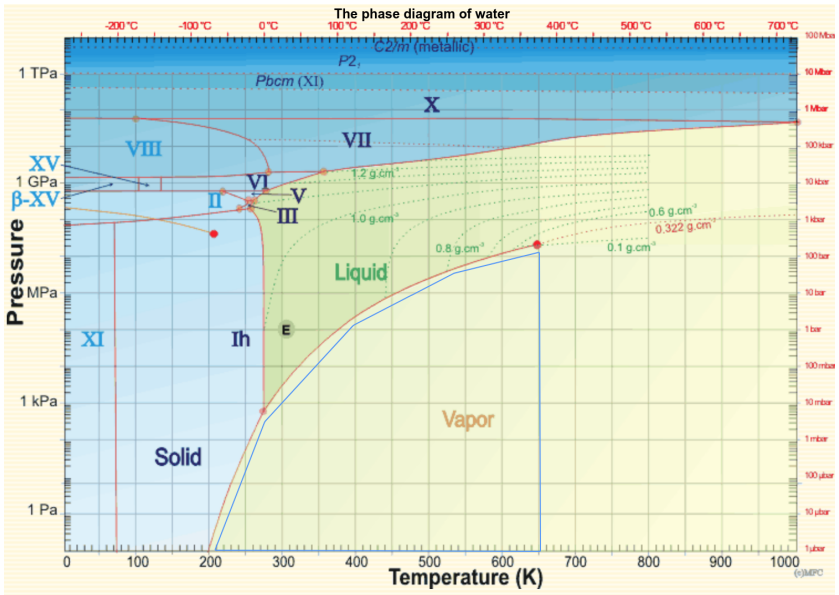
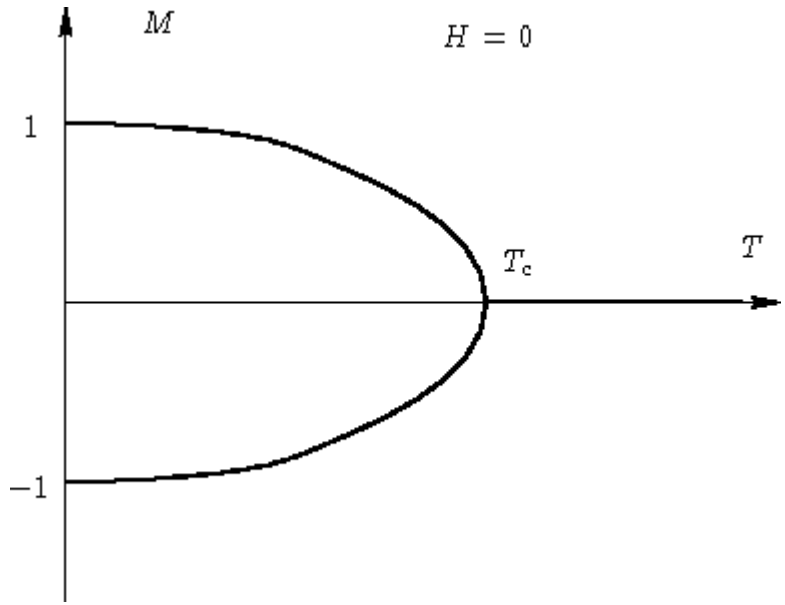
In many systems we observe phase change:
Ordered/Unordered, Solid/Liquid , Liquid/Gas, Magnetized/Unmagnetized
Variation of some parameter: Temperature, pressure, chemical potential, external field, ...
Often there is an observable called **Order parameter** that allows the differentiation of the phases macroscopically:
Density, magnetization, etc.

Phase diagram shows possible phases as the parameters are varied:



Water

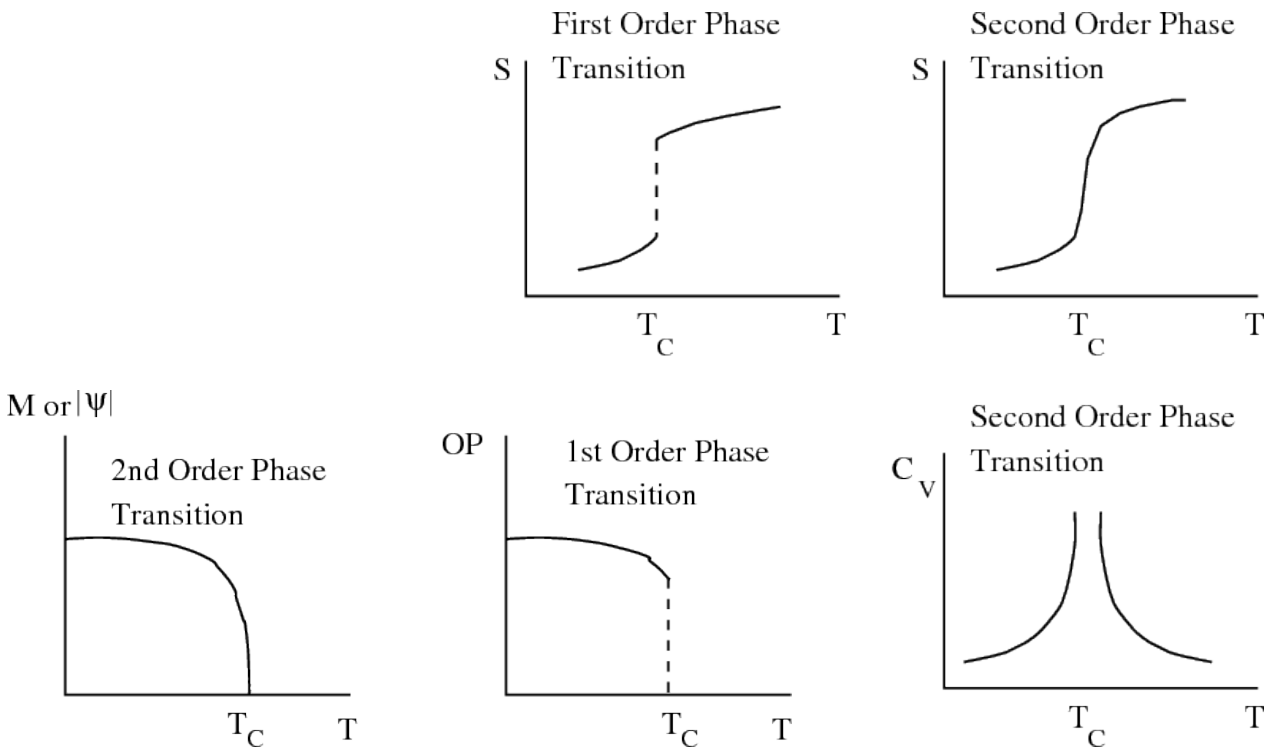


Ising model

First order phase transitions have discontinuities (jump) in e.g. the density Charactherised by a jump the first derivative of the free energy of the system. This corresponds to a jump in e.g. the energy: **Latent heat**, magnetization , ...

Second order phase transition has no discontinuity. Second derivative of the free energy is discontinous No latent heat but heat capacity diverges at T_c

Crossover is not a phase transition: the dependence is smooth (analytic) all the way but the change is "rapid"



Consider e.g. the Ising model.

$$Z = \sum e^{-\beta H[S]}, \quad F = -k_B T \ln Z \tag{1}$$

We investigate this system on a finite lattice. Sum of finitely many terms, each of which is an analytical function of the parameters β, h.

$\Longrightarrow$ No phase transition on a (finite) lattice

In the thermodynamical limit ($V \to \infty$) we can have discontinuities as (for example)

$$\partial_\beta \left(\sum_{i=0}^{\infty} e^{-\beta H_i} O_i \right) \neq \sum_{i=0}^{\infty} \partial_\beta (e^{-\beta H_i} O_i) \tag{2}$$

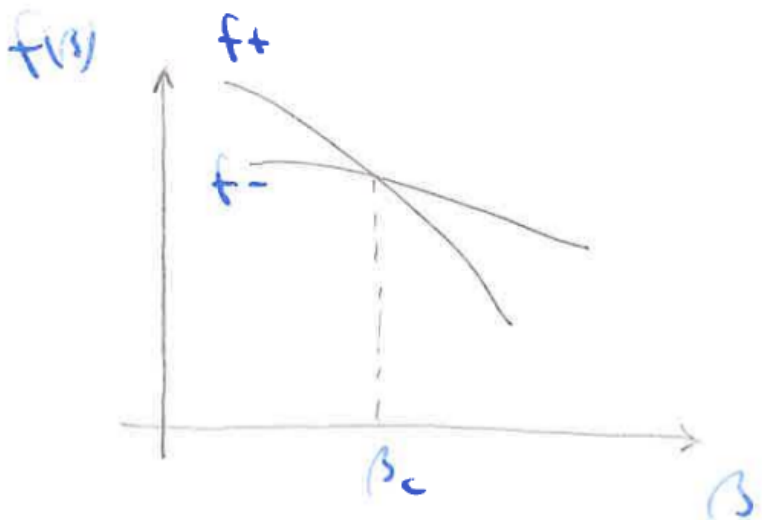
We need to investigate the $V \to \infty$ limit (or rather, finite size scaling) to investigate phase transitions on the lattice

Suppose there are two class of configurations: $+$ and $-$
The partition function is then written as $Z = Z_+ + Z_-$

$$Z = e^{-\beta f_+(\beta)V} + e^{-\beta f_-(\beta)V} \tag{3}$$

where $f_\pm$ is the free energy density of the two phases: $f_\pm = -(k_B T \ln Z_\pm)/V$

$$\beta > \beta_c \quad \Longrightarrow \quad f_+(\beta) < f_-(\beta) \tag{4}$$
$$\beta < \beta_c \quad \Longrightarrow \quad f_-(\beta) < f_+(\beta) \tag{5}$$
$$\beta = \beta_c \quad \Longrightarrow \quad f_+(\beta) = f_-(\beta) \tag{6}$$



We calculate the average energy:

$$E = \langle H \rangle = -\frac{\partial}{\partial \beta} \ln Z \tag{7}$$

energy density

$$\begin{aligned} \frac{E}{V} &= -\frac{1}{V}\frac{\partial}{\partial \beta} \ln \left(\sum_{\alpha=\pm} e^{-\beta f_\alpha V} \right) = -\frac{1}{VZ} \sum_{\alpha=\pm} (-f_\alpha - \beta f'_\alpha) V e^{-\beta f_\alpha V} = \\ &= \frac{h_+ e^{-\beta f_+ V} + h_- e^{-\beta f_- V}}{e^{-\beta f_+ V} + e^{-\beta f_- V}} \quad \text{with} \quad h_\alpha = f_\alpha + \beta f_\alpha \end{aligned}$$

$$\frac{E}{V} = \begin{cases} \frac{h_+ + h_- e^{-\beta(f_- - f_+)V}}{1 + e^{-\beta(f_- - f_+)V}} & \text{for} \quad \beta > \beta_c \implies f_+ < f_- \\ \frac{h_+ e^{-\beta(f_+ - f_-)V} + h_-}{e^{-\beta(f_+ - f-)V} + 1} & \text{for} \quad \beta < \beta_c \implies f_- < f_+ \end{cases} \tag{8}$$

In the infinite volume limit this gives:

$$\epsilon = \frac{E}{V} = \begin{cases} h_+ = f_+ + \beta f'_+ & \text{for} \quad \beta > \beta_c \\ h_- = f_- + \beta f'_- & \text{for} \quad \beta < \beta_c \end{cases} \tag{9}$$

No we can calculate the latent heat:

$$\begin{aligned} \frac{\Delta E}{V} &= h_+ - h_-|_{\beta=\beta_c} = f_+ + \beta f_+' - (f_- + \beta f_-')\big|_{\beta=\beta_c} \\ &= \beta_c (f_+' - f_-')\big|_{\beta=\beta_c} \end{aligned} \tag{10}$$

we continue with the heat capacity:

$$\begin{aligned} \frac{1}{V}\frac{C_v}{k_B\beta^2} &= \frac{\langle H^2\rangle - \langle H\rangle^2}{V} = \frac{1}{V}\frac{\partial^2}{\partial\beta^2}\ln Z = -\frac{1}{V}\frac{\partial}{\partial\beta}\langle H\rangle = \\ &= -\frac{1}{V}\frac{\partial}{\partial\beta}\frac{\sum_{\alpha=\pm}(-f_\alpha - \beta f_\alpha')Ve^{-\beta f_\alpha V}}{\sum_{\alpha=\pm} e^{-\beta f_\alpha V}} = \end{aligned} \tag{11}$$

$$= \frac{\sum[V(\overbrace{f_\alpha + \beta f_\alpha'}^{h_\alpha})^2 - f_\alpha' - f_\alpha' - \beta f_\alpha'']e^{-\beta f_\alpha V}}{\sum e^{-\beta f_\alpha V}} - V\frac{(\sum(-f_\alpha - \beta f_\alpha')e^{-\beta f_\alpha V})^2}{(\sum e^{-\beta f_\alpha V})^2}$$

Using only terms $\sim V$

$$= V\frac{\sum h_\alpha^2 e^{-\beta f_\alpha V}}{\sum e^{-\beta f_\alpha V}} - V\frac{(\sum h_\alpha e^{-\beta f_\alpha V})^2}{(\sum e^{-\beta f_\alpha V})^2}$$

Now we evaluate at the phase transition β_c

$$V\frac{\sum h_\alpha^2 e^{-\beta f_\alpha V}}{\sum e^{-\beta f_\alpha V}} - V\frac{\left(\sum h_\alpha e^{-\beta f_\alpha V}\right)^2}{(\sum e^{-\beta f_\alpha V})^2} = \tag{12}$$

$$= V\frac{(h_+^2 + h_-^2)e^{-\beta f_c V}}{2e^{-\beta f_c V}} - V\left(\frac{(h_+ + h_-)e^{-\beta f_c V}}{2e^{-\beta f_c V}}\right)^2$$

$$= \frac{V}{4}\left(2h_+^2 + 2h_-^2 - (h_+ + h_-)^2\right)\Big|_{\beta=\beta_c} = \frac{V}{4}(h_+ - h_-)^2\Big|_{\beta=\beta_c}$$

So we finally have

$$\frac{C_V}{V} = V\frac{k_B\beta^2}{4}(h_+ - h_-)^2\Big|_{\beta=\beta_c} = V\frac{k_B\beta^4}{4}(f_+' - f_-')^2\Big|_{\beta=\beta_c} \tag{13}$$

$\Longrightarrow$ At first order phase transitions c_v/V scales with the volume V
This is true for other susceptibilities as well

2nd order phase transitions are described by power law behaviors
reduced temperature: $t = \frac{T - T_c}{T_c}$
e.g. Magnetization, its susceptibility, heat capacity, correlation length: (defined for the intensive quantities)

$$\begin{aligned} M &\sim M_0(-t)^{\beta} \text{ for } t < 0 \\ M &\sim M_0'|h|^{1/\delta}\text{sign}(h) \text{ for } t = 0 \\ \chi &\sim \chi_0|t|^{-\gamma} \\ C &\sim C_0|t|^{-\alpha} \\ \xi &\sim \xi_0|t|^{-\nu} \end{aligned} \tag{14}$$

critical exponents: $\beta, \gamma, \alpha, \nu, \eta$
Some of these quantities also have a regular part, these dependencies describe the singular part: $\chi = \chi_r + \chi_s$

These exponents are calculated in some cases:
Ising model in 2d: $\alpha = 0,\ \beta = 1/8,\ \gamma = 7/4,\ \nu = 1,\ \eta = 1/4$

The critical exponents are not independent
Scaleing laws derived e.g. from Maxwell relations

$$\alpha + 2\beta + \gamma = 2, \quad d\nu = 2 - \alpha, \quad \gamma = \nu(2 - \eta) \tag{15}$$

2 independent exponents remain, these give the **Universality class** of the phase transition.
The universality class depends on

- Dimension of space
- Dimensionality and symmetry of the spins

e.g. the 2d Ising model belongs to the 2d Z_2 universality class
Details of the interactions or the dynamics does not matter, these give T_c and a regular part of the free energy

The power law behaviors can be extracted from **Widom scaling forms** (generalized homogeneous function) e.g.

$$M(st, s^{\beta\delta}h) = s^{\beta}M(t, h) \tag{16}$$

where this equation holds for any real number s.
use $h = 0$ and $s = -1/t \implies$

$$M(1, 0) = (-1/t)^{\beta}M(t, 0) \implies M(t, 0) \sim (-t)^{\beta} \tag{17}$$

Or use $t = 0$ and $s^{\beta\delta}h = 1$

$$M(0, 1) = (h)^{-1/(\beta\delta)^{\beta}}M(0, h) \implies M(0, h) = h^{1/\delta}M(0, 1) \tag{18}$$

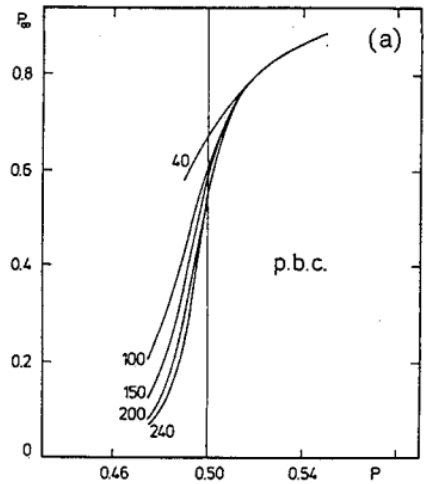
Widom scaling allows more: set $st = \mathrm{sign}(t) \implies s = 1/|t|$

$$M(\pm 1, |t|^{-\beta\delta}h) = |t|^{-\beta}M(t, h) \tag{19}$$

we can describe behaviors of the system where both $t \neq 0, h \neq 0$

$$M(\pm 1, |t|^{-\beta\delta} h) = |t|^{-\beta} M(t, h) \qquad (20)$$

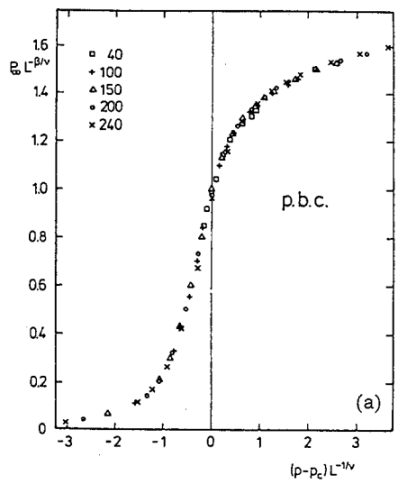
If we now measure $|t|^{-\beta} M_{t,h}$ and plot it as a function of $|t|^{-\beta\delta} h$ we see two universal curves: one for $t > 0$ and one for $t < 0$
This is called **data collapse**



Scaling forms for M, χ,.. etc. exist,
they are based on a scaling form for the free energy $f = f_r + f_s$

$$f_s(s^p t, s^q h) = s^d f_s(t, h), \quad \frac{q}{p} = \frac{\nu}{2}(d + 2 - \eta), \frac{1}{p} = \nu \qquad (21)$$

using e.g. derivativ with respect to h one gets the scaling form for M



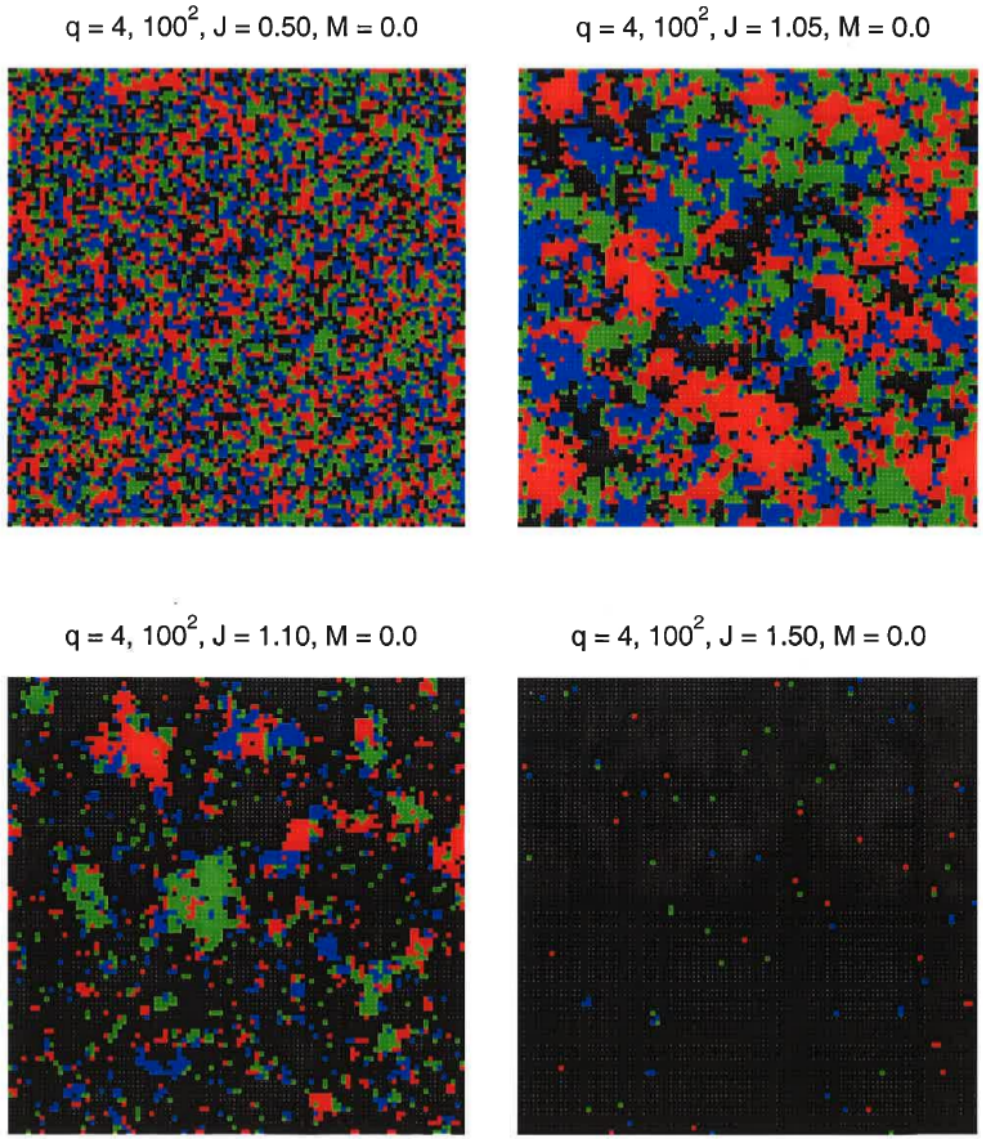
Phase transformation in the Potts model

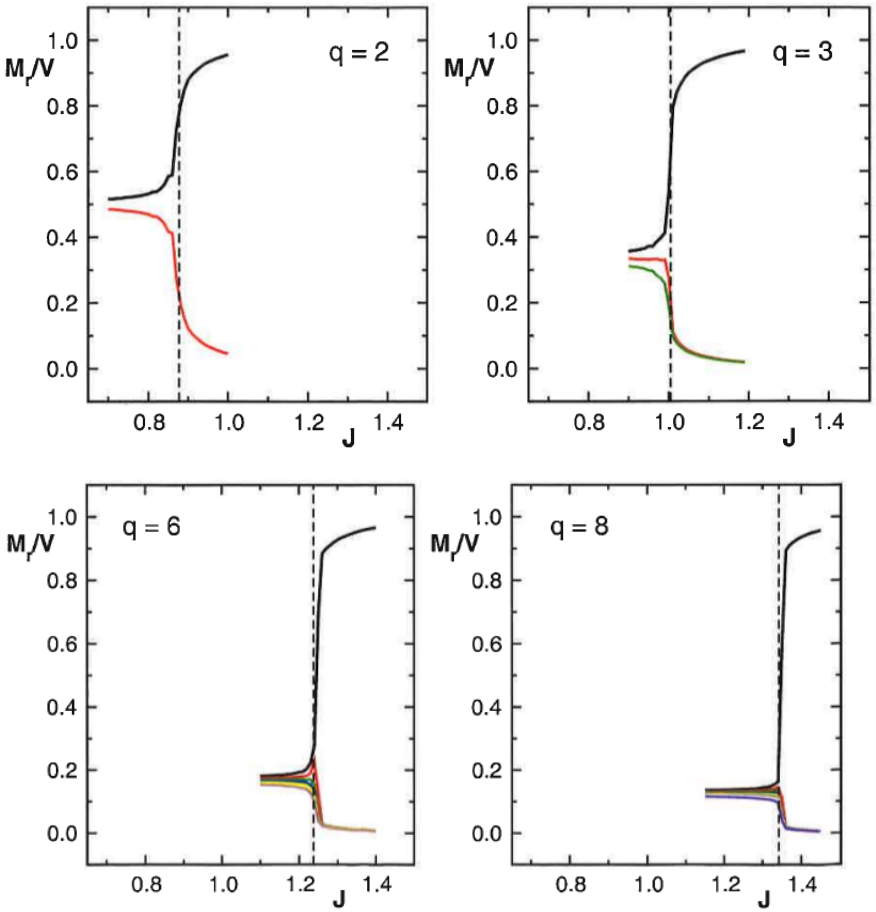
Sample configurations from $q = 4$ Potts model

$J = \alpha\beta$, the coefficient of the interaction term
$M = 0$ means here zero magnetic field

Colors show the 4 different spin states

Phase tr. clearly visible:
at $J = 0.5$ mostly random clusters
at $J = 1.5$ almost all spins in $q = 1$ state





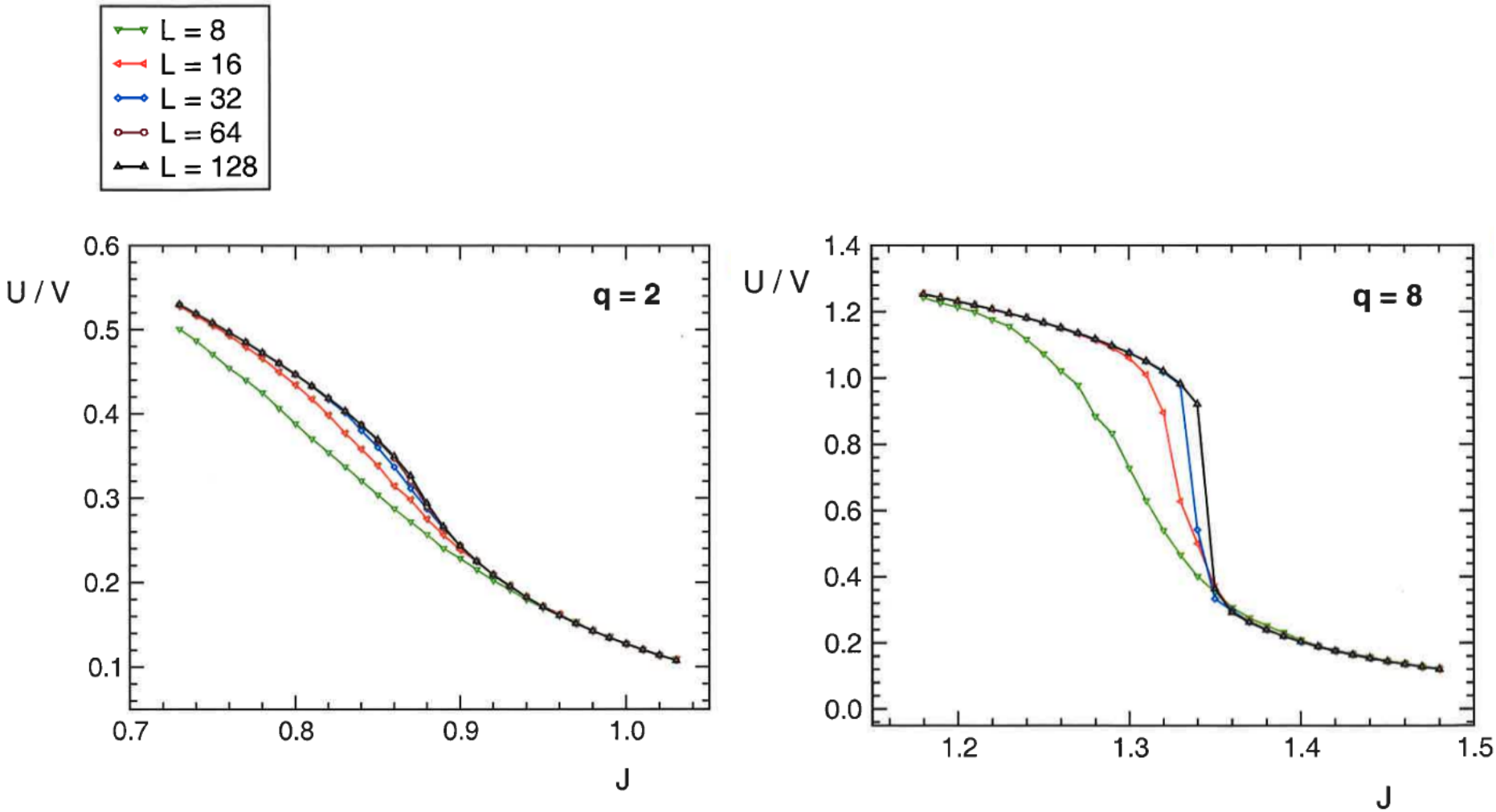
Measuring the components of the magnetisation
In practice the components are ordered:
$M_1 \geq M_2 \geq \ldots \geq M_q$
global permutation symmetry allows this

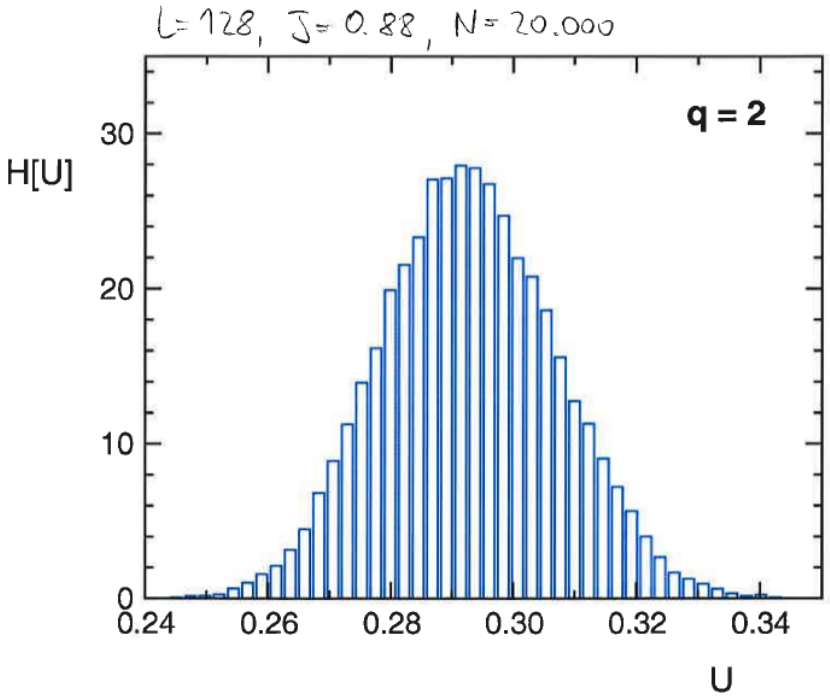
Which of these phasetransitions is 1st and 2nd order?

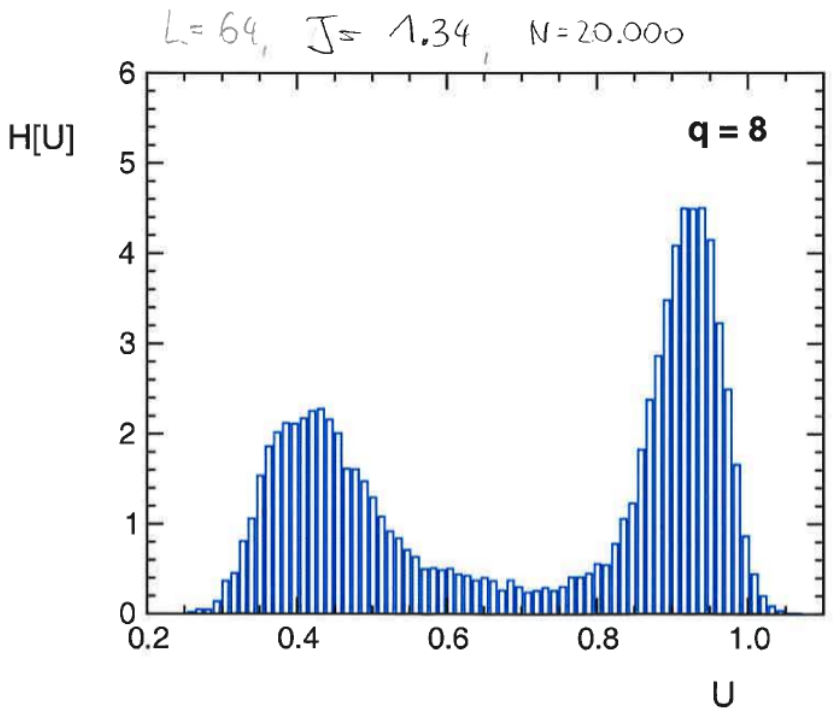
In the literature we can find the following table about the critical couplings:

q	J_c	order
2	0.881	2nd
3	1.005	2nd
4	1.099	2nd
5	1.174	1st
6	1.238	1st
7	1.298	1st
8	1.342	1st
9	1.386	1st
10	1.426	1st

Using different volumes shows the limiting curve:



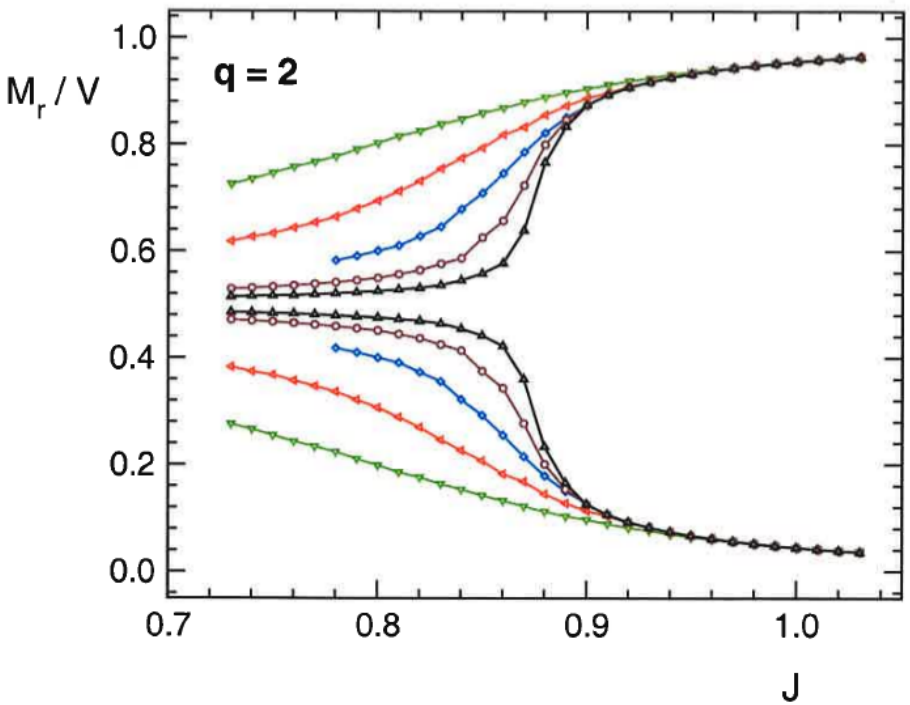


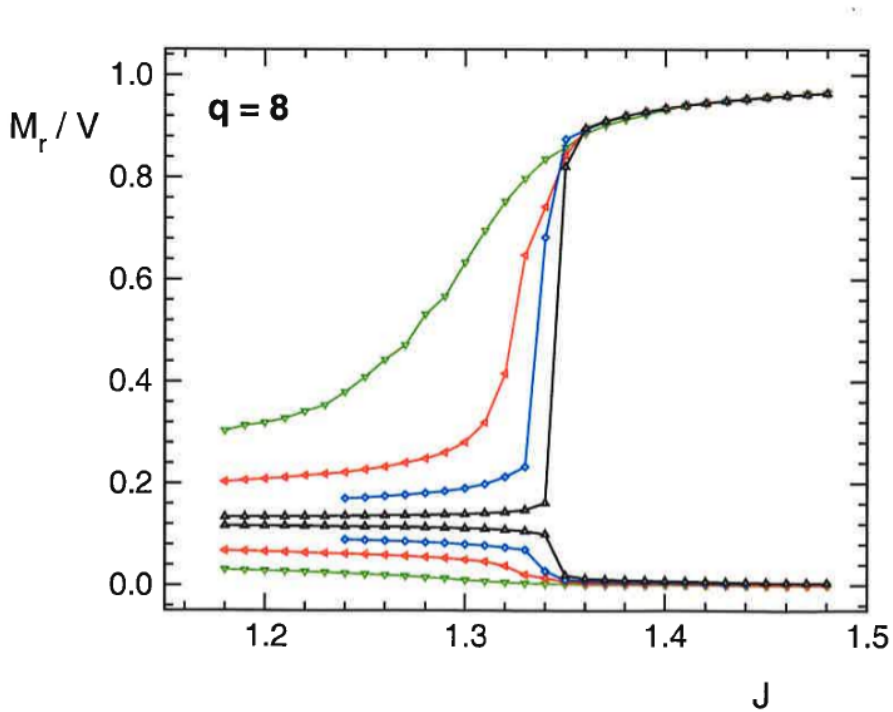


The internal energy is different on the two sides of the phase transition
$\Longrightarrow$ For a first order phase transition we see two distinct peaks

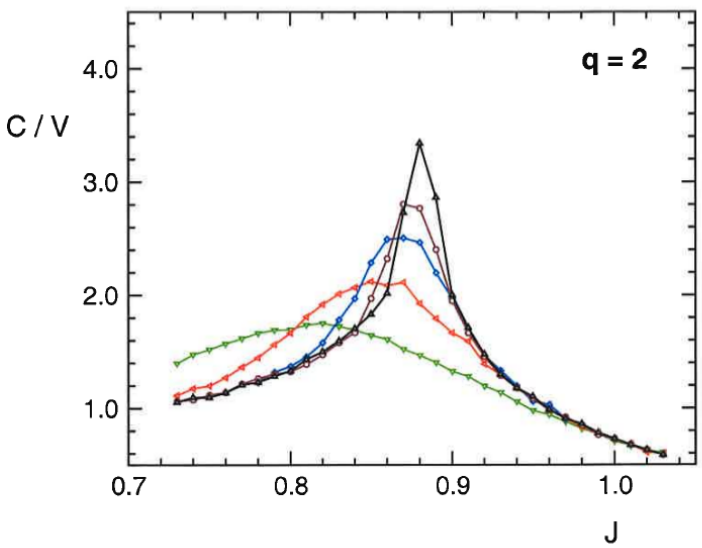
Peaks get more pronounced for increasing volume

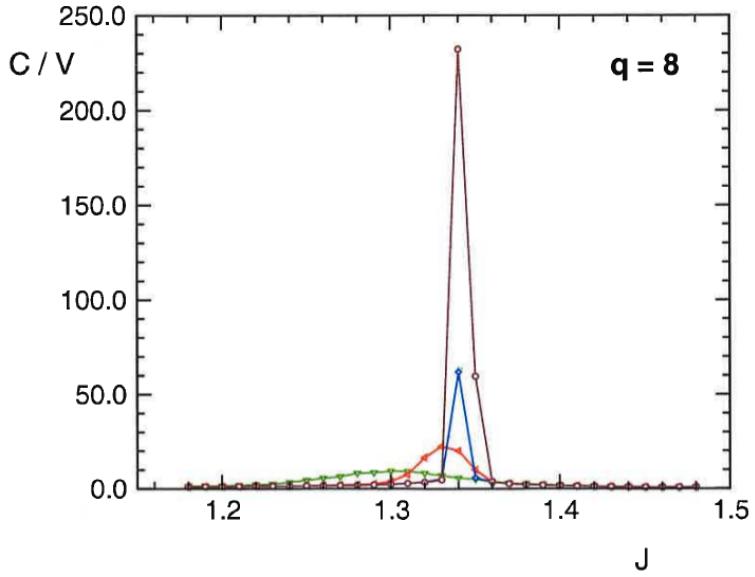
Potts Magnetizaton scaling





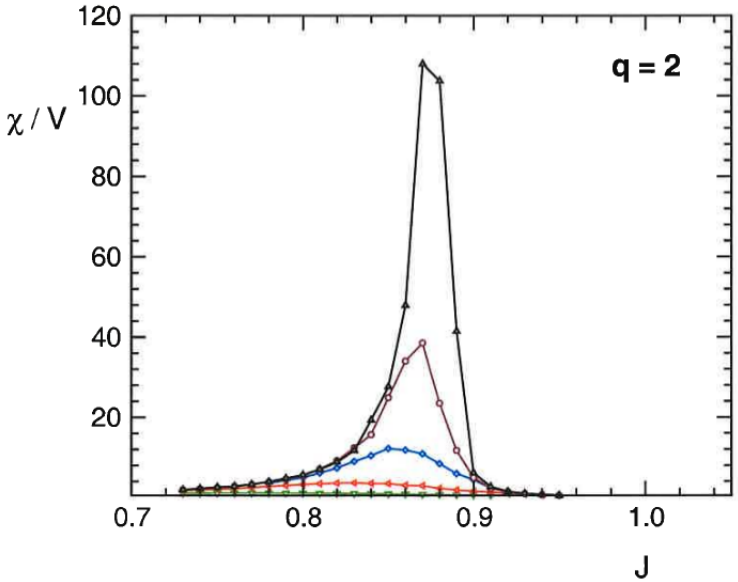
Potts heat capacity, magnetic susceptibility

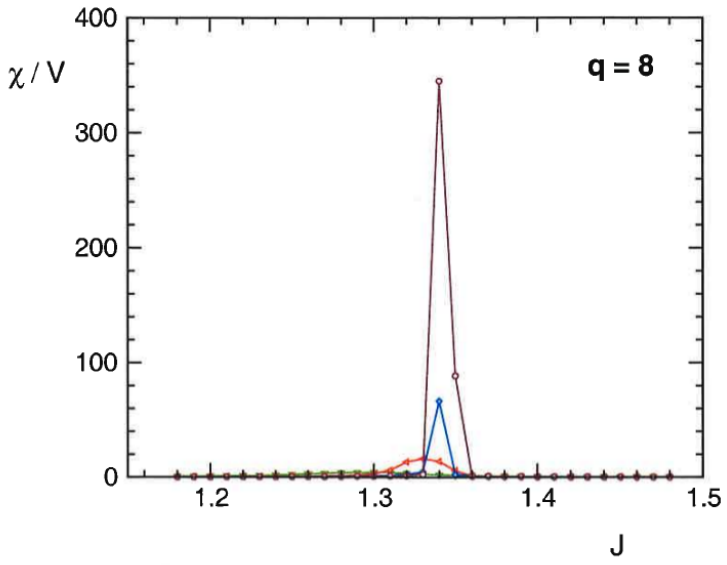




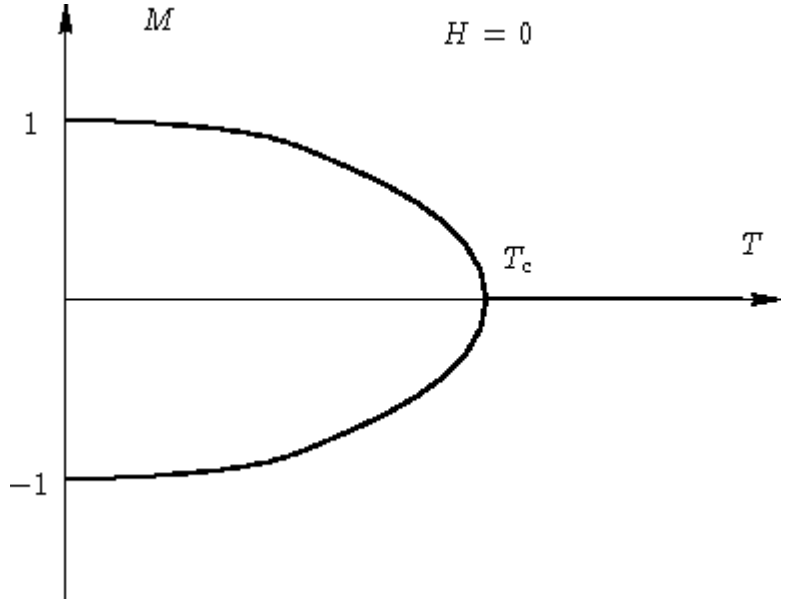
$T_c(L)$ is given by the peak of the susceptibility

Lattice size stops the growth of ξ at $\xi \approx L$
$\Longrightarrow$ in the temperature where $L \sim |T - T_c|^{-\nu}$ $\Longrightarrow$ width of the peak as a function of T: $\sigma(L) \sim L^{-\frac{1}{\nu}}$
we also have $T_c(L) - T_c(\infty) \sim L^{-\frac{1}{\nu}}$





Magnetic susceptibility behaves similarly



Consider the ising model:
Due to the symmetry $s_i \to -s_i$, for every configuration S we have an other configuration with opposite magnetisation and same interaction term.
$\Longrightarrow$ At zero magnetic field, we have:

$$M(T, h = 0) = \frac{1}{N} \sum_{i}^{N} \langle S_i \rangle = 0 \tag{22}$$

We therefore define the order parameter as the limit:

$$M(T) = \lim_{h \to 0} \lim_{N \to \infty} M(T, h) \tag{23}$$

Opposite order of limits is always zero.

We know that for macroscopic systems the magnetization can be nonzero for zero magnetic field.
The state with a given magnetization at $T < T_c$ is metastable
Tunnelings become increasingly rare as the system size is increased.
t_e ergodic time: typical time sent between spin flips. One can measure $M \pm \delta M$ if one uses simulations $t \ll t_e$, where δM is decreased as we increase the simulation time.
When we reach $t \sim t_e$ the average magnetization will be zero also below $T < T_c$
Especially hard in the critical region where we have large fluctuations: $\delta M \sim M$
Practically one uses (root mean square):

$$M_{abs} = M_{rms} = \sqrt{\langle M^2 \rangle} = \left\langle \left(\sum_{i=1}^{N} S_I / N \right)^2 \right\rangle^{1/2} = \frac{1}{N} \left(\sum_{i,j=1}^{N} \langle S_i S_j \rangle \right)^{1/2} \quad (24)$$

Especially important for isotropic spin systems such as $O(2)$ where there is no metastability at $h = 0$

$$M_{abs} = M_{rms} = \sqrt{\langle M^2 \rangle} = \left\langle \left(\sum_{i=1}^{N} S_I / N \right)^2 \right\rangle^{1/2} = \frac{1}{N} \left(\sum_{i,j=1}^{N} \langle S_i S_j \rangle \right)^{1/2} \tag{25}$$

M_{abs} is nonzero at all temperatures, no strict phase transition.
At infinite temperature: $\langle S_i S_j \rangle = \delta_{ij} \implies M_{abs} = 1/\sqrt{N}$

$G(r_{ij}) = \langle S_i S_j \rangle$ is a **correlation function** or **two point function**. At the critical temperature, we have

$$G(r_{ij}) = G_0 |r_{ij}|^{-(d-2+\eta)} \tag{26}$$

which defines the critical exponent η

Suppose we have periodic boundary conditions, than $\langle S_i S_j \rangle$ depends only on the relative position of i and j

$$M_{rms} = \frac{1}{N} \left(\sum_{i,j=1}^{N} \langle S_i S_j \rangle \right)^{1/2} = \left(\frac{1}{N^2} \sum_{i,k} \langle S_i S_{i+k} \rangle \right)^{1/2} = \left(\frac{1}{N} \sum_{k} \langle S_0 S_k \rangle \right)^{1/2} \tag{27}$$

if we have a finite system size, the maximal distance we can have is $L/2$
At the critical temperature

$$\sum \langle S_0 S_k \rangle \sim \int_0^{L/2} r^{d-1} G(r) dr \sim \int_0^{L/2} r^{d-1-d+2-\eta} dr \sim L^{2-\eta} \tag{28}$$

with $N = L^d$ we have for the OP:

$$M_{rms} \sim (L^{2-d-\eta})^{1/2} \sim L^{-\beta/\nu} \tag{29}$$

The second relation follows by usage of scaling laws
$2 - \eta = \gamma/\nu, \quad d\nu = 2\beta + \gamma$

Before we had:

$$\chi \sim \chi_0 |t|^{-\gamma}, \quad \xi \sim \xi_0 |t|^{-\nu} \tag{30}$$

$\Longrightarrow \chi \sim \xi^{\gamma/\nu}$. In a finite box ξ can not be larger than L.

$$\chi = \xi^{\gamma/\nu} \chi_o(L/\xi) \tag{31}$$

χ_0 should be constant for $x \gg 1$, and $\chi_0(x) \sim x^{\gamma/\nu}$ as $x \to 0$
Now define $\tilde{\chi}(x) = x^{-\gamma}\chi_0(x^{\nu})$

$$\begin{aligned} \chi &= \xi^{\gamma/\nu}\chi_o([(L/\xi)^{1/\nu}]^{\nu}) = \xi^{\gamma/\nu}(L/\xi)^{\gamma/\nu}(L/\xi)^{-\gamma/\nu}\chi_o([(L/\xi)^{1/\nu}]^{\nu}) \\ &= L^{\gamma/\nu}\tilde{\chi}((L/\xi)^{1/\nu}) = L^{\gamma/\nu}\tilde{\chi}(L^{1/\nu}|t|) = L^{\gamma/\nu}\tilde{\chi}(L^{1/\nu}t) \end{aligned} \tag{32}$$

$\tilde{\chi}$ is an unknown function, the **scaling function** of the susceptibility. Allows the measurement of critical exponents through data collapse.
Similarly one can derive:

$$c_v = L^{\alpha/\nu}\tilde{c}_v(L^{1/\nu}t), \quad m = L^{-\beta/\nu}\tilde{m}(L^{1/\nu}t) \tag{33}$$

(They all follow from a scaling form of the free energy, now also involving finite size L)

Starting from the scaling form

$$\chi(s^{y_t} t, s^{y_h} h, L/s) = s^x \chi(t, h) \tag{34}$$

We again obtain:

$$\chi = L^{\gamma/\nu} \tilde{\chi}(L^{1/\nu} t) \tag{35}$$

(This tells us how to expand the scaling form to the finite size)

Now we can measure the peak at $|t| = 0$

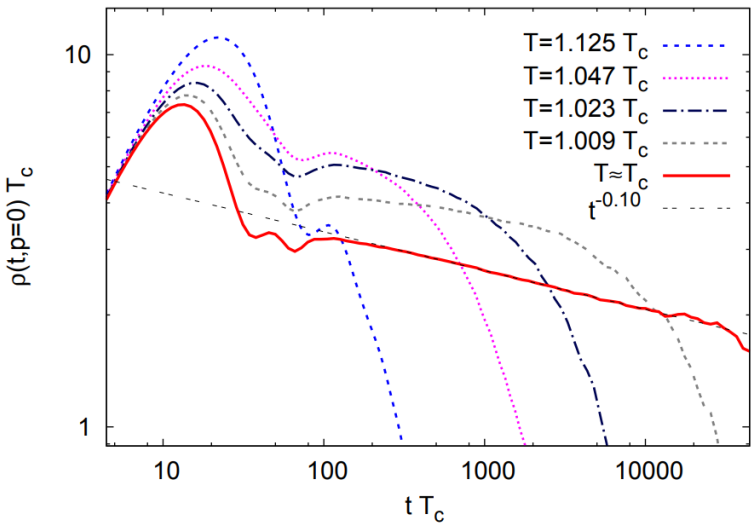
$$\chi(t = 0) \sim L^{\gamma/\nu} \tag{36}$$

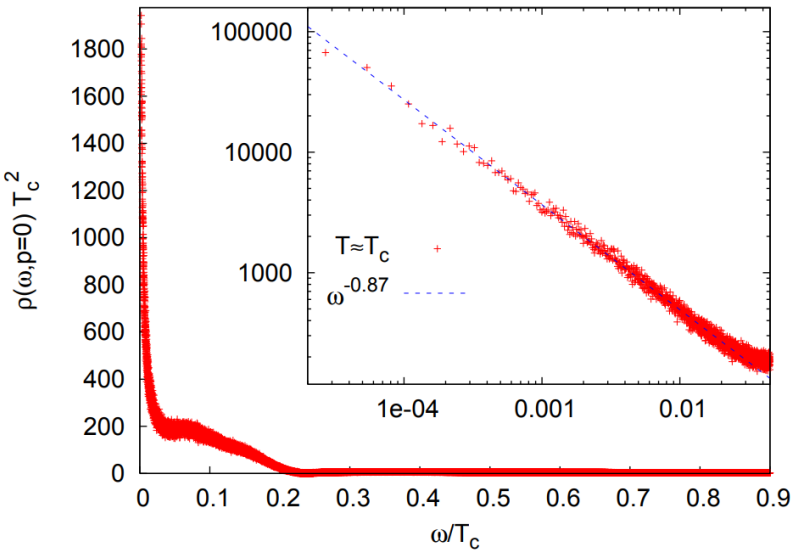
scaling corrections might make numerical calculations hard:

$$A(L) = L^x (A_1 + A_2 L^{-x_2} + \ldots + B \ln L + \ldots) \tag{37}$$

Possible if the system size is large enough and one gets close enough to critical parameters

Two point function of scalar model with Z_2 symmetry on 1024x1024 lattice:





Non universal behavior ($\sim$ regular part) is also visible – one judges where the universal part is by eye

One needs large lattices, well-tuned parameters, high accuracy $\rightarrow$ can be demanding

Otherwise one can use **Finite size scaling**

Simulations around the critical region are typically hard:
1.: Critical fluctuations are large $\Longrightarrow$ Statistical errors will be large
2.: correlation length diverges: cluster sizes increase. Local update inefficient in flipping clusters

The first property can not be changed, the physics of the 2nd order phase transitions dictates this.

The second property means that the autocorrelation time of the simulation grows around the critical point. This is called **critical slowing down**

$$\tau \sim |t|^{-z\nu} \sim \xi^z \tag{38}$$

z is called the dynamical exponent. z is algorithm dependent
Obtaining a new configuration thus costs $\sim L^{d+z}$ computer time

For 2d Ising model with the local Metropolis update: $z = 2.1665 \pm 0.0012$
Advanced algorithms Cluster algorithms, worm algorithm improve on this

We a given a function $f(x_1, \ldots, x_n)$. We want to find the minimum (or maximum) $\sim$ finding the ground state in some energy landscape
Finding a local maximum is relatively easy, finding the global minimum is usually hard (without more information on the function)

IF the landscape is rugged finding the minimum is very hard. Computational complexity grows faster than any power of the system size.

NP-complete optimization problems:

- Travelling Salesman problem
- Graph partitioning
- Graph coloring
- Knapsack problem

Sometimes we don't need the global minimum, we just want to find a minimum which is close to the global one, with preferably a fast algorithm.

Idea: Let's find the ground state by using a $T = 0$ MC simulation
We can get stuck at a local minimum $\rightarrow$ add heat and slowly cool down. $\Longrightarrow$ we control the temperature of the system in a predetermined way.
More heating and cooling cycles makes this effective: **Simulated Annealing**
Some experimentation with the *Annealing Schedule* is needed

Example: **Travelling Salesman problem**
we have to make a round trip getting to N cities by visiting each of them exactly once. Which round trip gives the minimal distance?

State of the system: permutation of the cities
Hamiltonian: total path length
Update proposal 1: exchange two random cities in the permutation
Update proposal 2: remove a set of cities along a path and replace them with the same cities in the opposite order
Update proposal 3: remove a set of cities along a path and insert them back into an other random place in the path

Another optimization method with inspiration from Darwinian evolution
Survival of the fittest $\rightarrow$ optimization problem

- genetic code
- cross breading
- mutations
- death of the least fit

In nature the environment keeps changing and the species represent the environment as well.
In our case the fitness criteria is constant $\rightarrow$ simpler problem

We need to implement a **Fitness function** which defines the optimization problem $f(s) =$min. where s is the **genetic representation** of the solutions to the problem (e.g. an ordering of the cities, a coloring of a graph, etc.)

We can implement sexual reporoduction in which two parents combine to give an offspring (easy if we have a binary genetic representation, can be complicated for e.g. permutations, see in the projects)

Chromosome s_1	111011 | 00100110110
Chromosome s_2	011011 | 11000011110
Offspring s_3	111011 | 11000011110
Offspring s_4	011011 | 00100110110

There can be asexual reproduction where we keep the best members of the pool with perhaps some mutations.

Important terms, parameters:
pool: A set of N "solutions" at a certain point in time. We generate offspring from it, kill off the weakest ones, then we have the next *generation*
Mutation rate: how often random mutations take place
Crossover rate: how often crossover takes place (generally parameters of the generation of offspring from two parents)
Selection principle: how parents are selected (random, elitistic)

Given a pool of items with weights and values, put items into a knapsack such that the value is maximal, and the weight is limited.

p_i = value
w_i = weight

genetic representation:
string of bits b_i
signalling whether we take an i-th item

Fitness function:
$f = \sum p_i b_i$
(we stop counting when we hit the weight limit)