Simulations in Statistical Physics

Course for MSc physics students

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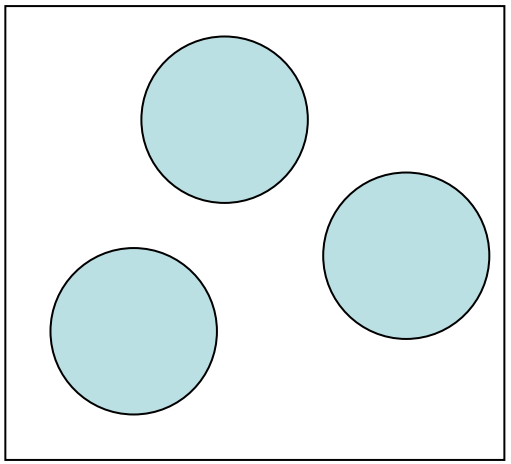
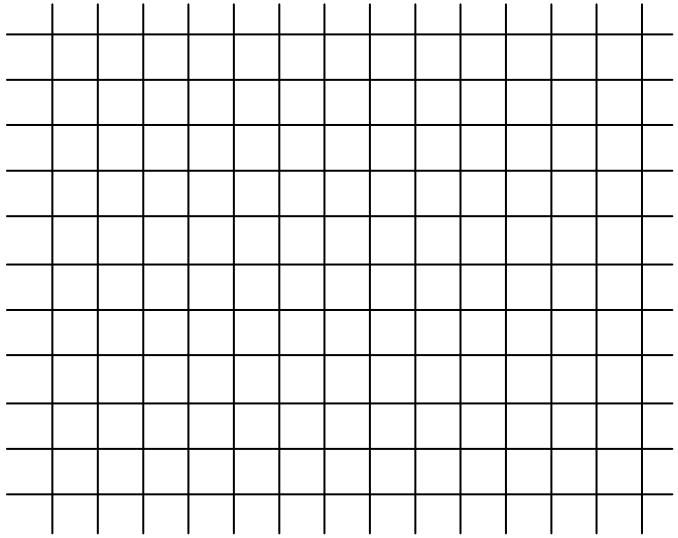
Lecture 3

Physics problem → model → algorithm
Depending on the computational capacity:
Sample size, # of runs
Boundary conditions (BC)

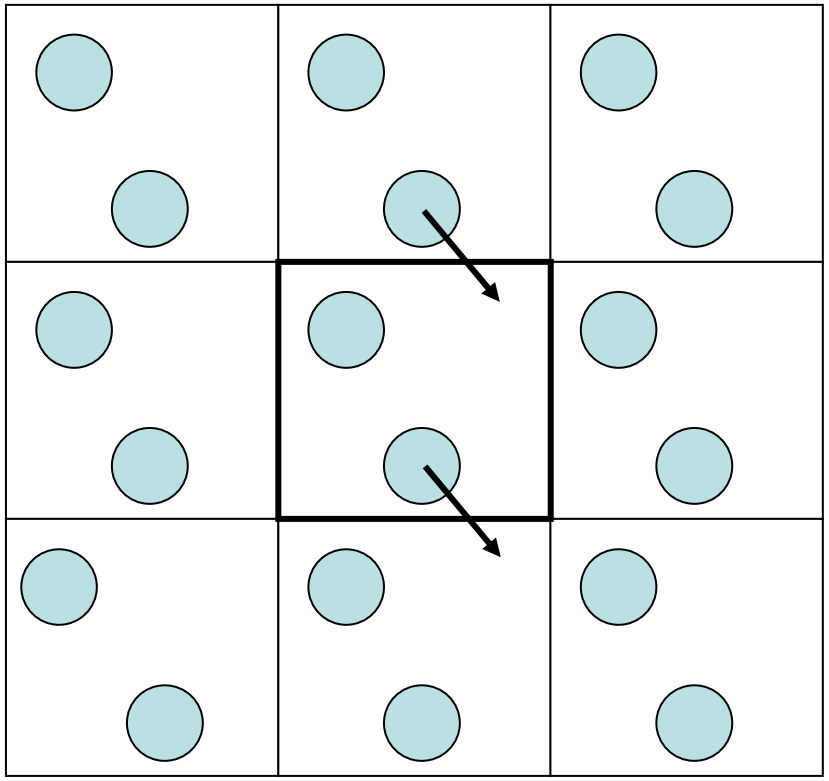
a) Free BC. Particles (spins) have no interaction outside the box. The walls have to be specified (e.g., elastic). For lattice models interactions are cut at the boundaries



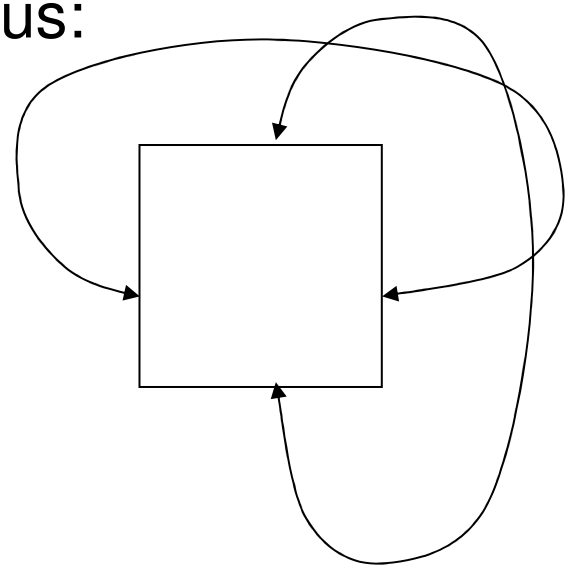


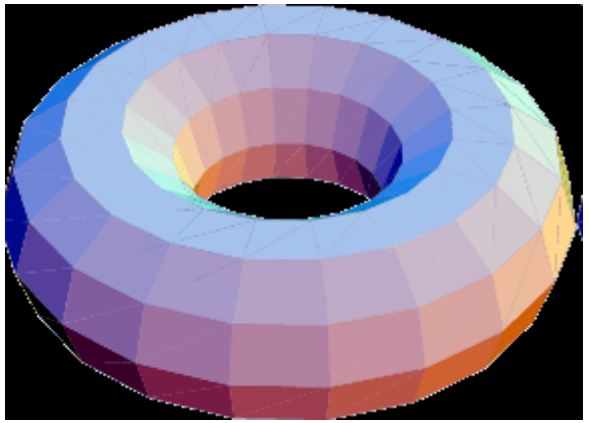
For small systems strong boundary effects leading to spurious behavior

b) Periodic BC. The opposite d-1 dimensional boundaries of the d-dimensional box are defined as neighbors.



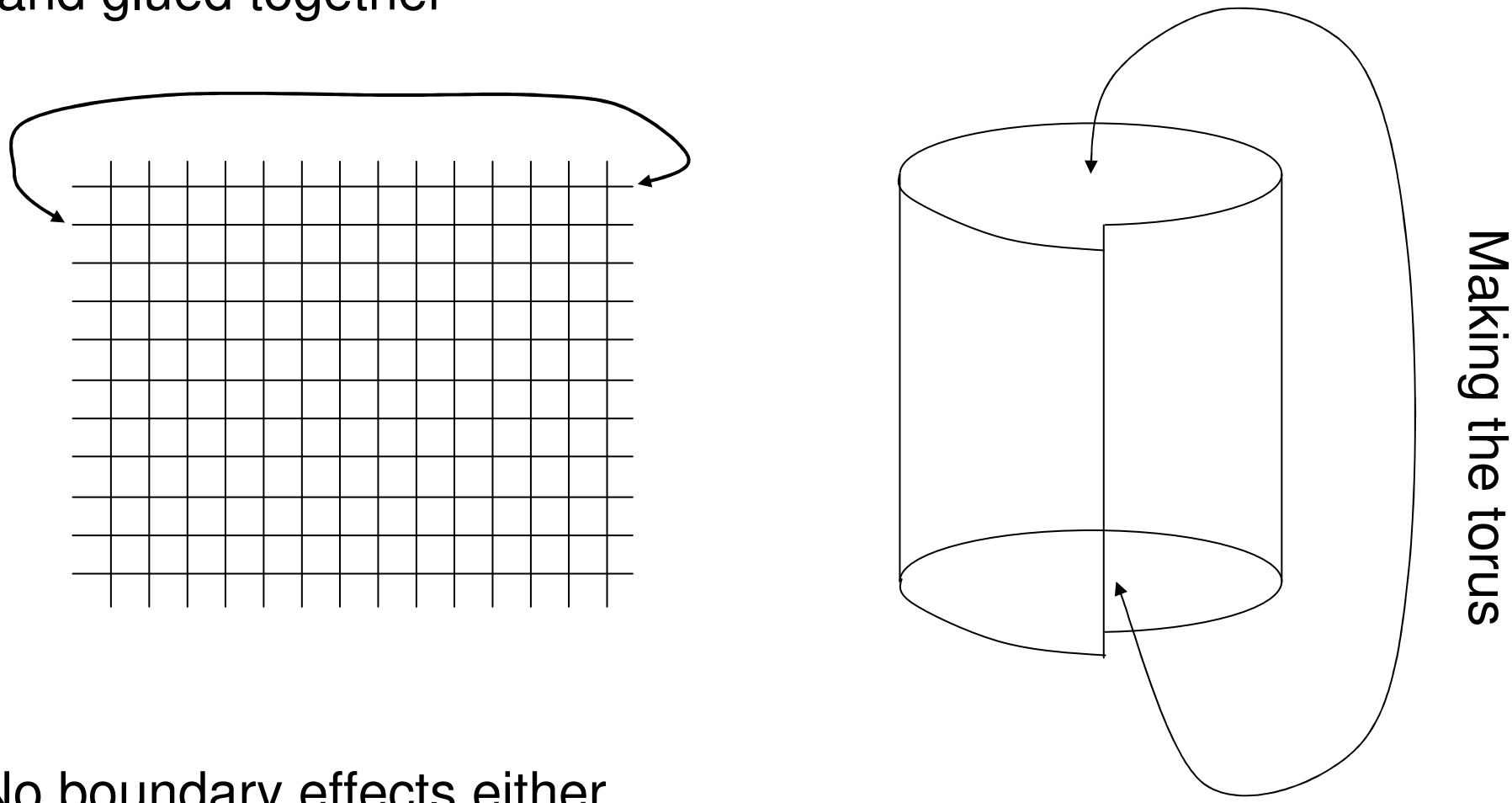
In d = 2 this corresponds to putting the system onto a torus:





No boundary effects
(But finite size effects are there!)

c) Helical boundary conditions. The opposite parts are shifted and glued together

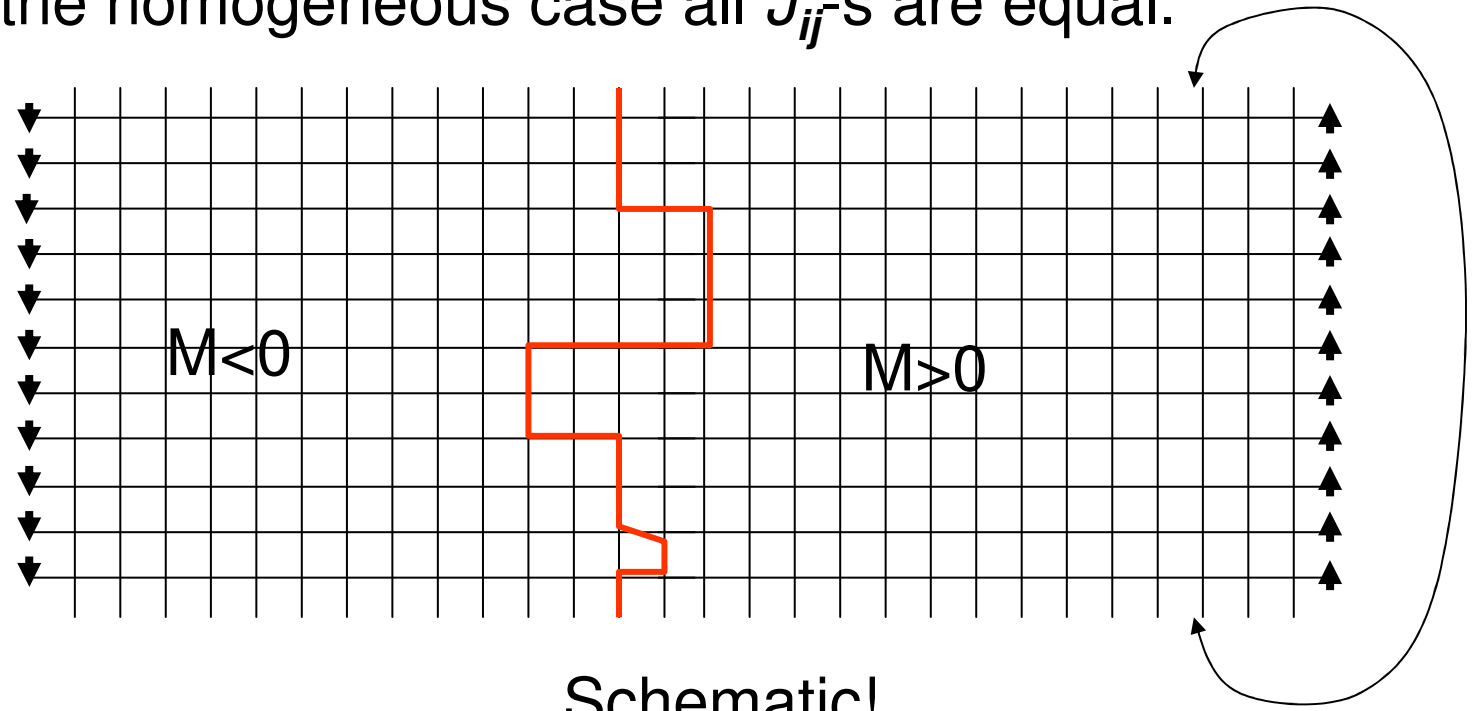


No boundary effects either.
Advantage: If information about a lattice is stored in an array of one variable, no special measures needed at the end of the rows (no „if” decisions or copying 1st and last rows).

d) Physical boundary conditions. Special BC-s may reflect physical situations. E.g., equilibrium interface fluctuations can be studied in an Ising model, where the two domains are prepared by the BC-s. The Ising model in zero external field is:

$$H = -\sum_{ij} J_{ij} S_i S_j$$

where S_i is an Ising „spin" with two possible states (+1 or -1). In the homogeneous case all J_{ij}-s are equal.



Schematic!

Basic approaches to calculating thermodynamic averages:

1. Molecular dynamics (MD). We try to reproduce what nature does: Solution of the equations of motion. Temporal averages can be calculated from the trajectories of the particles.
2. Monte Carlo (MC) method. We start from the equivalence of temporal and ensemble averages:

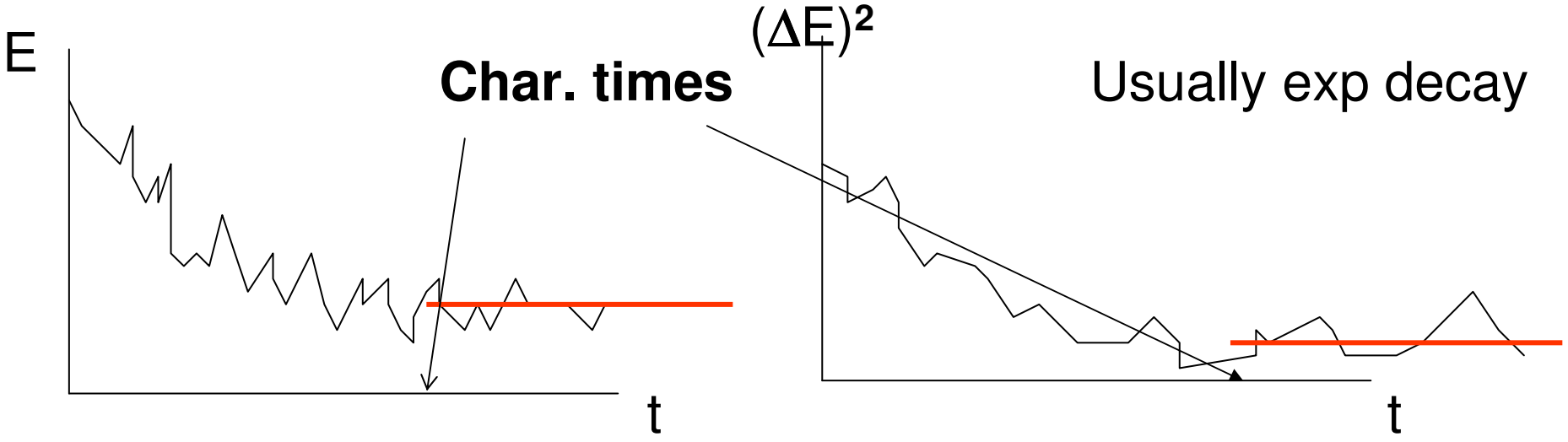
$$\overline{A} = \lim_{T\to\infty} \frac{1}{T} \int_0^T A\big(q(t), p(t)\big) dt \qquad\qquad \overline{A} = \sum A_i P_i^{eq}$$

However, the explicit calculation of P_i^{eq} is difficult, it contains information about the partition function – i.e., the solution of the problem. Moreover, the distributions of statistical physics are sharply peaked, therefore most trials in a simple sampling will lead to zero contributions. Therefore we will use „importance sampling", such that we generate a sequence of configurations according to their equilibrium statistical weights. This sequence defines an „artificial" time.

This way even MC averages are calculated as temporal averages.

Let us consider a dynamic quantity A (energy, kinetic energy, magnetization etc.) for which we are interested in the equilibrium expectation value.

First we have to decide if the system is already in equilibrium. Equilibrium means stationarity, so we have to find indicators for this. A good candidate is just the total energy of the system and its moments.



Measurements are time consuming.
Consecutive configurations are strongly correlated – no new information in the time integral.

Define correlation time τ through the time dependent corr. fn.

$$\phi_{EE}(t) = \frac{\langle E(t')E(t'+t)\rangle - \langle E\rangle^2}{\langle E^2\rangle - \langle E\rangle^2} \qquad \tau = \int_0^\infty \phi_{EE}(t)dt$$

Sampling is reasonable in intervals > τ. Only in this case can be expected that accuracy increases with the number *N* of sampling points as $1/\sqrt{N}$

Characteristic length and time finite only off the critical point.

What if we are interested in critical behavior?

Finite size scaling (FSS)

Close to the critical point it behaves like:

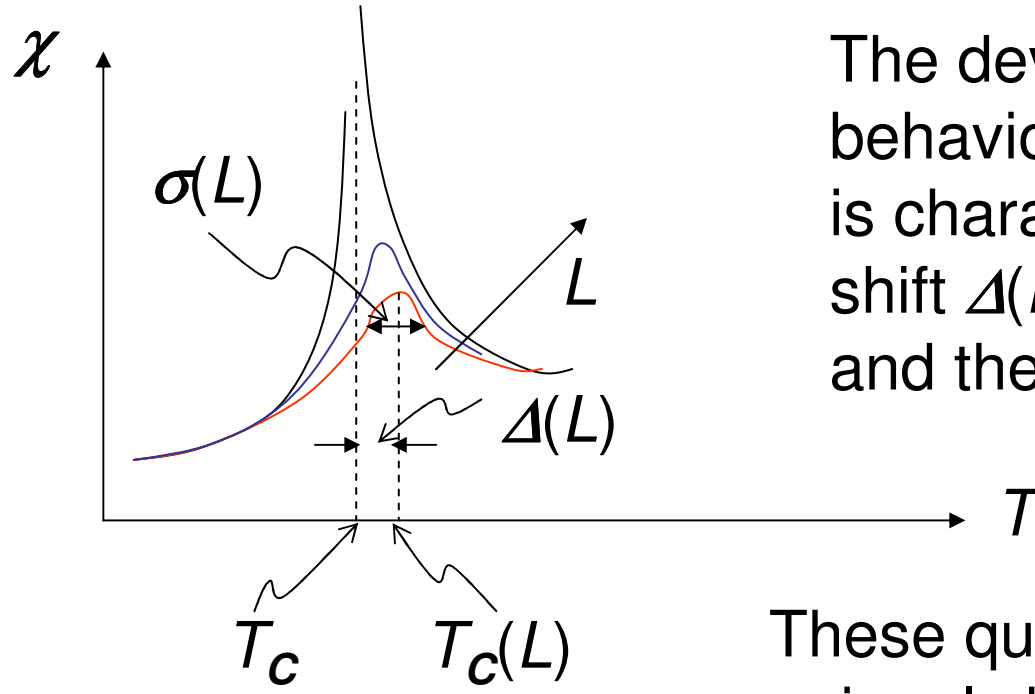
$$G(r,t,h) \propto b^{-2\beta/\nu} G(r/b, b^{y_t} t, b^{y_h} h) \quad \text{for } t \to 0^{\pm}, h \to 0.$$

where $\xi \propto |T - T_c|^{-\nu}$ is the correlation length.

$$C_{(h=0)} \sim |t|^{-\alpha}$$
$$M_{(h=0)} \sim (-t)^{\beta} \quad , \quad t < 0$$
$$\chi_{(h=0)} \sim |t|^{-\gamma}$$
$$M_{(t=0)} \sim h^{1/\delta}$$

Far from the critical point $\xi << L$, the behavior is similar to that of the bulk equilibrium in the TDL: no pronounced L-dependence
Near to the critical point $\xi >> L$: strong L-dependence

How to find TDL behavior? Use just this L-dependence! E.g., for the susceptibility in a PM-FM transition:



The deviation of the finite size behavior from that of the TDL is charaterized by th
shift $\Delta(L)$
and the width $\sigma(L)$

These quantities are not defined uniquely but simple factors do not matter (scaling is important)

$\xi \propto |T - T_c|^{-\nu}$ In a finite size sample the linear size L will play the role of the correlation length, if ξ exceeds L. The characteristic temperature, where this happens is

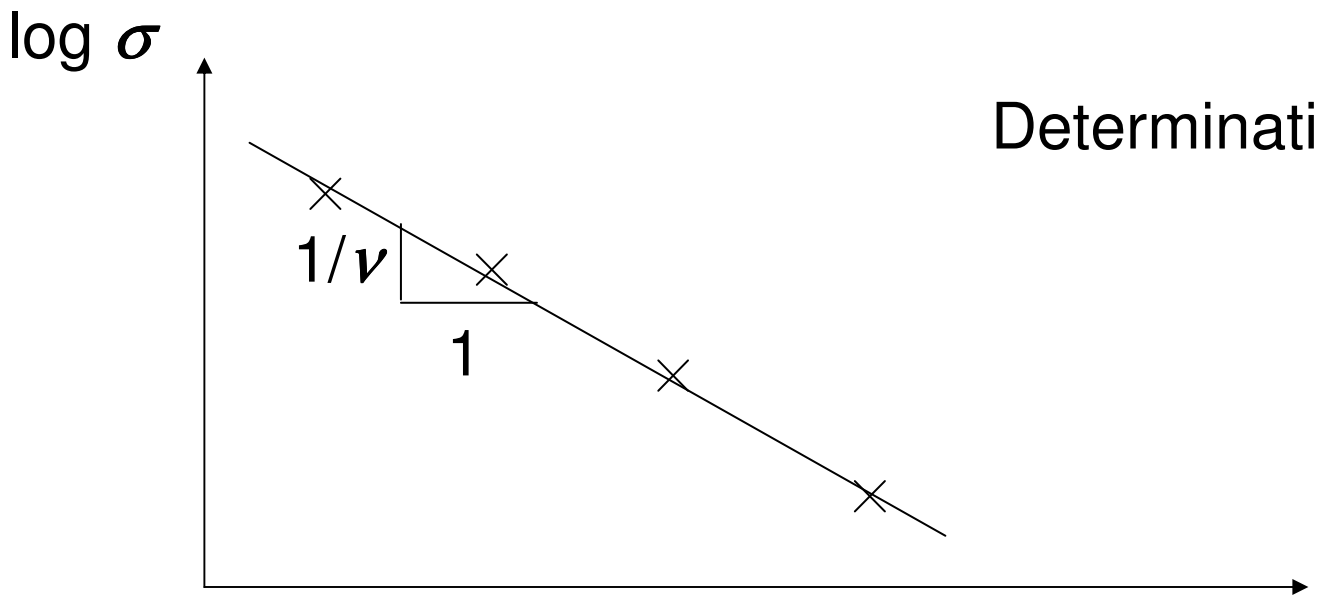
$$L \propto |T(L) - T_c|^{-\nu}$$

If we accept that there is only one characteristic size in the TDL, then there is only one characteristic temperature regime in the finite size system, where significant deviations from the TDL can be seen. It follows that

$\Delta(L) \sim L^{-1/\nu}$

$\sigma(L) \sim L^{-1/\nu}$ (*)

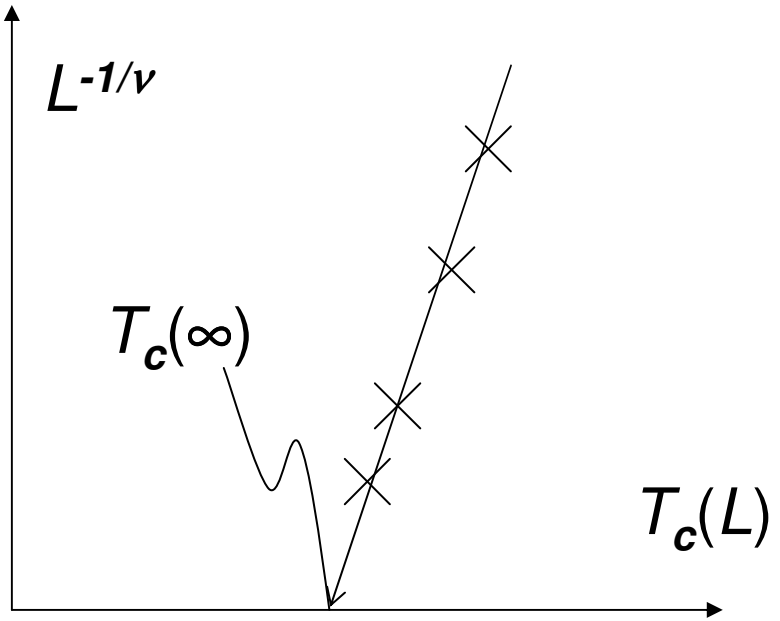
We measure σ and L and have to calculate T_c and ν
Fortunately (*) does not depend on T_c



Determination of ν

Using ν we can calculate $T_c(\infty)$

The straightness of the extrapolation line is a check of the goodness of ν



In critical phenomena we have usually two independent exponents: One more is needed

The generalized homogeneity assumption for the correlation function implies that (the critical part) of the susceptibility is also a gen. hom. fn. of its variables:

$$\chi(t,h) = b^{x}\chi(b^{y_t}t, b^{y_h}h)$$

Choosing $h = 0$ and $b = t^{-1/y_t} = t^{-\nu}$, we have

$$\chi(t,0) = |t|^{-\nu x}\chi(1,0) \sim |t|^{-\gamma} \quad \text{i.e.,} \quad x = \gamma/\nu$$

Let us extend the homogeneity assumption (*) to the variable L!

$$\chi(t,h,L) = b^{x}\chi(b^{y_t}t, b^{y_h}h, L/b)$$ Choosing now $t = 0,\ h = 0,\ b = L$

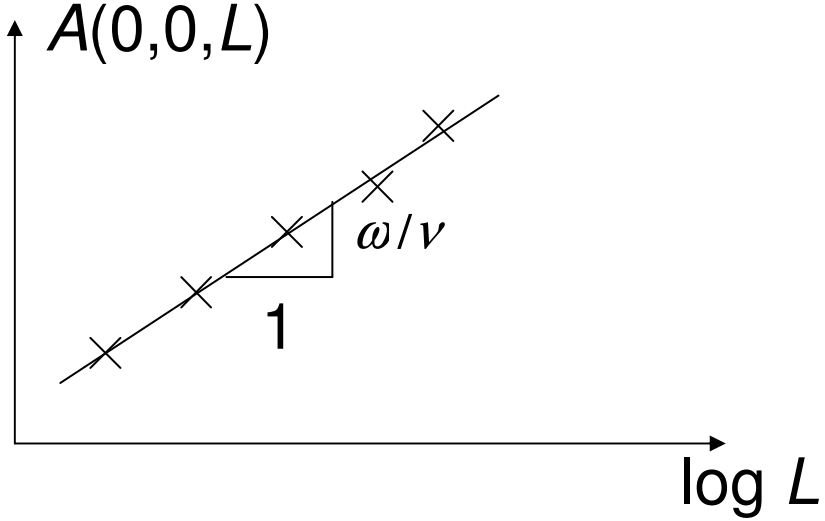
$$\chi(0,0,L) = L^{\gamma/\nu}\chi(0,0,1)$$

I.e., measuring χ at the critical point, we can calculate ν

Similarly for any quantity, which has the critical behavior in TDL

$A(t,0) \sim |t|^{-\omega}$, we have for finite size systems at the critical point

$A(0,0,L) \sim L^{\omega/\nu}$



If precise enough data are available the scaling is not so nice: the lines on the log-log plots bend. This is because the simple power law scalings are valid only asymptotically and what we measure by linear fits are „effective exponents”. Since we can never reach „Asymptotia”, there will be corrections to scaling:

$A(0,0,L) = A_1 L^{\omega/\nu}(1 + \mathrm{A}_2 L^{-x_2} + ...)$

The numerical handling of these corrections is a major challenge.

Cluster counting and critical behavior in percolation

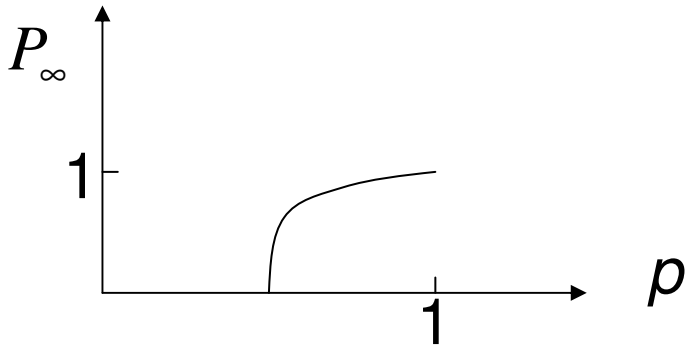
We have a mixture of conducting and insulating grains and are interested in the electrical properties of this ensemble. Or monomers build a three dimensional web by random link formations and we are interested in when the whole gets interconnected (gelation). In these (and many other) problems disorder plays a crucial role. A paradigmatic model is: Percolation.

Let us take a square lattice where the lattice sites can have two states: Occupied/empty, conducting/insulating, black/white etc. We occupy these sites with an uncorrelated probability *p* (occupation probability). The configurations will depend on this control parameter *p.*

Although the sites are independently occupied we ask particular questions about these systems such that the related behavior is highly non-linear. The questions are about the connectivity properties of such random systems. We define a cluster as a set of points, which can be mutually reached from each other using only nearest neighbor paths through occupied sites. If p is small, we have only small clusters. At the other extreme, we have almost a giant connect part, with some finite clusters and clusters of empty sites. The giant component becomes infinitely large in the TDL ($L \rightarrow \infty$, $p =$ const).

Naturally we can assume that there is a transition at p_c from the state, where there is no infinite cluster to that where there is.

The indicator (order parameter) is: P_∞ the percolation probability, which is the probability that an occupied site belongs to the infinite cluster.



A basic quantity is the number of s-size clusters per site: n_s

$$n_s = \frac{\#\text{ of s - size clustes}}{N}$$ where $N = L^d$ is the total number of sites.

The probability that an occupied site belongs to a cluster of size s is $p_s = sn_s$. Therefore the following equation is valid:

$$\sum_s p_s + P_\infty + (1-p) = 1$$ The average size S of finite clusters is

$$S = \frac{\sum_s s^2 n_s}{\sum_s s n_s}$$

There is an intimate relationship between thermal critical phenomena and the percolation transition, which can be established using the theory of diluted magnets as well as that of the Potts magnetic models. P_∞ corresponds to the magnetization (order parameter), S to the susceptibility with p being the control parameter (~temperature). There is possibility to introduce the analogue of the magnetic field (ghost site).

The connectivity function $G(\mathbf{r})$ is the probability that two occupied sites belong to the same *finite* cluster. It is a generalized function of its variables and the connectivity length ξ diverges at p_c as

$$\xi \sim |p - p_c|^{-\nu}$$

where even the notation reminds to the thermal phase transitions. Then it is not surprising that we have:

$$P_\infty \sim (p - p_c)^{\beta}$$

$$S \sim |p - p_c|^{-\gamma}$$

indicating that S plays the role of the susceptibility (no wonder, it contains the second moment of n_s.

The key task in simulating percolation systems is cluster counting, i.e., calculating n_s-s.