Simulations in Statistical Physics

Course for MSc physics students

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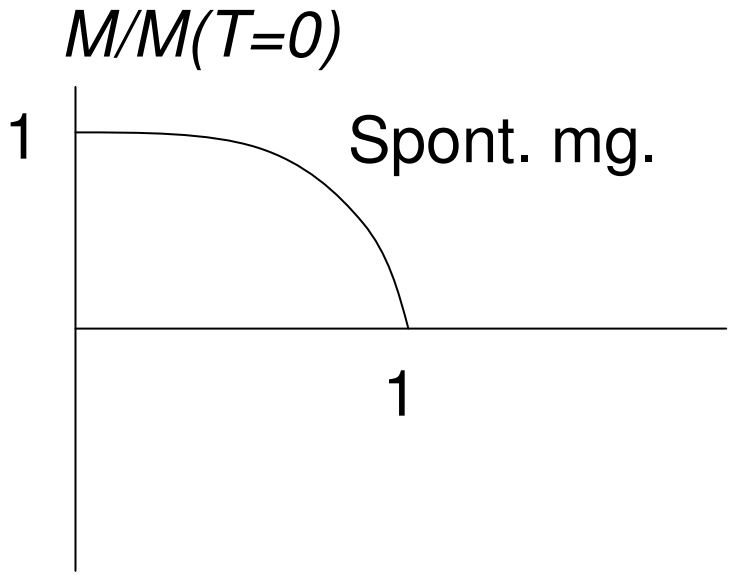
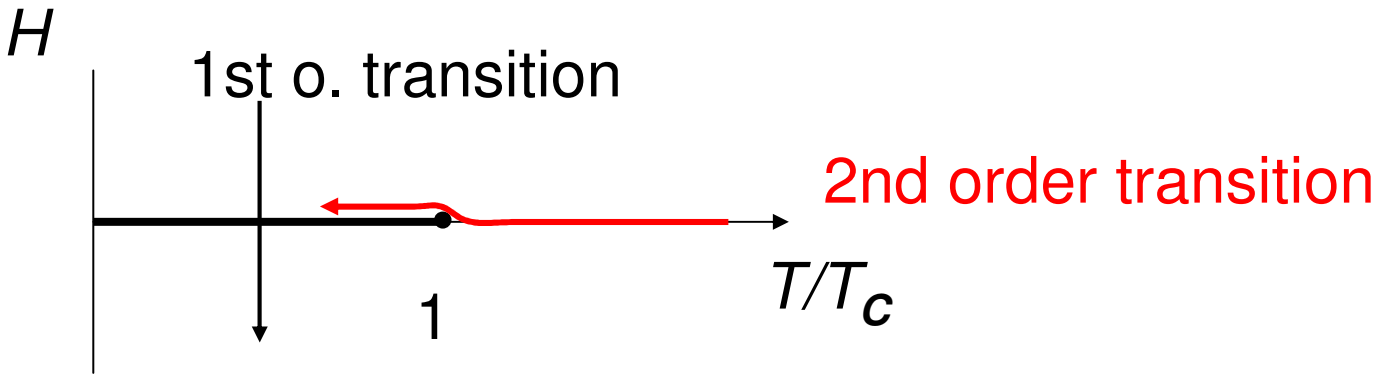
Lecture 2

Para- ferromagnetic phase transition:

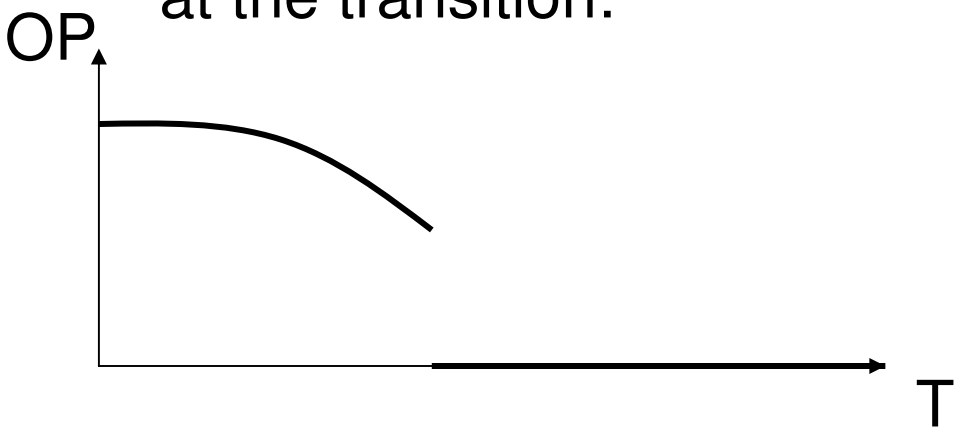


Above the Curie temperature T_c ($H = 0$) there is no spontaneous magnetization (paramagnetic phase).

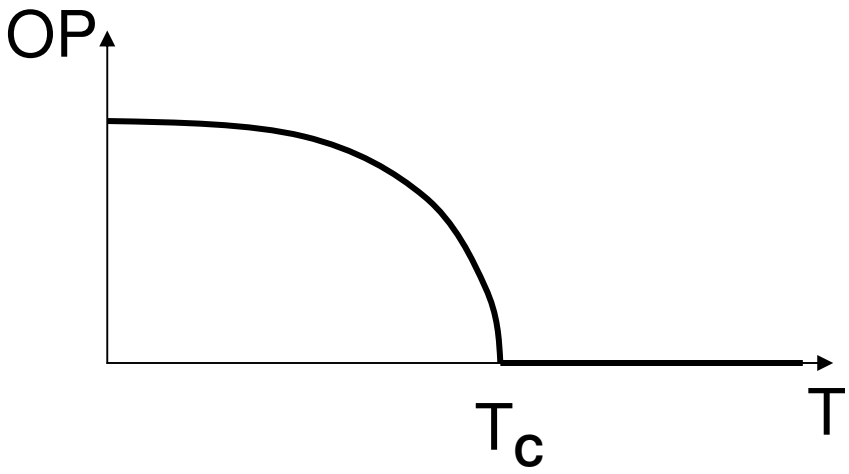
Low temperature phase: Broken symmetry.
Order parameter: Normalized magnetization
Phase diagram:



First order transitions are discontinuous: The order parameter changes discontinuously at the transition:



Second order transitions are continuous:



The continuous transition point is also called critical point (c.f. liquid-gas transitions) and the related phenomena are critical phenomena:

1. Many physical quantities show power law behavior
2. Critical behavior of different systems can be ordered into universality classes, which can be identified by the critical exponents

E.g., he correlation function in a magnetic system is:

$$G(r) = \langle \mathbf{s}(R) \cdot \mathbf{s}(R+r) \rangle \; - \langle \mathbf{s} \rangle^2$$

Where **s** is the local magnetic moment („spin”), and the bracket means thermal average.

Close to the critical point it behaves like:

$$G(r) \approx \frac{1}{r^{d-2+\eta}} \exp\left(\frac{-r}{\xi}\right)$$

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

The correlation length, i.e., the characteristic size of the regions, where the fluctuations are correlated diverges at the critical point, $T = T_c$ and $h = 0$ (h is the external field.)

ν and η critical exponents.

Near to the critical point G is a generalized homogeneous function of its variables:

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

Where $t = (T - T_c) / T_c$ is the reduced temperature. The notation of the exponents follows the conventions. We will use the following relationships:

$$\chi = \beta V \int G(\mathbf{r}) d^3 r = \beta V < (\mathbf{s} - < \mathbf{s} >)^2 >$$

$$\chi = \frac{\partial M}{\partial h} \qquad M = \frac{\partial F}{\partial h} \qquad C = \frac{\partial F}{\partial T}$$

M: magnetization (OP), χ: susceptibility C: specific heat

Starting from the generalized homogeneity of *G,* we obtain:

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

We have altogether 8 exponents ($\alpha, \beta, \gamma, \delta, \eta, \nu, y_t, y_h$)
$y_t = 1/\nu$, $y_h = d - \beta/\nu$,

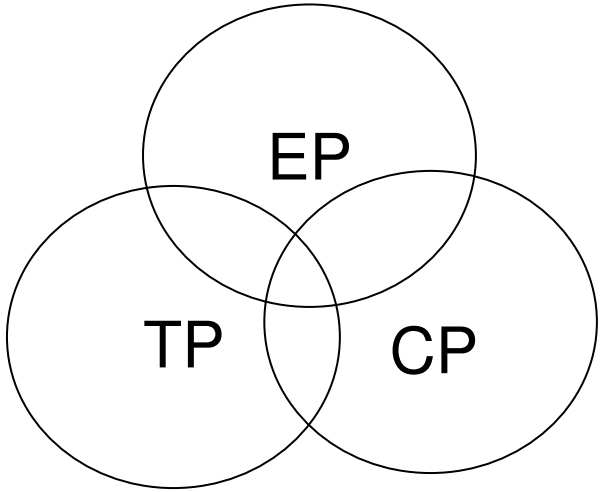
Scaling relations:

$$\alpha + 2\beta + \gamma = 2$$
$$\delta = 1 + \gamma/\beta$$
$$d\nu = 2 - \alpha$$
$$\nu = \gamma/(2 - \eta)$$

Two independent exponents to identify universality classes

COMPUTATIONAL PHYSICS

A new, third methodoligical branch of physics, beside *theoretical* and *experimental* physics



Computational physics: When the MAIN tool of investigating nature is the computer. It operates on models, like theoretical, but analyses data like experimental physics.

Experiments		*Simulations*
Principle of measurement		Algorithm
Apparatus		Program
Calibration		Debugging
Sample		Model
Measurement		Run
	Data collection	
	Statistical analysis	

Basic problem of equilibrium statistical physics: Calculate averages

Simulations:
1. „Do what nature does” → calculate temporal averages
2. Make use of stat. phys.: $< A >= \sum_i A_i P_i^{eq}$

Method 1 is „Molecular dynamics”
2 is „Monte Carlo method”

We start with investigating the equilibrium properties of macroscopic systems. If the characteristic length $\xi << L$, where L is the linear size of the system we can symulate, no much difference between the finite size and the TDL is expected. The opposite situation is more interesting.

Very large systems have to be simulated.
Program efficiency is crucial!

MC trivially needs random numbers.
Although – in principle – MD is fully deterministic rn-s are needed there too, at least for the initial conditions.

We need many „good” random numbers!
Many: They have to be generated on the computer.
I.e., they cannot be random:

Pseudo-random number generators

Algorithms, which produce sequences of numbers $r \in (0,1)$ with behaviors similar to those of uniformly distributed, independent random numbers.

Most high level languages (C, C++, FORTRAN…) and programing environments (MATHLAB, R…) provide System Supplied RNG-s

DANGEROUS!

General remark: **It is good to know what the compouter does!**

„Portable RNG-s”

1. Multiplicative congruential algorithm

$$I_{j+1} = aI_j + c \qquad \mathrm{mod}(m)$$

Needs 3 parameters (*a, c, m*) and – as all RNG-s – a seed, I_0

$$r_{j+1} = I_{j+1} / m$$ Normalization to (0,1)

A simple and efficient version:

$$a = 7^5 = 16807$$

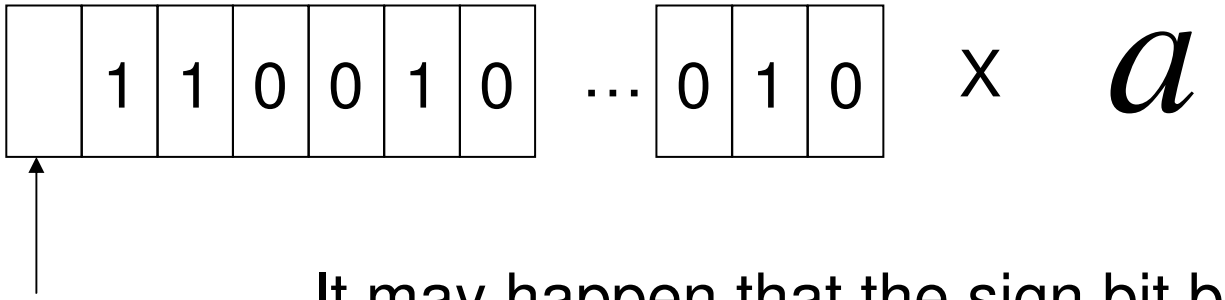
$$m = 2^{31} - 1 = 2147483647$$

$$c = 0$$

$$I_{j+1} = aI_j$$

Automatic type declaration: Variables with first letter *I,J,K,L,M,N* are integers

On a 32 bit machine, where the maximum integer is just *m,* if integer overflow does not cause fatal error the remaining digits are just the appropriate ones:



It may happen that the sign bit becomes 1

$$I_{j+1} = aI_j$$

$$\mathrm{IF}(I_{j+1}.\mathrm{LE}.0)\ \ I_{j+1} = I_{j+1} + m$$

This has to be normalized:

$$r_{j+1} = \mathrm{FLOAT}(\mathrm{I}_{\mathrm{j+1}}) / m$$

In many applications a little trick helps to save time:
Transfer the MC decisions betwenn 0 and m, instead of using numbers (0,1).

Is this a good RNG? Density function: $P(x) = 1 \text{ if } \ 0 \le x \le 1$

independence

Test:

- moments $\int_0^1 x^n dx = \frac{1}{n+1}$
- correlation functions and ratios $C_{q,q'}(t) = \int_0^1 \int_0^1 x^q x'^{q'} P(x, x'(t)) dx dx' = \frac{1}{(q+1)(q'+1)}$
- Fourier spectra

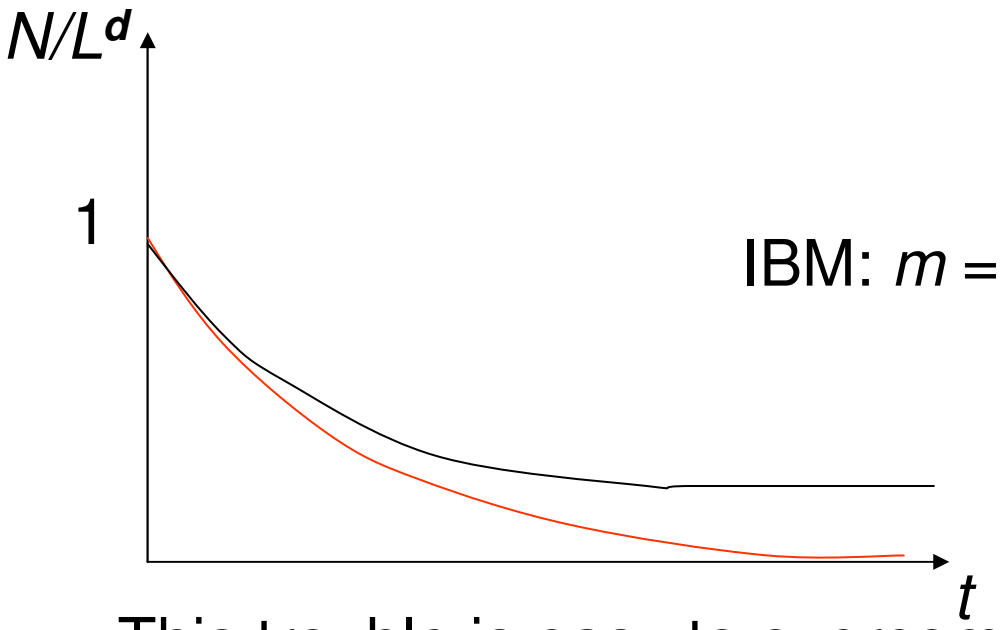
Most RNG-s pass these tests well.
More sophisticated tests of correlations needed. Marsaglia effect

Let us fill an L^d d-dimensional lattice using RNG!

```
IX1=L*RND(IJK)+1
IX2=L*RND(IJK)+1
.
.
IXD=L*RND(IJK)+1
```

If a point is hit, we consider it occupied. Let $N(t)$ be the # of empty points at time t, where time is measured with trials. $N(t)$ should approximately follow an exponential decay.

The Marsaglia effect is that for all congruential multiplicative generators there will be unavailable points (on hyperplanes) if d is large enough.



IBM: $m = 65539$ bad already in $d = 3$!

This trouble is easy to overcome by putting all the points into a single index array of size $L3D = L^3$ (in three dimensions):

```
I3D=L3D*RND(IJK)+1
IZ=I3D/L2D
IY=(I3D-IZ*L2D)/L
IX=I3D-IZ*L2D-IY*L
```

However, the M-effect indicates correlations!

Tausworth (shift register, Kirkpatrick-Stoll) generator

Instead of 1, it has 250 integer random numbers as seeds.

$$J(K) = \mathrm{XOR}(J(K-250), J(K-103))$$

Where $\mathrm{XOR}(L,M)$ means bitwise exclusive or between *L* and *M*

XOR	1	0
1	0	1
0	1	0

This generator is not perfect either. Ziff discovered short range correlations. There is no „good” generator, it depends on the purpose, which one is appropriate.
Two tricks: Warm up the RNG (folklore: throw away ~10000 numbers). Mix different RNG-s (helps also to increase cycle).

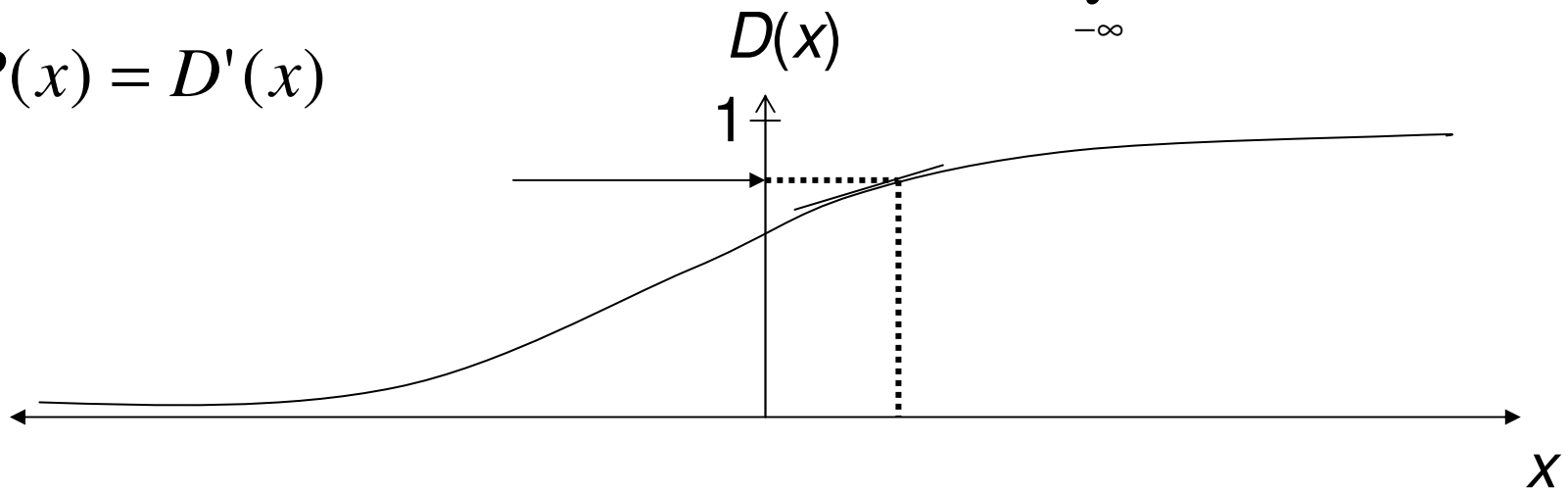
Random numbers with distributions different from uniform

Starting point: We have a „good” RNG generating independent uniformly distributed random numbers between (0,1)

Let *P*(x) be the prob. density function we are interested in.

The probability distribution is $D(x) = \int_{-\infty}^{x} P(x')dx'$

$P(x) = D'(x)$



Generate random numbers $r \in (0,1)$. Then $D^{-1}(r)$ will be distributed according to $P(x)$.

Normally distributed random numbers

$$P(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

Box-Müller method:
Generate two independent, uniformly distributed random numbers r_1 ,$r_2 \in$ (0,1). We obtain two normally distributed numbers:

$$x_1 = \sqrt{-2\ln r_1}\cos 2\pi r_2$$

$$x_1 = \sqrt{-2\ln r_1}\sin 2\pi r_2$$

$$P(x,y) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} = \frac{1}{2\pi} e^{-(x^2+y^2)/2}$$

Radial symmetry → 1d distribution