Statistical Mechanics
E0415

Fall 2023, lecture 5
Percolation: a phase transition

Take home (previous)

…. we skip to the next time….

Summary of a geometrical phase transition

- What is percolation?
- How does it depend on typical parameters like the dimension?
- What kind of physics might be important for?
- What kind of quantities turn out to be important?

What is percolation?

The study of connectedness

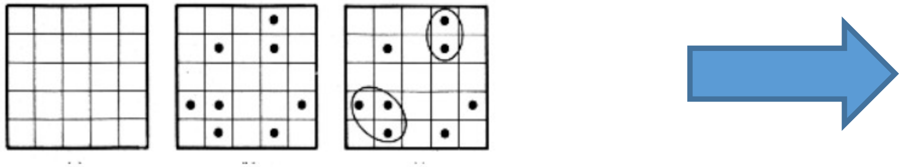
“How far can I go?” – idea of a cluster (of size s, with a given p).

What is this transition at a p_c like?

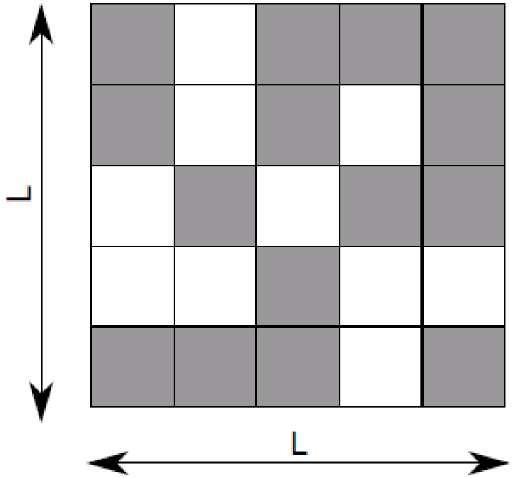
What does it depend on and not depend on?

Why is it relevant?

Suppose a large porous rock is submerged under water for a long time, will the water reach the center of the stone?
(Broadbent and Hammersley, 1957)



Main definitions



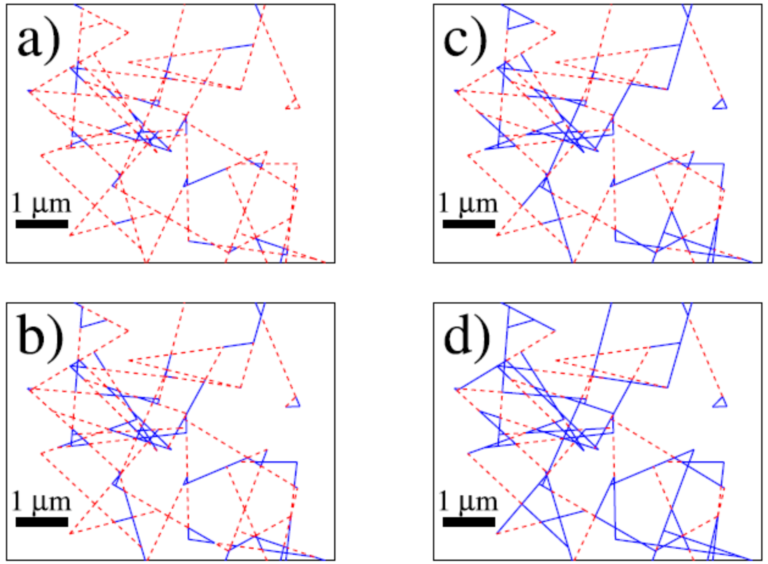
- a cluster is a group of nearest-neighbor occupied sites
- the size *s* of a cluster is the number of sites in this cluster
- the critical occupation probability p_c is the probability *p* at which an infinite cluster appears for the first time in an infinite lattice

Conductivity of random systems


Electrical transport properties of percolating random networks of carbon nanotube bundles


EPL, **91** (2010) 47002

CNT bundle systems: some CNT segments are semiconducting, some are metallic due to impurities (or not). Make a network: is it a good transistor? Which network conducts or in other words percolates?



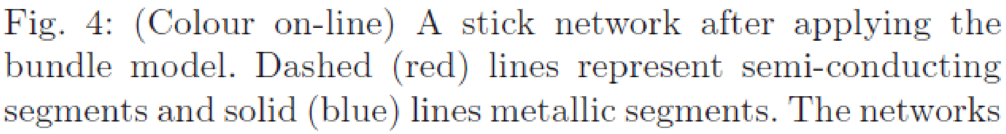
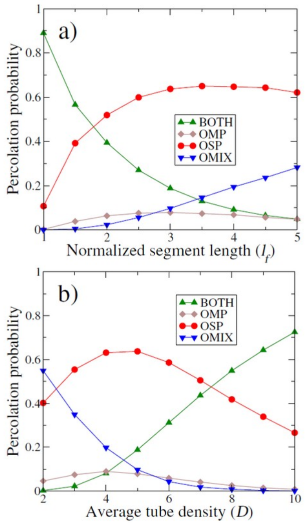
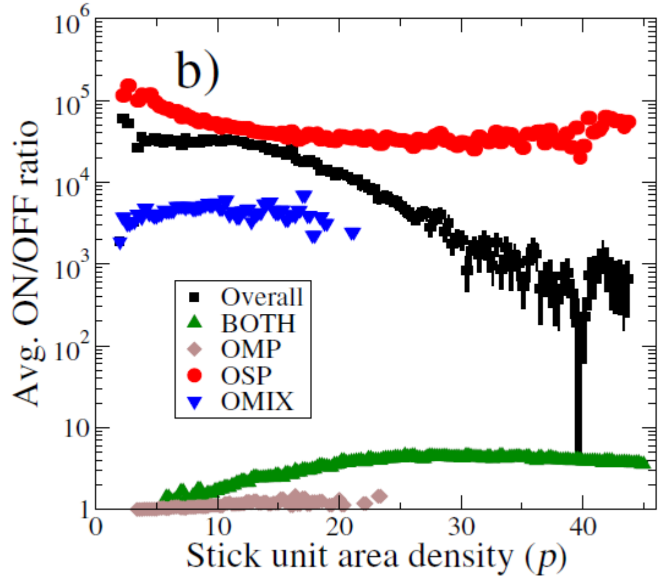
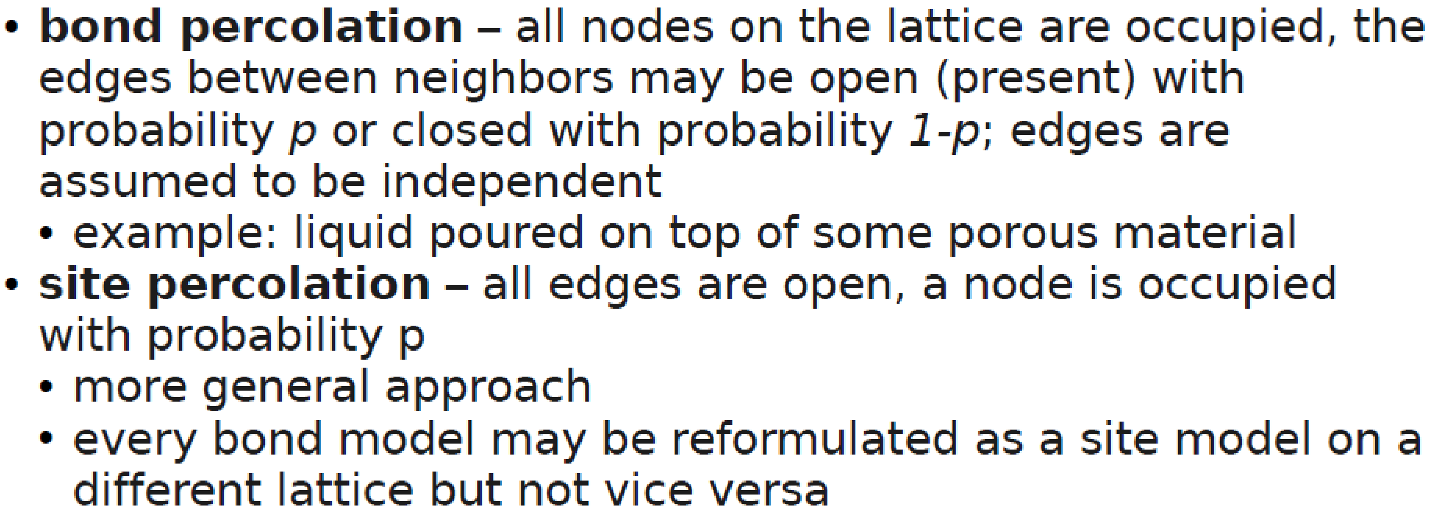


Fig. 4: (Colour on-line) A stick network after applying the bundle model. Dashed (red) lines represent semi-conducting segments and solid (blue) lines metallic segments. The networks



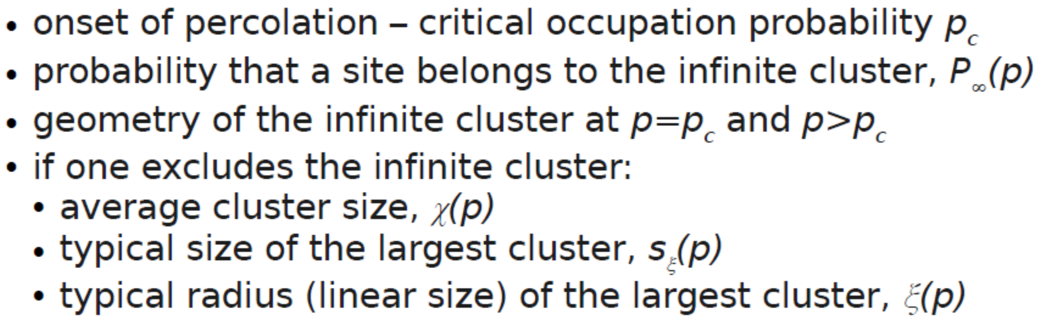


Main properties in a lattice



- **bond percolation** – all nodes on the lattice are occupied, the edges between neighbors may be open (present) with probability p or closed with probability $1-p$; edges are assumed to be independent
  - example: liquid poured on top of some porous material
- **site percolation** – all edges are open, a node is occupied with probability p
  - more general approach
  - every bond model may be reformulated as a site model on a different lattice but not vice versa

Main quantities or questions



- onset of percolation – critical occupation probability p_c
- probability that a site belongs to the infinite cluster, $P_\infty(p)$
- geometry of the infinite cluster at $p=p_c$ and $p>p_c$
- if one excludes the infinite cluster:
  - average cluster size, $\chi(p)$
  - typical size of the largest cluster, $s_\xi(p)$
  - typical radius (linear size) of the largest cluster, $\xi(p)$

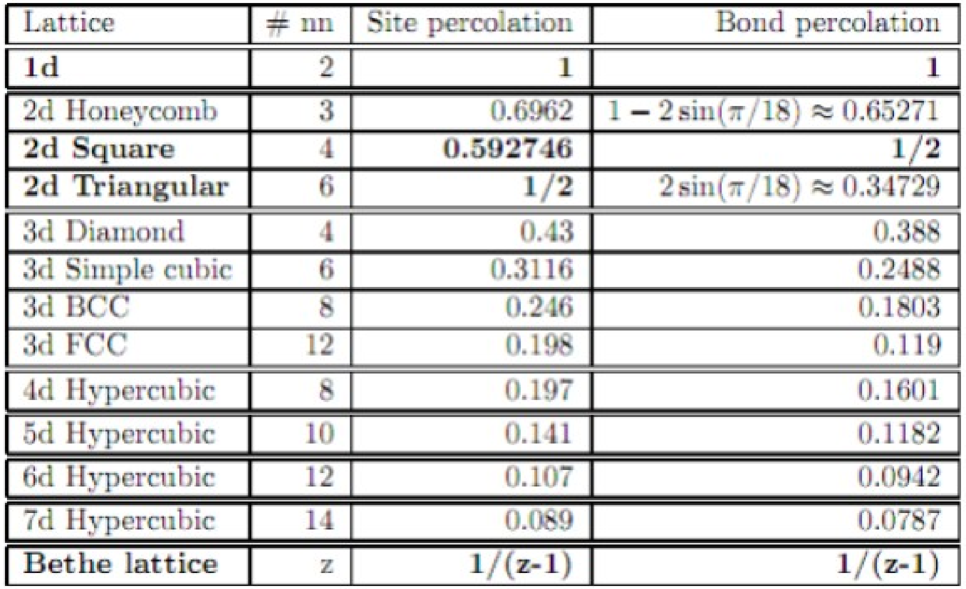
Examples of thresholds

2D vs 3D (or ND): p_c and its trends

Site vs. bond thresholds

In a fixed dimension: threshold vs. lattice type

(Value: math vs. physics vs. numerics)



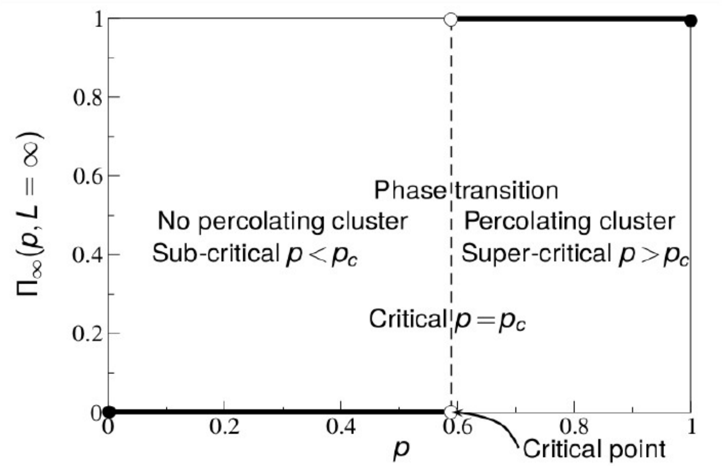
Lattice	# nn	Site percolation	Bond percolation
1d	2	**1**	**1**
2d Honeycomb	3	0.6962	$1 - 2\sin(\pi/18) \approx 0.65271$
2d Square	4	**0.592746**	**$1/2$**
2d Triangular	6	**$1/2$**	$2\sin(\pi/18) \approx 0.34729$
3d Diamond	4	0.43	0.388
3d Simple cubic	6	0.3116	0.2488
3d BCC	8	0.246	0.1803
3d FCC	12	0.198	0.119
4d Hypercubic	8	0.197	0.1601
5d Hypercubic	10	0.141	0.1182
6d Hypercubic	12	0.107	0.0942
7d Hypercubic	14	0.089	0.0787
Bethe lattice	z	**$1/(z-1)$**	**$1/(z-1)$**

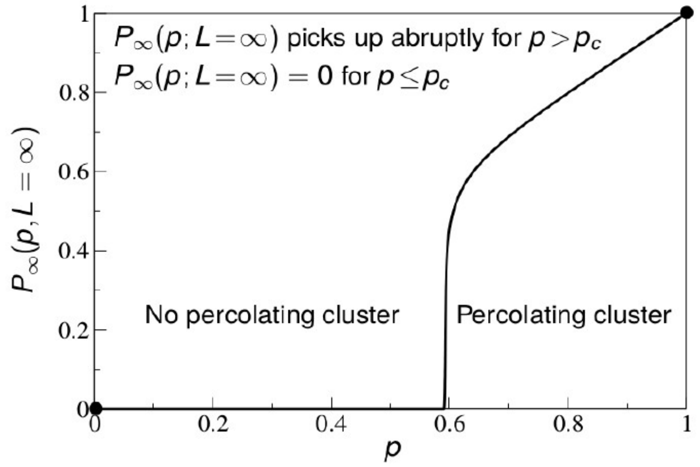
Percolation property

The largest cluster either percolates or not.

This defines a probability and a phase transition.

The transition is second order: correlation length diverges continuously. (Or: it is usually 2nd order.)



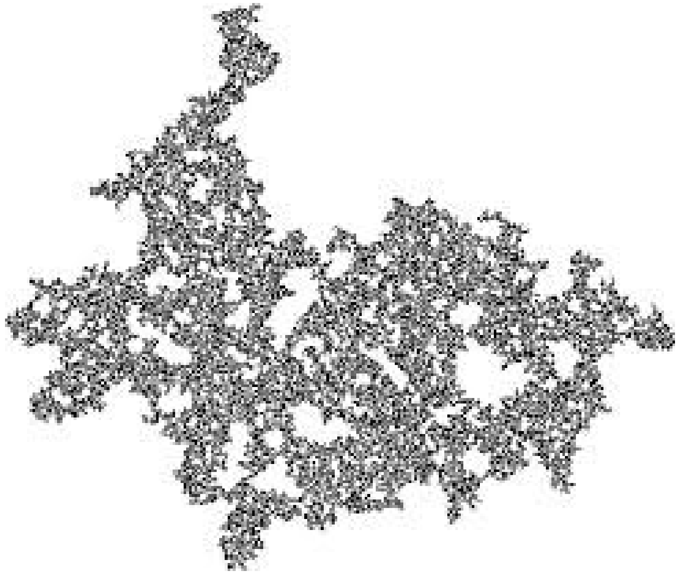


What is the percolating cluster like?

The mass is not volume-like

The structure is “tenuous” – the cluster can be broken up by “cutting” or “red bonds” – if you do transport phenomena (conductivity…) on the cluster the physics comes from these.

The perimeter is an interesting random walk-process – Stochastic Lowner Evolution….



Mass of the spanning cluster, correlation length

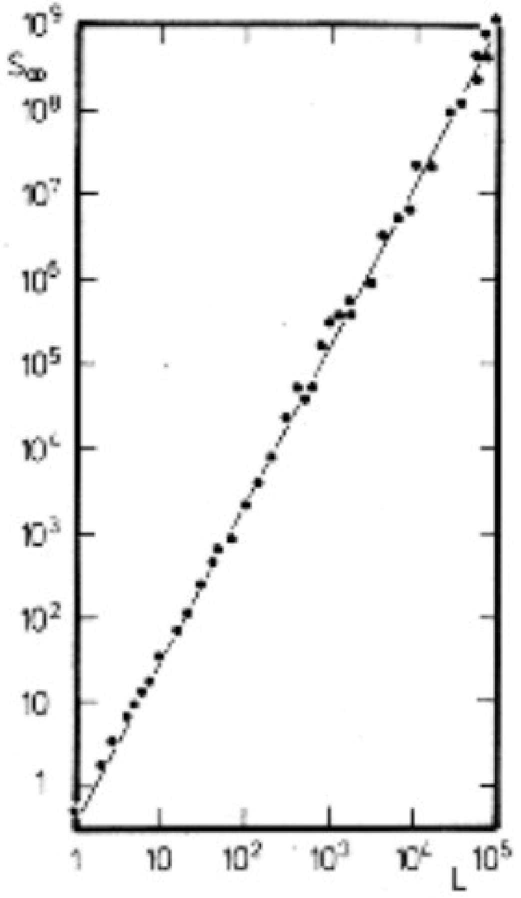
fractal dimension D_f

91/48 in 2D, an universal value (little bit less than 2!)

Mass scaling above defines an exponent for the mass above the transition, β, 2D 5/36, 3D 0.14

Correlation length exponent ξ, 2D 4/3, 3D 0.88

Exponents universal! (Bond/site, lattice type)

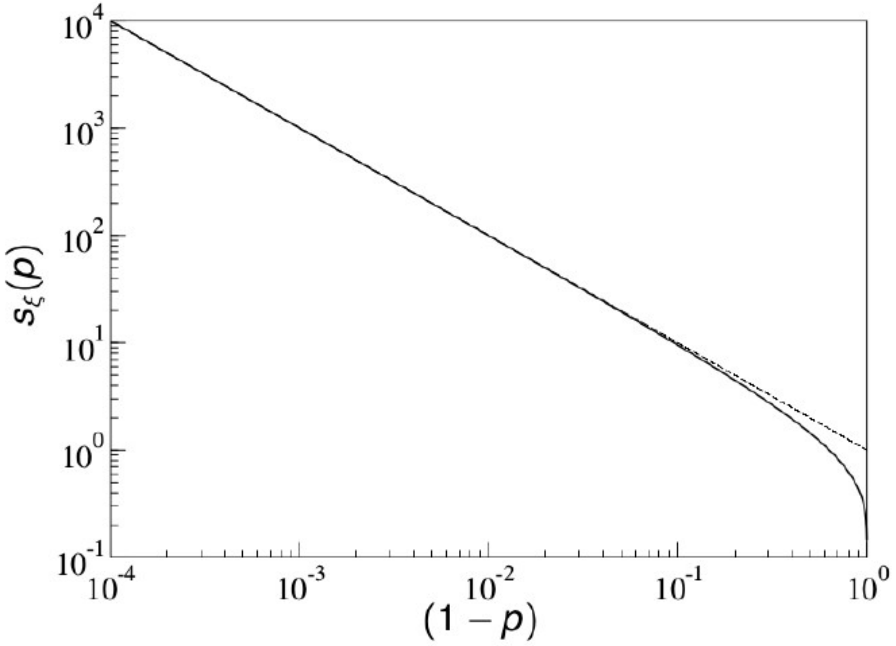


Example: 1D case (in probability)

Exactly solvable, but boring case.

Similar problems are found on trees (Bethe lattice, Cayley tree).

They generalize into other connectivity problems (“2-connectivity” or rigidity, combinatorial optimization/Satisfiability problems…).



Notes on scale-free behavior

Re-scale lengths (or time) – avalanche/cluster size and the pdf also re-scale.

Pdf invariant, solve for D(S).

More complicated examples (book).

$$\begin{aligned}\xi' &= \xi/B = \xi/(1+\epsilon),\\ S' &= S/C = S/(1+c\epsilon),\\ D' &= AD = D(1+a\epsilon).\end{aligned}$$

$$D'(S') = AD(S) = AD(CS') = (1+a\epsilon)D\big((1+c\epsilon)S'\big).$$

$$\begin{aligned}D(S') = D'(S') &= (1+a\epsilon)D\big((1+c\epsilon)S'\big),\\ 0 &= a\epsilon D + c\epsilon S'\frac{\mathrm{d}D}{\mathrm{d}S},\\ \frac{\mathrm{d}D}{\mathrm{d}S} &= -\frac{aD}{cS},\end{aligned}$$

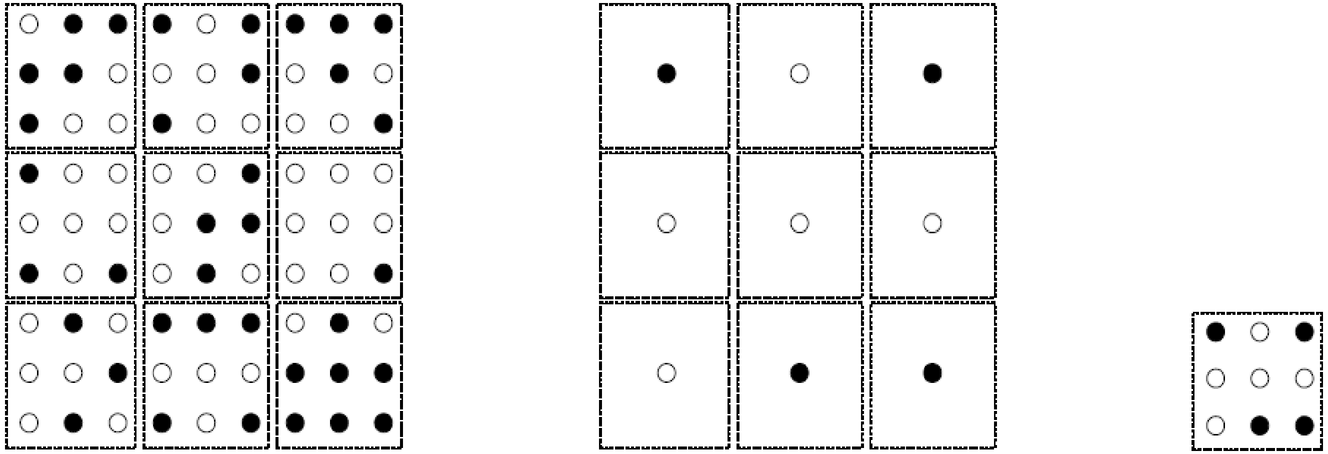
$$D = D_0 S^{-a/c}.$$

Renormalization (easy case)

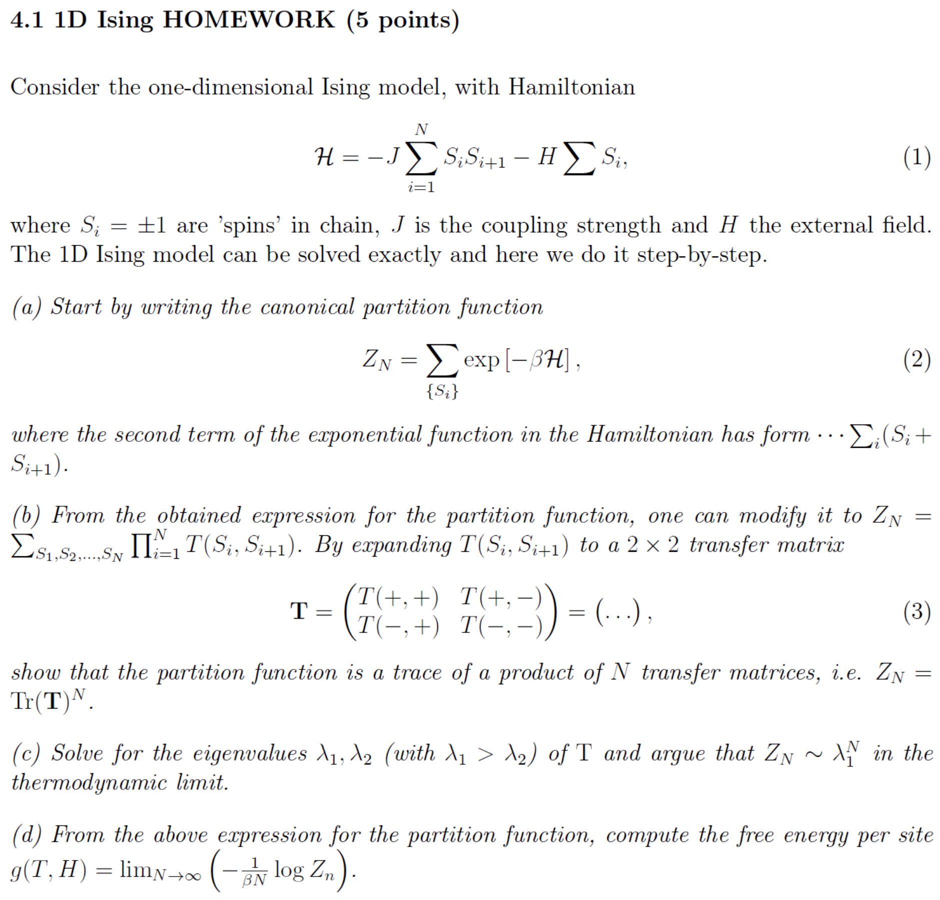
1. *Divide the lattice into blocks of linear size b (in terms of the lattice constant) with each block containing a few sites (spin).*
2. *Next, the coarse graining procedure takes place. The sites in the blocks are* averaged in some way *(to be specified more precisely shortly) and the* **entire** *block is replaced by a single super site (spin) which is occupied with a probability according to the renormalisation group transformation $p' = R_b(p)$.*

   In the combined procedure 1 and 2, one should keep the symmetry of the original lattice such that we can repeat the coarse graining procedure again. The result of these two operations are to create a new lattice whose fundamental spacing is b times as large as the original lattice.
3. *Restore original lattice constant by rescaling the length scales by the factor b.*

Real-space, k-space is the usual and hard case...



Next exercise



4.1 1D Ising HOMEWORK (5 points)

Consider the one-dimensional Ising model, with Hamiltonian

$$\mathcal{H} = -J \sum_{i=1}^{N} S_i S_{i+1} - H \sum S_i, \tag{1}$$

where $S_i = \pm 1$ are 'spins' in chain, J is the coupling strength and H the external field. The 1D Ising model can be solved exactly and here we do it step-by-step.

(a) Start by writing the canonical partition function

$$Z_N = \sum_{\{S_i\}} \exp\left[-\beta \mathcal{H}\right], \tag{2}$$

where the second term of the exponential function in the Hamiltonian has form $\cdots \sum_i (S_i + S_{i+1})$.

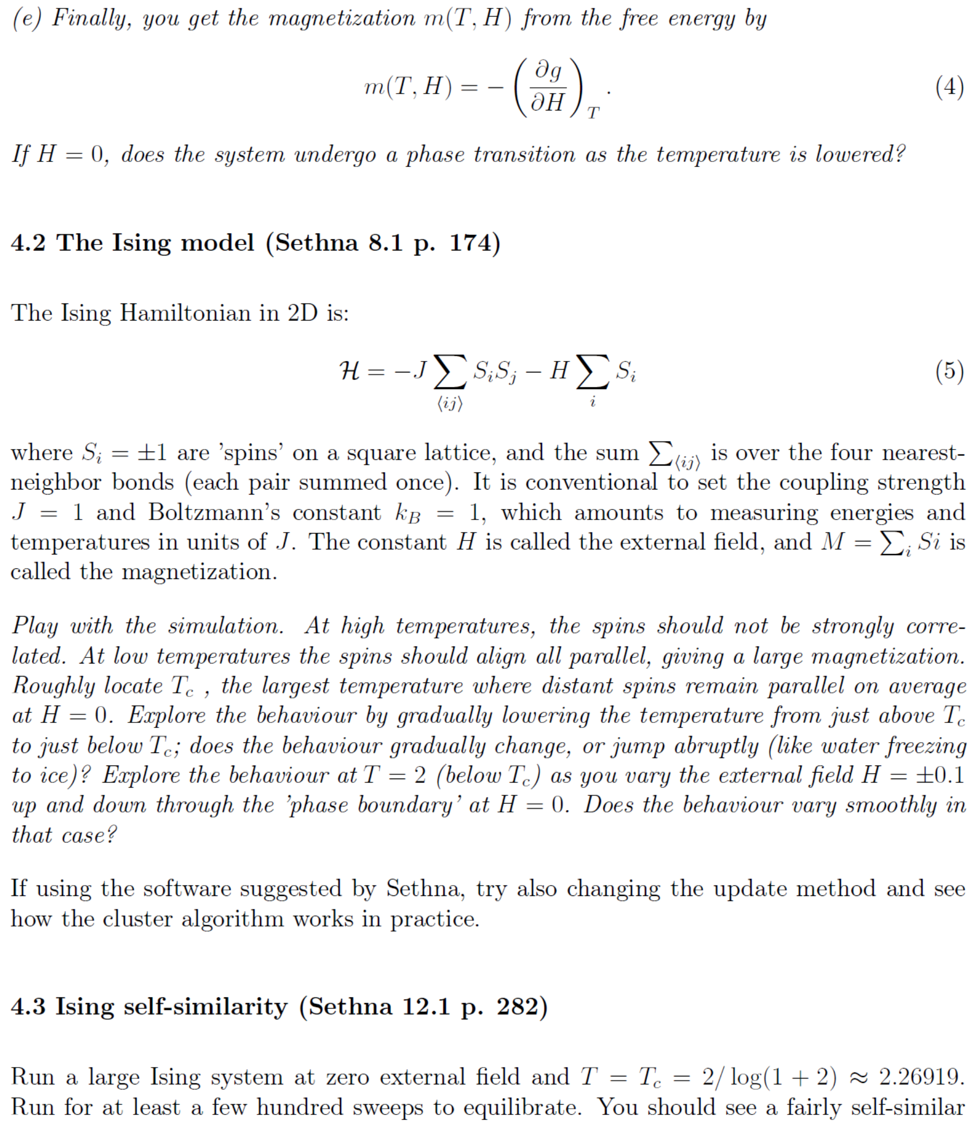
(b) From the obtained expression for the partition function, one can modify it to $Z_N = \sum_{S_1, S_2, \ldots, S_N} \prod_{i=1}^{N} T(S_i, S_{i+1})$. *By expanding* $T(S_i, S_{i+1})$ *to a* 2×2 *transfer matrix*

$$\mathbf{T} = \begin{pmatrix} T(+,+) & T(+,-) \\ T(-,+) & T(-,-) \end{pmatrix} = (\ldots), \tag{3}$$

show that the partition function is a trace of a product of N *transfer matrices, i.e.* $Z_N = \mathrm{Tr}(\mathbf{T})^N$.

(c) Solve for the eigenvalues λ_1, λ_2 *(with* $\lambda_1 > \lambda_2$*) of* T *and argue that* $Z_N \sim \lambda_1^N$ *in the thermodynamic limit.*

(d) From the above expression for the partition function, compute the free energy per site $g(T, H) = \lim_{N \to \infty} \left(-\frac{1}{\beta N} \log Z_n \right)$.



(e) Finally, you get the magnetization $m(T, H)$ *from the free energy by*

$$m(T, H) = -\left(\frac{\partial g}{\partial H} \right)_T. \tag{4}$$

If $H = 0$*, does the system undergo a phase transition as the temperature is lowered?*

4.2 The Ising model (Sethna 8.1 p. 174)

The Ising Hamiltonian in 2D is:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i \tag{5}$$

where $S_i = \pm 1$ are 'spins' on a square lattice, and the sum $\sum_{\langle ij \rangle}$ is over the four nearest-neighbor bonds (each pair summed once). It is conventional to set the coupling strength $J = 1$ and Boltzmann's constant $k_B = 1$, which amounts to measuring energies and temperatures in units of J. The constant H is called the external field, and $M = \sum_i Si$ is called the magnetization.

Play with the simulation. At high temperatures, the spins should not be strongly correlated. At low temperatures the spins should align all parallel, giving a large magnetization. Roughly locate T_c *, the largest temperature where distant spins remain parallel on average at* $H = 0$*. Explore the behaviour by gradually lowering the temperature from just above* T_c *to just below* T_c*; does the behaviour gradually change, or jump abruptly (like water freezing to ice)? Explore the behaviour at* $T = 2$ *(below* T_c*) as you vary the external field* $H = \pm 0.1$ *up and down through the 'phase boundary' at* $H = 0$*. Does the behaviour vary smoothly in that case?*

If using the software suggested by Sethna, try also changing the update method and see how the cluster algorithm works in practice.

4.3 Ising self-similarity (Sethna 12.1 p. 282)

Run a large Ising system at zero external field and $T = T_c = 2/\log(1 + 2) \approx 2.26919$. Run for at least a few hundred sweeps to equilibrate. You should see a fairly self-similar

Take home 5

- We concentrate on Sethna Ch 12 and percolation. Study the first two sections (12.1, 12.2). You may also read through the rest of the chapter. On percolation, there is a lot of material available. We would recommend http://www.ams.org/publicoutreach/feature-column/fcarc-percolation for a mathematical viewpoint, which may be entertaining. It shortly explains how percolation is related to conformal invariance.

  Check out also Kim Christensen's lecture notes on easily solvable percolation problems, https://web.mit.edu/ceder/publications/Percolation.pdf. Spend a moment in understanding how the cluster size distribution is derived (Equations 1.1-1.3) and the same for the correlation length in 1D (1.9-1.10, roughly). The analysis of the Bethe lattice percolation is entertaining but it is useful for our purposes (at most) for showing what kind of quantities one might want to compute.

  A final piece of reading is the lecture note for engineers, http://www.idc-online.com/technical_references/pdfs/chemical_engineering/Percolation.pdf, which introduces to some practical applications.

Note on take-home’s

Please remember, that the purpose is NOT to answer correctly. The purpose is that you answer SOMETHING (and think about the question and the material).

That is sufficient for “passing” the question (read: getting the points).

…. Questions…

The take-home questions are two. Check the real-space renormalization part of the KC (1.9 section). Try out that for 1D percolation, eg. draw what happens to the system as you coarse-grain it (to larger scales).

The last set of notes in particular mentions again the conductivity problem (e.g. take a system of insulating/conducting sticks, look at the conductivity when such sticks percolate by varying their fraction and assuming the system is connected anyways, or a bond percolation system say in 2d). Another variant of this is the elasticity of the percolation cluster, imagine that the sticks are very very soft or very hard springs so that the percolation transition leads to the stiffening of the whole thing.

Both of these "transport quantities" are described by their own exponents (conductivity and elasticity). The question to answer is: which of these has a bigger value? Does the conductivity or the elastic modulus increase faster? Do you have an argument why?