

Firstly, a few words about this exercise course. You can form groups up to 3 persons. The solutions should be uploaded to StudIP in form of a PDF file or a Mathematica notebook into the corresponding folder. I will look at the latest version uploaded before 12:00 on the submission day. The solutions should contain the code, its output and comments describing what you do and why.

The preferred program is Mathematica. You can use other tools and languages (e.g. Python), but support is not guaranteed.

There is no strict grading system as these exercises are not about following a recipe. There are several ways to approach the problem, and many ways to shape your approach into a code. The exercises are not extensive: if you know what you're doing, you can solve them in a few lines.

If you have questions about this exercise, or if you're stuck, you can contact me via zhilin@math.uni-hannover.de.

[H13] The Ising model

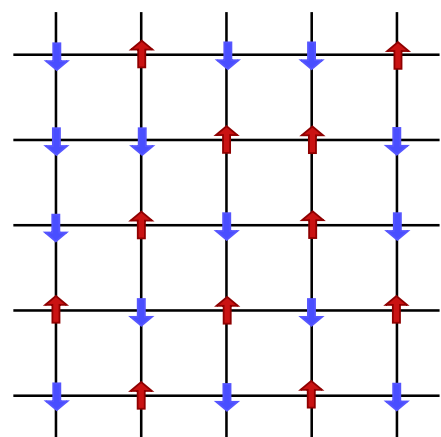
(12 points)

Let us play a bit with the Ising model. It is a famous toy model for ferromagnetism. Imagine a square lattice (we will stick to two dimensions), each site occupied by a spin s . Each spin can either point up ($s = +1$) or down ($s = -1$). Each link (i, j) connects two spins (s_i and s_j) and contributes $\epsilon_{ij} = -s_i s_j$ to the total energy. One can also turn on an external magnetic field h , so that each spin contributes additional $\epsilon_i = -h s_i$. Hence the total energy of a spin configuration $\{s\}$ is

$$E(\{s\}) = - \sum_{(i,j)} s_i s_j - h \sum_i s_i.$$

You can see that it is energetically favourable for spins to point in the same direction. One might expect that at high temperatures the spins will point randomly, while at low temperatures they will spontaneously align. This is exactly what happens in ferromagnetic materials.

In what follows we will consider a 64×64 periodic square lattice. Periodic means that, for example, a spin at site $(1, 1)$ interacts with spins at $(1, 2)$, $(2, 1)$, $(1, 64)$, $(64, 1)$. Even for such a modest lattice it is hardly possible to sum over all $2^{64 \times 64}$ configurations. The best we can do is to sample this sum by a stochastic process — in this exercise we will use the Metropolis algorithm.



An example of a spin lattice.

Please turn

To implement the Metropolis algorithm you can start with a lattice of randomly chosen spins. Then repeat the following steps:

1. Pick a random lattice site.
2. Calculate the energy ΔE needed to flip the chosen spin.
3. If $\Delta E < 0$, flip this spin. Otherwise flip it with probability $e^{-\Delta E/\tau}$ (τ is the temperature).

This process generates a sequence of spin configurations $\{s(t)\}$, where t is the number of repetitions and can be thought of as a „time“ variable. If simulation time T is large enough, one can compute statistical averages $\langle O \rangle = \frac{1}{Z} \sum_{\{s\}} O(\{s\}) e^{-E(\{s\})/\tau}$ as time averages $\langle O \rangle_T = \frac{1}{T} \sum_{t=0}^{t=T} O(\{s(t)\})$.

Your **task** is to make an animation of the Metropolis algorithm at work. You can represent the lattice as an array of coloured squares, the colour representing the state of the corresponding spin. Make it possible to adjust the value of temperature τ and magnetic field h in real-time without resetting the animation. **Explore** the behaviour of the system at different values of τ and h (make sure that you update the lattice fast enough to see „thermal fluctuations“). **Estimate** roughly the critical temperature τ_c that separates the ordered and disordered phases at $h = 0$.

Compute the correlation function $\langle s_i s_j \rangle$ at zero magnetic field. This function depends on the temperature and on the distance $d = |i - j|$ between the spins. For simplicity you can average over all pairs of spins that lie on the same vertical or horizontal line and are separated by distance d . Plot the correlation function as a function of d for several values of temperature above and below τ_c . Check whether your computation is reliable, i.e. gives the same result every time you run your program.

Bonus (4 points) Compute the heat capacity (per site) and the disorder correlation function $\langle \sigma_a \sigma_b \rangle$ at zero magnetic field. Plot the former as a function of τ , and the latter as a function of separation $d = |a - b|$ for several values of τ . The disorder variables σ_a live on the dual lattice, i.e. on the centres of the squares formed by the links. Again, for simplicity let „dual“ sites a and b lie on a vertical or horizontal line. Connect these sites with a (shortest) line and mark the links crossed by the line. The presence of $\sigma_a \sigma_b$ insertion is equivalent to flipping the interaction sign on the crossed links, i.e. each crossed link contributes $s_i s_j$ instead of $-s_i s_j$ to the energy. Compare the behaviour of $\langle \sigma_a \sigma_b \rangle$ to that of $\langle s_i s_j \rangle$.

Remark You can learn more about the Metropolis algorithm and its use in statistical physics on the corresponding Wikipedia page.