FYSA2041 Statistical fysiikka
ISING-MODEL MONTE-CARLO SIMULATION

Python3 version

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Course participation in year _____

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Instructions and simulation code
Ising model and its Monte Carlo simulation is described in the lecture notes.
Python Monte Carlo program can be downloaded from
http://users.jyu.fi/~veapaja/Ising-simulaatio/python
the directory contains files

ising.py	Ising simulation code
analyze.py	plotting etc.
ising_2022_worksheet.pdf	this document (pdf format)
ising_2022_worksheet.doc	this document (doc format)

The program requires Python version 3 + modules matplotlib, numpy,
and optionally numba.
They can be installed with the command
python3 -m pip install matplotlib numpy numba --user

Task: Run the code as instructed below and aswer the questions.

1. Question: What makes the Ising model classical, not quantum?
   Hint: This has nothing to do with the assumption on spin-spin interactions, but
   to the way spin values can be chosen.

2. *Motivation to use Monte Carlo*
   The partition function sums all possible spin arrangements.

   Question: How many years would it take to go through all spin states in a tiny
   10x10 two-dimensional Ising model, assuming the computation of one state takes
   only a nanosecond?

3. *Critical slowing down*
   Monte Carlo efficiency depends essentially on how quickly and comprehensively different states of the system are sampled.

   Question: What does critical slowing down mean in a simulation, where individual spin are probed one by one icient near the critical temperature?
   Tip: Near T_c spins form large parallel enclaves. Imagine how fast different states are sampled.

4. *Ideal paramagnet*
   Let's turn off the spin-spin interaction for the moment.
   Run the simulation for a 50x50 lattice
     python3 ising.py 0 50 1000 30 0.1 0.1 40 0.1 0.1 40 1 0 3
   and for a 10x10 lattice
     python3 ising.py 0 10 1000 30 0.1 0.1 40 0.1 0.1 40 1 0 3

   Question: Why is the result in this case independent of the grid size?

5. *Ferromagnet J>0, no magnetic B=0*
   Run the simulation
     python3 ising.py 1 100 1000 50 0.1 0.1 50 0 0 1 0 0 2
   At the beginning spins are parallel, and as the temperature is increased we continue from the previous spin configuration. The first 50 Monte Carlo steps are thermalization, the next 1000 are used for measurements.
   The finite system results won't exactly follow Onsager's infinite system results, but exhibit, nevertheless, same characteristics.

Comments:
a) In theory, finite systems can't have phase transitions. This is due to the   fact that the conditions are not fulfilled until infinitely many terms are   summed in the partition function. However, even a finite number of terms shows features that resemble a phase transition, since the sum converges rapidly toward the thermodynamic limit.
b) Heat capacity can be measured either from the derivative dE/dT, or from energy fluctuations at a given temperature. Calculating a numerical derivative of noisy data is tricky. The presented code is ineffective near the critical temperature.


Run the simulation from high to low temperature,
        python3 ising.py 1.0 100 10 20 5.0 50 -0.1 0 0 1 1 0 2
Repeat this a few times. Sometimes you may end up with a low-temperature result, where spins are not aligned, which shows also in magnetization and energy.
Question: Why didn't the simulation always find the minimum energy state, where all spins are in the same direction?
Hint: The ground state is either all spins up or all spins down, but which one? The cooling rate in the simulation is pretty fast.

6. The figure below shows the simulation to produce the instantaneous spin distribution (up=black, down=white). The simulation uses periodic boundary conditions.
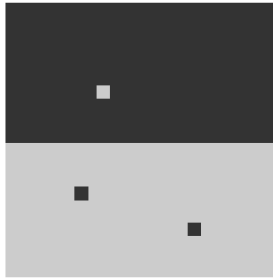
Question: Which of the two figures below describes the simulated space, expanded a bit?
Hint: periodic boundary conditions is the word; copy the image space endlessly in x- and y-directions.

a)

b)
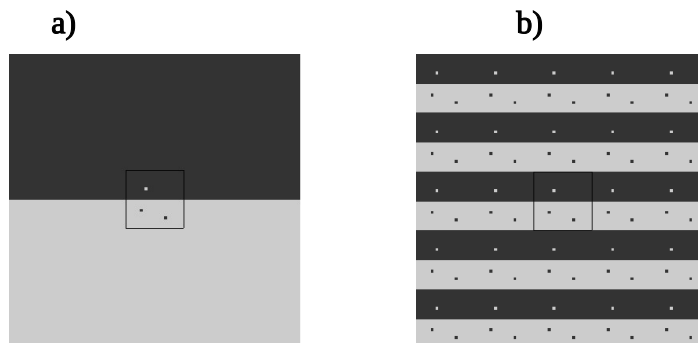
Answer: _____

7. *Ferromagnet J>0, magnetic field B> 0*
   Run the simulation with B = 1,
   python3 ising.py 1.0 50 1000 0.1 30 0.1 50 1 0 1 0 1 2
   and with B = 3,
   python3 ising.py 1.0 50 1000 0.1 0.1 30 50 3 0 1 1 2 0
   Question: How does increasing B affect the magnetization |M| and why does this happen?

8. *Antiferromagnetic*, J <0.
   Run the simulation
    python3 ising.py -1.0 50 100 30 5.0 -0.1 100 0 0.1 1 2 0 3
   Observe how a completely disordered structure at high temperatures turns into an
   ordered one as temperature decreases; this is due to antiferromagnetism.
   Question: None, this is just for fun.

9. *Hysteresis*
   Question: What causes hysteresis in ferromagnetic materials?

   Hysteresis in simulation: Run the following two simulations, in this order:
        python3 ising.py 1.0 50 500 100 2.2 0.0 1 -5.0 0.1 100 0 0 3
        python3 ising.py 1.0 50 500 100 2.2 0.0 1 5.0 -0.1 100 0 0 2
   Here magnetic field is first increased, then decreased.
   After the second simulation you'll get M(B), which shows a hysteresis loop.
   Question: What happens to the hysteresis loop at a lower/higher temperature?

10. *Boiling*
    In the simulation, small areas of gas phase form inside liquid and may quickly
    disappear. Finally the gas phase becomes stable, and gas regions expand: liquid
    boils.
    Boiling can be triggered by
    a) increased temperature
         python3 ising.py 1 100 500 0 0.8 0.01 100 -1 0 1 2 0 2
    b) reduced pressure (now: magnetic field)
         python3 ising.py 1 100 500 0 1 0 1 -0.8 -0.01 100 2 0 2
    Stable gas bubbles should form roughly aroud B ~ -0.87; this depends on the
    grid size.
                  Question: Monitor the spins during the simulation.
    Stable gas bubbles seem to form

    in a _____ x _____ grid, when B ~ _____

Final Note: Monte Carlo configurations have actually only a statistical significance. Here they are used to illustrate situations, where the state develops to a state that qualitatively differs from the initial quess.