Exercise 3: Finite size scaling

In this exercise, we will determine the critical temperature and critical exponents of the Ising model.

- a) First, we need finite size data. Since generating the data takes some time, it is useful to save it to disk. Generate your own finite size data from last weeks program (which can take some time to get well converged results), and/or download finite size data provided on the GitLab page. Inspect generate_data.py to find out how the data is structured and how to load the data. Plot the specific heat C_V and magnetic susceptibility χ .
- b) The specific heat C_V and magnetic susceptibility χ have maxima, which move with increasing system size L. Determine the temperature corresponding to the maxima for various system sizes and plot them versus $\frac{1}{L}$. Extrapolate to $L \to \infty$ to obtain an estimate for the critical temperature T_c .

Hint: You can use the functions np.argmax and np.polyfit.

c) Another quantity which is especially good to obtain the critical temperature is the so-called Binder cumulant, introduced by Binder in 1981 and defined as

$$U_B = \frac{3}{2} \left(1 - \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2} \right) \tag{1}$$

Plot the Binder cumulant for various system sizes. Find the crossings of U_B between curves corresponding to L and 2L, and include them into the previous plot from b).

Right at the critical temperature T_C , the (infinite) system becomes scale invariant. As one approaches the critical point, different macroscopic quantities scale with a power law in $\tau \equiv \frac{T-T_C}{T_C}$. The exponents of these power laws are universal, i.e., they can coincide for systems with different microscopic descriptions (which defines the "universality class"). For example, the correlation length diverges as $\xi \propto |\tau|^{-\nu}$, the specific heat as $C_V \propto |\tau|^{-\alpha}$, the order parameter in the ordered phases as $|M| \propto (-\tau)^{\beta}$, and the susceptibility as $\chi \propto |\tau|^{-\gamma}$. The correlation length of a finite system is bounded by the system size L. From that, one can derive a universal finite size scaling near the critical point.

d) Instead of viewing finite-size effect as a nuisance in cutting off power laws, one can exploit the dependency of critical exponents on system size L to extract the exponents. Recall the maxima value of specific heat C_V and magnetic susceptibility χ are cut off by

$$\chi \sim L^{\frac{\gamma}{\nu}} \tag{2}$$

$$C_V \sim L^{\frac{\alpha}{\nu}}$$
 (3)

Find out the ratio $\frac{\gamma}{\nu}, \frac{\alpha}{\nu}$.

Hint: You can use the functions plt.loglog and np.polyfit.

e) The binder cumulant has the finite size scaling

$$U_B = \Phi_{U_B} \left(\tau L^{\frac{1}{\nu}} \right), \tag{4}$$

where Φ_{U_B} is an unknown, universal function. Plot U_B versus $\tau L^{\frac{1}{\nu}}$ for various L. Vary the unknown exponent ν until the curves all appear on a single line.

f) The susceptibility and specific heat scale as

$$\chi = L^{\frac{\gamma}{\nu}} \Phi_{\chi} \left(\tau L^{\frac{1}{\nu}} \right) \tag{5}$$

$$C_V = L^{\frac{\alpha}{\nu}} \Phi_{C_V} \left(\tau L^{\frac{1}{\nu}} \right) \tag{6}$$

with other unknown scaling functions Φ_{χ} , Φ_{C_V} . Try to find the exponents γ and α by plotting $\chi/L^{\frac{\gamma}{\nu}}$ and $C_V/L^{\frac{\alpha}{\nu}}$ versus $\tau L^{\frac{1}{\nu}}$ and varying the exponents until you get a data collapse. How well is the hyperscaling relation $\nu d = 2 - \alpha$ fulfilled?

Hint: While for an exponent $\alpha = 0$ formally $C_V \propto \tau^{-\alpha} = \text{const.}$, the leading scaling behaviour is in this case $C_V \propto -\log(\tau)$. For the finite size scaling, this means $C_V = \log(L)\Phi_{C_V}\left(\tau L^{\frac{1}{\nu}}\right)$.

g) Modify the program generating the Monte carlo data to simulate the (ferromagnetic) Ising model on a triangular lattice. (For the provided program, this requires only to add 2 lines (and maybe changing output filename)!). Find the critical temperature. Are the critical exponents the same as on the square lattice, i.e., are these two models in the same universality class?

Comment: In order to obtain the critical exponents in a systematic way, we have to estimate the quality of the data collapse in some algorithm. The reduced chi-square method quantifies the deviation between the data points and some master curve (note that the master curve is dependent of the data itself!), and thus gives an estimate of the quality of the data collapse. Finally to obtain the critical exponents, we have to minimize this estimate in function of the exponents.

This scaling analysis is implemented in the pyfssa package, you could try to use it to extract the critical exponents γ , ν and the critical temperature T_c . The documentation can be found here https://pyfssa.readthedocs.io/en/stable/ and the source code here https://github.com/andsor/pyfssa. You just need the files fssa.py and optimize.py. [Ref. Andreas Sorge. (2015). pyfssa 0.7.6. Zenodo.]