Exercise sheet 4

The two-dimensional Ising model
PUE Advanced Computational Physics
University of Vienna - Faculty of Physics

11 The two-dimensional Ising model

For the square-lattice Ising model in two dimensions, an analytic solution is only known for the special case $H = 0$, first derived by Lars Onsager in the 1940s. Below the critical temperature

$$\frac{k_\mathrm{B} T_c}{J} = \frac{2}{\ln(1+\sqrt{2})} \approx 2.26918531421, \tag{1}$$

the spontaneous magnetization is

$$m = \left[1 - \sinh^{-4}(2\beta J)\right]^{1/8}. \tag{2}$$

The magnetization is zero for any $T > T_c$.

Use the provided example program *2dising* for this exercise. If you want, feel free to implement your own version, for example by extending the Python code from the previous sheet. *Hint:* we employ periodic boundary conditions and a square lattice. This means that each spin as four neighbors: left, right, top, bottom.

a. Run *2dising* with the default parameters given in *options.dat*: 20x20 lattice, $k_\mathrm{B} T/J = 2.1$, *ntskip* = 500, *ntjob* = 2000. Plot the magnetization as a function of simulation time. How does the result relate to to Eq. (2)?

b. Run further simulations with a larger system (40x40 lattice or more) at various temperatures approaching T_c from below. A reasonable choice is $k_\mathrm{B} T/J = \{1.0, 1.5, 1.75, 2.0, 2.1, 2.2\}$, and (if you use the provided Fortran code) good results can be achieved by running just a few minutes for each simulation. How would you choose your initial configuration, and why? Plot the resulting magnetization as a function of temperature and compare with the analytic result.

12 Acceptance probabilities

Consider a one-dimensional system with the potential energy

$$U(x) = \varepsilon\,\theta(x)\theta(1-x),$$

where $x \in [0,2]$ (without periodic boundary conditions) and $\theta(x)$ is the Heaviside step function. We want to generate a sample from the canonical probability distribution with the probability density

$$\Pi(x) = \frac{1}{Z} e^{-\beta U(x)}$$

using the Metropolis Monte Carlo algorithm. To do so we use two different methods to generate trial positions y given that we are at position x:

i. choose a random number ξ from a uniform distribution on the interval $[-\delta, \delta)$ and set $y = x + \xi$.

ii. choose a random number ϕ from a uniform distribution on the interval $[1, 1+\delta)$. With probability $1/2$ invert ϕ (i.e. perform a transformation from $\phi \to 1/\phi$) and calculate $y = \phi x$.

The acceptance probability has to fulfill the equation

$$\frac{p_{\mathrm{acc}}(x \to y)}{p_{\mathrm{acc}}(y \to x)} = \frac{P(y)\, p_{\mathrm{gen}}(y \to x)}{P(x)\, p_{\mathrm{gen}}(x \to y)}. \tag{3}$$

a. What is the ratio of generation probabilities $p_{\mathrm{gen}}(y \to x)/p_{\mathrm{gen}}(x \to y)$ for method (i.)? What is the acceptance criterion that follows?

b. Calculate the probability distribution $P_\Phi(\phi)$ that results from the procedure given in ii. both analytically and numerically. Compare your results. *Note:* recall that given a coordinate transformation $x \to y(x)$ the probability density transforms like

$$P_Y(y) = P_X(x(y)) \left| \frac{\mathrm{d}y(x')}{\mathrm{d}x'} \right|^{-1}_{x'=x(y)}.$$

c. Use $P_\Phi(\phi)$ to derive the acceptance criterion for method ii..

d. Implement a Metropolis Monte Carlo scheme in order to calculate a sample from $\Pi(x)$ using both methods. Demonstrate numerically that you are sampling the right distribution. What happens if you use the acceptance criterion of method *i.* together with the trial generation of method ii.?

13 Fluctuation formulas

The heat capacity at constant pressure, C_p, and the isothermal compressibility, χ_T are given by

$$C_p = T\left(\frac{\partial S}{\partial T}\right)_{p,N},$$

and

$$\chi_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_{T,N},$$

respectively. Use the relation between the Gibbs potential

$$\mathrm{d}G = -S\mathrm{d}T + V\mathrm{d}p + \mu\mathrm{d}N$$

and the corresponding partition function

$$Q_{NpT} = e^{-\beta G} = \frac{1}{N!(2\pi\hbar)^{3N}}\frac{1}{V_0}\int_0^\infty \mathrm{d}V \int \mathrm{d}\mathbf{r}^N \mathrm{d}\mathbf{p}^N \exp\left\{-\beta\left[H(\mathbf{r}^N,\mathbf{p}^N)+pV\right]\right\}$$

to derive fluctuation formulas for C_p and χ_T that can be used to calculate these quantities in the isothermal-isobaric ensemble. *Hint:* for the calculation of C_p, it is useful to express the derivative with respect to T as a derivative with respect to β.

The normalization of the volume integration in the (classical) isothermal-isobaric partition function is still a matter of debate. Here, we use a constant reference volume V_0 to ensure that Q_{NpT} has no dimension. In the literature, one will often find βp, which also has the dimension of inverse volume and leads to the correct equation of state for an ideal gas. However, in the case of this exercise, this will lead to inconsistencies when taking the derivative of the partition function with respect to β and p. Ultimately, it is not clear at all how to properly "count" a volume, which is a continuous quantity. The problems encountered in this context might even stem from an internal inconsistency of classical mechanics and could only be fixed by employing quantum statistics.