Assignment 11

Handout 05.02.2021 – Return 12.02.2021 – Discussion 18./19.02.2021

Exercise 11.1 [3 points]: Weiss mean field theory for the Ising model

Consider the Ising model on a cubic lattice in $d = 1$ and 2 dimensions. So the number of nearest neighbours is $z = 2$ for $d = 1$ and $z = 4$ for $d = 2$. Using the argument introduced by Weiss, we will rederive here the mean field result obtained in the lecture through the Bogoliubov inequality. The idea is to consider a spin s_0 and to take only the mean value $\langle s_i \rangle = \langle s \rangle$ of the neighbouring spins i:

$$\mathcal{H}_{\text{Ising}} = -J \sum_{\langle ij \rangle} s_i s_j \;\rightarrow\; \mathcal{H}_{\text{Weiss}}(s_0) = -J s_0 \sum_{i=1}^{z} \langle s_i \rangle \,. \tag{1}$$

The second step in the argument is that the chosen spin is not special, hence $\langle s_0 \rangle = \langle s \rangle$, which constitutes a self-consistency condition.

1. What is the value of the 'mean field' $\tilde{B}$, i.e. the effective field the spin s_0 experiences if the Hamiltonian is rewritten as $\mathcal{H}_{s_0} = -s_0 \tilde{B}$?
   Derive an equation for the magnetization $m = \langle s \rangle$ using the self-consistency condition. *(2 points)*

2. Solve this equation graphically. How many solutions are there as a function of T ? Show that the critical temperature for the phase transition is given by $k_B T_c = zJ$. Discuss the result in comparison to the full analytical solutions in $d = 1$ and 2 given in the lecture. *(1 point)*

Exercise 11.2 [8 points]: Bethe mean field theory for the Ising model

Bethe proposed a refined mean field theory, where one considers *clusters* of spins. The simplest (smallest) cluster is the one taking the nearest neighbours of a chosen spin, s_0, into account. Those neighbours interact exactly with s_0, but see their own further neighbours only via an effective mean field $\bar{B}$. The Hamiltonian hence reads:

$$\mathcal{H}_{\text{Bethe}}(s_0, \{s_i\}) = -J s_0 \sum_{i=1}^{z} s_i - \bar{B} \sum_{i=1}^{z} s_i \,. \tag{2}$$

Self-consistency again demands $\langle s_0 \rangle = \langle s_i \rangle$ for any i.

1. Calculate the partition sum and use it to determine $\langle s_0 \rangle$ and $\langle s_i \rangle$. *(3 points)*

2. Show that the consistency condition then implies
$$\left(\frac{\cosh \beta (J + \bar{B})}{\cosh \beta (J - \bar{B})} \right)^{z-1} = \exp(2\beta \bar{B}) \,. \tag{3}$$
   Show that this equation always has one solution and that (two) more may exist. *(3 points)*
   HINT: Study the behavior for large $\bar{B}$ as well as the slopes of the left and right sides at $\bar{B} = 0$.

3. Show that the critical temperature for the phase transition is $k_{\mathrm{B}}T_c = \frac{2J}{\ln\left(\frac{z}{z-2}\right)}$. *(1 point)*
   HINT: $\mathrm{arcoth}(x) = \frac{1}{2}\ln\frac{x+1}{x-1}$.
4. Discuss in how far this result is better than the one developed in 11.1. *(1 point)*

Exercise 11.3 [4 points]: Tonks gas

Consider a one-dimensional gas of N particles of length a confined to a strip of length L. The particles cannot overlap with each other (hard core repulsion) and otherwise do not interact with each other (no attraction like in the van der Waals gas).

1. Calculate the canonical partition sum Z by integrating over all possible values for the midpoints of the gas particles. *(2 points)*
   HINT: The result should be:

   $$Z(T, L, N) = \lambda^{-N}\frac{1}{N!}(L - Na)^N, \tag{4}$$

   where λ is the thermal wavelength (which is not needed for what comes later, but required to make Z dimensionless). Use this expression to proceed.
2. Calculate the free energy $F = -k_B T \ln Z$ and the pressure $p = -\partial_L F$. Evaluate the virial coefficient B_2 from the appropriate Mayer function and show that your result agrees with the virial expansion based on the exact solution. *(2 points)*

Exercise 11.4 [10* points]: Computer exercise: Ising model

Consider a two-dimensional lattice of $N \times N$ spins. Every spin can take values $s_{i,j} = \pm 1$ and the system is governed by the Hamiltonian

$$\mathcal{H} = -J\sum_{NN} s_{i,j}s_{k,l}\,, \tag{5}$$

with J being the interaction strength. The sum is only over nearest neighbors (NN), meaning that the spin $s_{i,j}$ at $x = i$, $y = j$ interacts only with spins at $s_{i\pm1,j}$ and $s_{i,j\pm1}$. Assume periodic boundary conditions in both directions, meaning that, for instance, spin $s_{0,j}$ interacts with $s_{1,j}$ and with $s_{N-1,j}$ on 'the other side'. In the following, put $J = 1$ and $k_B = 1$ for simplicity.

1. Write a code (and submit it along with your results) that implements the following algorithm (called "importance sampling with the Metropolis algorithm"):
   - Initialize the spins with $s = \pm 1$ randomly chosen in an array.
   - Pick a spin (i, j) at random.
   - Calculate the energy change ΔE upon flipping only this spin (i, j).
   - If $\Delta E < 0$, accept the spin flip.
   - If $\Delta E > 0$, accept the flip with Boltzmann probability $e^{-\beta\Delta E}$, otherwise reject.
   - After every N^2 of such spin 'tests', evaluate the mean magnetization $\langle M\rangle = \frac{1}{N^2}\sum_{i,j} s_{i,j}$ (note that the sum here is over all spins).

Why does this simple method sample phase space (rather) efficiently?

2. Study the system numerically for $N = 32$ or higher and for the two temperatures $T = 3$ and $T = 1.5$ (note again that $J = 1 = k_B$, hence T is the only parameter). Continue running the algorithm, until $\langle M \rangle$ does not change anymore except for small fluctuations around a constant value. Discuss your results.
   If you are more ambitious, you may wish to measure a full curve $\langle M \rangle(T)$ for temperatures in the interval $T \in [0.5, 3]$.

* **Bonus points**