Exercise sheet 1

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Exercise 1

Consider the Ising Hamiltonian,

$$\mathcal{H} = -J \sum_{<ij>} \sigma_i \sigma_j - h \sum_i \sigma_i$$

.

Imagine that this is a d-dimensional lattice where each lattice site is occupied by a spin like variable (say the z-component of a spin 1/2 operator). Each spin interacts with its nearest neighbors but we also consider an external magnetic field H. In the previous Hamiltonian $h = \mu_B/2H$ where μ_B is the magneton of Bohr. In two-dimensions there is an exact solution by Onsager. But as we mentioned in the class this is not the case for three dimensions so one needs to resort to either numerics or some approximation. In this exercise you will attack this problem employing the *mean field approximation*(MFA). It is a very simple concept. Each spin "feels" an average of the spin of its nearest neighbors.

- how many neighbors does each site have?
- what is the Hamiltonian of any spin "i"?
- what is the Ising Hamiltonian within the MFA.
- what is the Ising partition function?
- make your solution self consistent by requiring that the average value of σ_i is the same as the input value of $\bar{\sigma}$.
- give the expression of the magnetization
- plot the magnetization as a function of $\bar{\sigma}$.
  (hint: any intersection is a solution. Which solution is trivial? Which condition do you need to impose for non-trivial solutions?).
- from the previous condition define a characteristic temperature (T_c). Analyze the behavior of the magnetization when $T \approx T_c$ (both when T_c is approached from above and below). You might find convenient to use in your formulae the reduced temperature $t = 1 - T/T_c$.
- what is the free energy?
- what is the average energy?
- what is the constant volume specific heat?
- Do you expect the MFA to work better when the dimensionality is small or large? Why?

Exercise 2

Now consider an Ising model where instead of the nearest neighbor interaction all spins are allowed to interact with each other. In this case the Hamiltonian reads

$$\mathcal{H} = -\frac{1}{2N} \sum_{i,j} \sigma_i \sigma_j - h \sum_i \sigma_i$$

. In this case the MFA will be exact.

- why is there an explicit factor $1/N$ in the Hamiltonian?
- why is there a factor 1/2 in the Hamiltonian?

- show that the Boltzmann weight of this model can take the following form

$$e^{-\beta\mathcal{H}} = \sqrt{\frac{N\beta}{2\pi}} \int_{-\infty}^{\infty} d\lambda \exp[-\frac{N\beta\lambda^2}{2} + \sum_i \beta(\lambda + h)\sigma_i]$$

- show that the partition function can take the following form

$$\mathcal{Z} = \sqrt{\frac{N\beta}{2\pi}} \int d\lambda e^{-N\beta A(\lambda)}$$

  where

$$A(\lambda) = \frac{\lambda^2}{2} - \frac{1}{\beta} \ln(2\cosh[\beta(\lambda + h)])$$

  . hint: use the steepest descent method.

- which equation should λ satisfy in order for it to be the maximum of the argument in the exponent? Show that your partition function (in the large-N limit) takes the form $\mathcal{Z} = e^{N\beta f}$. Where f is the Taylor expansion of the function $A(\lambda)$ around λ_0, up to second-order. In this expansion think of f as the free energy per spin and of λ_0 as the minimum of the function $A(\lambda)$. Show that actually λ_0 is the average magnetization per spin, namely $< \sigma_i >$. How does this result compare to the MFA result?