617, Homework IV

Problem 1

Consider a density matrix ρ for a quantum system with Hamiltonian H. The Gibbs variational principle states that, if we define a generalized free energy as

$$A(\rho) = E - TS = \mathrm{Tr}(\rho H) + k_B T\, \mathrm{Tr}(\rho \ln \rho) \tag{0.1}$$

and we minimize it as a function of ρ with the condition that $\mathrm{Tr}\rho = 1$ and T fixed, then the minimum is attained by the canonical density matrix $\rho = \frac{1}{Z} e^{-\beta H}$ (do the calculation!)

a) If we now have the Ising model in dimension d, take a diagonal density function with no correlations and given by

$$\rho(s_1, \ldots, s_N) = g(s_1) \ldots g(s_N) \tag{0.2}$$

that depends on two numbers $g(+1) = g_+$ and $g(-1) = g_-$. Find a relation between $g_\pm$ so that the density matrix in normalized and write both $g_\pm$ in terms of the mean value of the spin per site $\langle s \rangle$.

b) Use the Gibbs variational principle to find an equation for $\langle s \rangle$.

c) Compare the equation you obtained in **b)** with the eqaution obtain from the mean field approximation.

Problem 2

Consider the Ising model in d dimensions in the mean field approximation (for example using problem 1).

a) For zero external magnetic field, compute the magnetization as a function of temperature and compute the corresponding critical exponent in this approximation.

b) For $T > T_c$ compute the magnetic susceptibility at zero external field $\chi = \frac{\partial M}{\partial B}\Big|_{B=0}$ and determine the corresponding critical exponent.

c) Again, for zero external field, compute the specific heat and evaluate it at the critical temperature. What is the corresponding critical exponent in this aproximation?

Problem 3

Consider the Ising model in d dimensions using the mean field approximation.

a) Work out the equivalence with the lattice gas.

b) Plot the phase diagram in the pressure-temperature plane. Identify the two phases and the critical point. Can you go continuously from one phase to the other?