Midterm Exam for Advanced Statistical Physics: NS-370B

Date: October 8th, 2019

Time : 13:30 - 15:30

This exam consists of 3 questions. Total points possible: 56.
This is a closed-book exam, i.e. notes and electronic devices are not allowed.
Please start every exercise on a new sheet of paper, with your name clearly written on every page.
Exam can be written in either English or Dutch. Please write clearly!

A few formulas and information that may or may not be useful in this exam:

- The canonical partition function of a classical thermodynamic system of N identical particles in a volume V a temperature T with Hamiltonian $H(\Gamma)$ is written as $Z(N, V, T) = 1/(N!h^{3N}) \int d\Gamma \exp[-\beta H(\Gamma)]$, where $\beta^{-1} = k_B T$.
- The grand partition function of identical particles is $\Xi(\mu, V, T) = \sum_{N=0}^{\infty} \exp(\beta\mu N) Z(N, V, T)$, and the grand-canonical distribution is $f_g(\Gamma, N) = \exp[\beta\mu N - \beta H(\Gamma)]/[N!h^{3N}\Xi(\mu, V, T)]$, with μ the chemical potential.
- $k_B = 1.13 \times 10^{-23}$J/K, $e = 1.6 \times 10^{-19}$C, and $R = 8.31$J/K/mol.
- The binomial coefficient (i.e. m choose n, which is the number of ways n objects can be chosen from m objects) is given by $\left(\frac{m!}{(m-n)!n!}\right)$.
- Stirling's approximation to order $O(N)$ is given by $\log(N!) = N \log N - N$.
- Gaussian Integral: $\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}$
- The Taylor series of $f(x)$ around $x = a$ is given by $f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots$.
- From the Taylor series we get: $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$

1. (16 points) Consider a single-component system that, at sufficiently low temperatures (i.e. below the critical temperature T_C) can phase separate into a gas and a liquid.

   (a) Under what three conditions does this system exhibit a coexistence between the gas phase and the liquid phase?

   (b) Sketch the free energy per volume as a function of the density i) below the critical temperature T_C, ii) above the critical temperature T_C.

   (c) Explain why or show why we can ignore the contributions from the interface between the gas and liquid phases when we are deriving the equilibrium conditions for coexistence between the two phases.

   Consider a system of blocks on a square lattice. Assume that each block is occupied with a probability p and that there are no interactions between the blocks. Here we will use renormalization group theory to predict the percolation threshold. Consider superblocks of size 3x3. Consider a mapping where the superblock percolates only when a majority of the subblocks are filled (i.e. 5 of the 9).

   (d) Determine the renormalization transformation $R(p)$. *(You should leave the answer in terms of binomial coefficients. Do not try and solve this!)*

   (e) Describe how one would use $R(p)$ to determine the percolation threshold.

   (f) Describe briefly what would happen to the system if one were to apply $R(p)$ repeatedly to the system i) just below the percolation threshold, ii) just above the percolation threshold, and iii) at the percolation threshold.

2. (20 points) Consider a gas of hydrogen molecules in contact with a wall at temperature T. Assume that the wall has M sites where the hydrogen molecules can adsorb, and that the binding energy between the lattice sites and a hydrogen molecule is given by $-\epsilon$, with $\epsilon > 0$.

   a) Make the rather ridiculous assumption that each binding site can adsorb any number of hydrogen molecules, and assume that exactly N hydrogen molecules are bound to the surface. i) What is the partition function for this system? ii) Show that the associated free energy is given by

   $$F(N, M, T) = k_B T N \left[\log(\rho) - 1\right] - N\epsilon$$

   where $\rho = N/M$.

   b) Instead, we now assume that the each binding site can adsorb only a single hydrogen molecule and that $N < M$ molecules are currently bound to the surface. i) What is the partition function for this system? ii) Show that the associated free energy can be written

   $$F(N, M, T) = k_B T \left[N \log(\rho) + (M - N) \log(1 - \rho)\right] - N\epsilon$$

   where $\rho = N/M$.

   As a next step, divide the surface into two subsystems 1 and 2. Assume M_1 and M_2 are the number of binding sites associated with subsystems 1 and 2 respectively. Define N_1 and N_2 to be the number of particle in subsystems 1 and 2 respectively. Assume that particles are free to hop between subsystems 1 and 2, but that the total number of particles is fixed to be N.

c) What are the total number of microstates available for this system?

d) Write down the fundamental assumption of statistical physics.

e) Let $\Omega_1(N_1)$ be the number of microstates with N_1 particles in system 1, and $\Omega_2(N_2)$ be the number of microstates with N_2 particles in system 2. Use the fundamental assumption of statistical physics to show that

$$\left.\frac{d\ln\Omega_1(N_1)}{dN_1}\right|_{N_1=N_1^*} = \left.\frac{d\ln\Omega_2(N_2)}{dN_2}\right|_{N_2=N_2^*},$$

where N_1^* and N_2^* are the most likely numbers of particles in systems 1 and 2 respectively.

3. (20 points) Consider a simple extension of the Ising Model. In this extension, in addition to having nearest neighbour interactions, there is also next nearest neighbour interactions. Assume we are interested in a 2d simple square lattice, so that each spin has 4 nearest neighbours and 4 next nearest neighbours. The Hamiltonian is given by

$$\mathcal{H} = -\frac{J_{nn}}{2}\sum_i\sum_j{}' S_iS_j - \frac{K_{nnn}}{2}\sum_i\sum_j{}'' S_iS_j \tag{1}$$

with $J_{nn} > 0$, $K_{nnn} > 0$. Additionally, $\sum_j{}'$ indicates a sum over nearest neighbors, and $\sum_j{}''$ indicates a sum over next nearest neighbours. Here we will consider a mean field approximation where we focus on a single spin.

(a) Let m be the magnetization per particle. Write down the mean field Hamiltonian so that it is of the form

$$\mathcal{H}_{MF} = C\sum_i S_i + D \tag{2}$$

where C and D can depend on m, and the coupling constants J_{nn} and K_{nnn}.

(b) Show that the magnetization m can be written as:

$$m = \tanh\left(4m\beta(J_{nn} + K_{nnn})\right)$$

The Landau free energy to order m^4 for this system is given by

$$\frac{\beta F}{N} = -\log[2] + 2\beta(J_{nn} + K_{nnn})\left(1 - 4\beta(J_{nn} + K_{nnn})\right)m^2 + \frac{64}{3}(J_{nn} + K_{nnn})^4 m^4\beta^4$$

Do not try and show this!

(c) Sketch the Landau free energy i) below the critical temperature, ii) above the critical temperature. Make sure to label the axes.

(d) Sketch the magnetization as a function of the temperature associated with this Landau free energy. Make sure to label the axes.

(e) What type of phase transition is this?

(f) At what temperature is the phase transition?