Midterm Exam for Advanced Statistical Physics: NS-370B

Date: October 12th, 2021

Time for Regular Students: 15:15 - 18:15

Extra-Time Students Only: 15:15 - 18:45

This exam consists of **7** questions of varying length.

The total number of possible points is: 100.

This is a **closed-book** exam, no notes are allowed.

You will not require a calculator or any other electronic device and are consequently not permitted one.

Please **start every exercise on a new PAGE of paper**.

Write your name clearly on every four-page sheet of paper.

The exam can be written in either English or Dutch.

Please write clearly and using pen!

Equation Cheat Sheet

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 $H(\mathbf{\Gamma})$ — $\mathbf{\Gamma}$ is a point in phase space — is written:

  $Z(N, V, T) = \frac{1}{N!h^{3N}} \int d\mathbf{\Gamma} \exp[-\beta H(\mathbf{\Gamma})]$, where $\beta^{-1} = k_B T$.

- The grand partition function of identical particles is given by:

  $\Xi(\mu, V, T) = \sum_{N=0}^{\infty} \exp(\beta\mu N) Z(N, V, T)$,

  and the grand-canonical distribution is given by:

  $f_g(\mathbf{\Gamma}, N) = \frac{\exp[\beta\mu N - \beta H(\mathbf{\Gamma})]]}{[N!h^{3N}\Xi(\mu, V, T)]}$, with μ the chemical potential.

- The second virial coefficient B_2 for an isotropic pair potential $\phi(r)$ is given by:

  $B_2 = -\frac{1}{2}\int_V \mathrm{d}r \; (\exp(-\beta\phi(r)) - 1)$.

- $k_B = 1.13 \times 10^{-23}$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:

  $\binom{m}{n} = \frac{m!}{(m-n)!n!}$.

- 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 obtain:

  $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$

  and

  $\log(1-x) = -\sum_{n=1}^{\infty} \frac{x^n}{n}$.

1. Entropy: (6 points)

Determine the Legendre transform of the entropy which is a natural function of $1/T$, V, N. Start from the definitions of the first and second law and write these down. Show that your transformation works.

2. Spins: (16 points)

Consider a system of N distinguishable, non-interacting spins, in an external magnetic field denoted $H > 0$. Assume that each spin carries a magnetic moment μ, which points either parallel or anti-parallel to the applied field. The energy of a specific state can then be expressed as

$$-\sum_{i=1}^{N} n_i \mu H; \quad n_i = \pm 1, \tag{1}$$

where $n_i\mu$ is the magnetic moment in field direction.

(a) What do the microstates of this system look like? Draw a few.

(b) What is the internal energy of this system as a function of $\beta = 1/k_B T$, H, and N (use the ensemble characterized by these variables).

(c) Determine the entropy of this system as a function of β, H, and N.

(d) Determine the behavior of the energy and entropy for this system as $T \to \infty$.

3. Percolation: (10 points)

Consider a square lattice. Assume that a 2×2 subset in this lattice 'spans' if there is an edge-connected cluster that goes from the top to the bottom of the square. Show that $R(p) = 2p^2(1-p)^2 + 4p^3(1-p) + p^4$ and support your argumentation toward this result using sketches. Determine the analytic expression for the corresponding non-trivial fixed point.

4. Equipartition: (16 points)

Show that a Hamiltonian of the form

$$\mathcal{H} = \sum_{i=1}^{M} a_i s_i^2 \tag{2}$$

with $a_i > 0$ some constant and s_i a generalized coordinate of the system leads to

$$\langle \mathcal{H} \rangle = \frac{1}{2} k_B T M. \tag{3}$$

Use what you have proven above to determine the internal energy per particle for:

(a) An ideal gas in 5 dimensions

(b) A diatomic gas with rigid bond in 3D

(c) A diatomic gas with flexible bond in the direction of the molecule's symmetry axis in 3D

(d) A gas of rigid L shapes in 3D

Justify your answer for each point (a-d) in a few words (no long-winded stories please).

The exam continues on the next page ⇒

5. Ising with more Neighbors: (20 points)

The one-dimensional, zero-field Ising model with nearest and next-nearest neighbor interactions can be written as

$$\mathcal{H} = -J_{nn} \sum_{i=1}^{N-1} S_i S_{i+1} - J_{nnn} \sum_{i=1}^{N-2} S_i S_{i+2}. \tag{4}$$

The partition function for this system can be shown to be

$$\frac{1}{N} \log Z \propto \log \left[e^{\beta J_{nnn}} \cosh(\beta J_{nn}) + \left\{ e^{-2\beta J_{nnn}} + e^{2\beta J_{nnn}} \sinh^2(\beta J_{nn}) \right\}^{1/2} \right]. \tag{5}$$

(a) Write down the free energy per particle.

(b) Show that

$$\langle S_i S_{i+1} \rangle = \frac{\sinh(\beta J_{nn})}{\left[\exp(-4\beta J_{nnn}) + \sinh^2(\beta J_{nn}) \right]^{1/2}}. \tag{6}$$

Via the same procedure, you can show that $\langle S_i S_{i+2} \rangle =$

$$1 - \frac{2\exp(-4\beta J_{nnn})}{\left[\exp(-4\beta J_{nnn}) + \sinh^2(\beta J_{nn})\right]^{1/2} \left[\cosh(\beta J_{nn}) + \left(\exp(-4\beta J_{nnn}) + \sinh^2(\beta J_{nn})\right)^{1/2}\right]}. \tag{7}$$

(c) Using these answers compute $\langle S_i S_{i+1} \rangle$ and $\langle S_i S_{i+2} \rangle$ in the limit as $J_{nnn} \to 0$ and explain your result in a few words.

6. Landau Free Energy: (20 points)

Let us assume that we have a system for which the Landau free energy is given by

$$f(T, m) \approx b'(T - T_0)m^2 - cm^3 + dm^4. \tag{8}$$

where $b' > 0$, $c > 0$, and $d > 0$ are constants and T_0 is a temperature.

(a) What happens as $T < T_0$? Explain this using a few words in terms of the disordered phase.

(b) What kind of phase transition does this system exhibit? Explain your answer with two sketches. One should show free-energy curves as a function of m for several (relevant) temperatures. The other should show how this leads to variation of the minima as a function of temperature. Label the curves by temperature where appropriate and indicate the stable minima clearly. Finally, properly label your axes.

(c) Compute the temperature at which the phase transition occurs and express the result in terms of b', c, and/or d.

7. Fluctuations: (12 points)

Show that at fixed V and N within the canonical ensemble, the constant-volume heat capacity

$$C_V = \left(\frac{\partial U}{\partial T} \right)_{N,V} \tag{9}$$

can be written as

$$\frac{\langle \epsilon_s^2 \rangle - \langle \epsilon_s \rangle^2}{k_B T^2}. \tag{10}$$

where ϵ_s is the energy associated with a microstate 's' and the brackets denote averages. Hint: you have to make several steps to get to the final answer, start by defining U in the ensemble.

The exam ends here!