Preliminary Exam: Statistical Mechanics, Tuesday January 15, 2019, 9am-noon

Answer a total **THREE** questions out of **FOUR**. If you turn in excess solutions, the ones to be graded will be picked at random. Each answer must be presented **separately** in an answer book, or on consecutively numbered sheets of paper stapled together. Make sure you clearly indicate who you are and the problem you are solving. Double-check that you include everything you want graded, and nothing else.
Some possibly useful information:

$$\text{Sterling's asymptotic series}: \quad \ln N! \approx N\ln N - N + \frac{1}{2}\ln[2\pi N] \quad \text{as} \quad N \to \infty,$$

$$\int_0^{\infty} dx\ x\ \exp(-\alpha x^2) = \frac{1}{2\alpha}, \qquad \int_{-\infty}^{+\infty} dx\ \exp(-\alpha x^2\ +\ \beta x) = \sqrt{\frac{\pi}{\alpha}}\exp(\frac{\beta^2}{4\alpha}) \text{ with } \mathrm{Re}(\alpha) > 0.$$

1. An ideal gas of identical atoms is enclosed in a large spherical container of volume V. Atomic particles can be bound by container walls and form a two-dimensional (2D) ideal gas with the particle energy $\varepsilon(p) = -\varepsilon_0 + p^2/2m$, where ε_0 is a positive constant describing the surface binding energy, m is the atomic mass, and p is the 2D momentum. The gas temperature T is high and the atomic particles obey the Boltzmann statistics.
   (a) Calculate the partition functions $Z_S(N_S, T)$ and $Z_V(N_V, T)$ of surface and volume gases, if the container wall and volume particles are considered as two non-interacting subsystems with the fixed numbers of surface and volume atoms N_S and N_V respectively. Determine the partition function $Z(N_S + N_V, T)$ for the entire system.
   (b) Calculate the system free energy $F(N_S + N_V, T) = E - TS$ and find the average particle energy $\langle\varepsilon\rangle$ for the entire container gas using the results obtained in (a).
   (c) Calculate the system partition function $Z'(N_S + N_V, T)$, the free energy $F'(N_S + N_V, T)$ and the average particle energy $\langle\varepsilon'\rangle$ if the volume and wall gases merged isothermally into a single gas, exchanging atoms and energies.
   (d) Explain the difference between results obtained for (b) and (c), and compute an average number of the surface atoms N'_S at conditions of part (c).

2. The gas of non-interacting Fermi atoms with the spin $s = 1/2$ is embedded into a thermal bath, supporting the constant chemical potential μ and temperature T of the gas particles. The Fermi system includes n_0 non-degenerate energy levels ($1 \le n \le n_0$) and the single particle energy of the n-th level depends on the quantum number n as $\varepsilon_n = \varepsilon_0 \log(n)$, where ε_0 is a positive constant.
   (a) For the given value of the chemical potential μ and temperature $T = \varepsilon_0/k$ (where k is the Boltzmann constant), calculate an average number of particles $N = N(\mu, \varepsilon_0, n_0)$ in the fermionic system, assuming that $n_0 \gg 1$.
   Hint: The sum over n can be replaced with an integral over dn, if $n_0 \gg 1$.
   (b) From the results obtained in (a), determine the leading terms of the low-temperature asymptotic behavior of N, if the parameter $\gamma = \exp(-\mu/kT) = \exp(-\mu/\varepsilon_0) \ll 1$ ($\gamma \to 0$).
   (c) Determine the number of atoms N_b in the system with the same energy levels, if the particles are bosons with the spin $s = 0$ and the thermal bath temperature $T = \varepsilon_0/k$. The chemical potential is negative: $\mu < 0$. Describe the behavior of the Bose system, if $\mu \to 0$.

3. Consider the Hamiltonian for an Ising anti-ferromagnet

$$H = J \sum_{<i,j>} S_i S_j - h \sum_i S_i,$$

where $J > 0$, $S_i = \pm 1$, h is the magnetic field, and $< i, j >$ designates all pairs i and j that are nearest neighbors. For simplicity, assume a one-dimensional lattice of N spins with periodic boundary conditions, i.e., $S_0 = S_N$. For strong interaction energy J, one expects the spins in this system to anti-align.

(a) Derive the mean-field theory for this system by dividing it into two sub-lattices (e.g., sublattice 1 consists of all odd i, sublattice 2 of all even i). Write the mean-field Hamiltonian and the magnetizations for both sublattices directly. Show that the the self-consistent resulting equations are given by

$$\begin{aligned} m_o \equiv \langle S_{i,odd} \rangle &= \tanh(\beta h - 2\beta J m_e), \\ m_e \equiv \langle S_{i,even} \rangle &= \tanh(\beta h - 2\beta J m_o). \end{aligned}$$

(b) Find the value of the sub-lattice magnetizations m_o and m_e in the paramagnetic regime for small magnetic field h, i.e., linear order in h. (*Hint: Remember the series expansion*

$$\tanh x = x - \frac{1}{3}x^3 + \mathcal{O}(x^4).)$$

(c) Derive the transition temperature to the anti-ferromagnetic phase for zero magnetic field. Describe, qualitatively or graphically, the anti-ferromagnetic solutions for the two magnetizations.

(d) From the previous parts, argue why the difference in the magnetizations can serve as an order parameter for this system, i.e., the transition between the paramagnetic and anti-ferromagnetic phases happens where this quantity changes between zero and non-zero values. Thus, the critical temperature changes in this case – does it get higher or lower? For this, find a self-consistent equation (similar to the one in part (a)) for the difference in magnetizations, using the formula

$$\tanh x - \tanh y = \tanh(x - y)(1 - \tanh x \tanh y).$$

The only terms that now still contain h can be resolved to the lowest order in h, using the paramagnetic solution for m_o and m_e from part (b). While this is a form that is hard to resolve, the qualitative answer to the question above can now be read off immediately.

4. A material is found to have a thermal expansion coefficient $\alpha_P = v^{-1}(R/P + a/RT^2)$ and an isothermal compressibility $\kappa_T = v^{-1}(Tf(P) - b/P)$ Here $v = V/n$ is the molar volume, T is the temperature, P the pressure, and R the molar Boltzmann constant ($= N_{\text{mol}} k_B$). Both a and b are constants. *(Hint: remember that both the thermal expansion coefficient and the compressibility are derivatives of the volume – by what? –, normalized by the volume, to keep the quantities intensive.)*

(a) Find $f(P)$.

(b) Find the equation of state.

(c) Under what condition is this material stable? (*Hint: Look at the compressibility.)*