Statistical Mechanics WS 2013/14 Sheet 3

Please hand in your solutions (in pairs) before the Monday lecture.

Problem 1 : Microcanonical and Canonical Ensemble (10 points)

The ensemble average $\langle f \rangle$ of a physical observable $f(\{q,p\})$ in the phase space $\mathbf{\Gamma} \equiv \{q_1, \ldots, p_1, \ldots\}$ with the total phase volume v, is given by

$$\langle f \rangle = \frac{\int f(\{q,p\})\rho(\{q,p\};t)dv}{\int \rho(\{q,p\};t)dv}, \tag{1}$$

where $\rho(\{q,p\};t)$ is the density function. The dimensionless Hamiltonian is denoted by $\mathcal{H}(\{q,p\})/(k_B T) \equiv \beta\mathcal{H}(\{q,p\})$ with the Boltzmann's constant k_B and the absolute temperature T.

a) (2 points) Write down the condition for $\rho(\{q,p\};t)$ to yield the "*stationary ensemble*" which represents a system in *equilibrium*.

b) (4 points) Write down the condition for $\rho(\{q,p\})$ (over the relevant region of $\mathbf{\Gamma}$) to yield the microcanonical ensemble. Express $\langle f \rangle$.

c) (4 points) Write down the condition for $\rho(\{q,p\})$ to yield the canonical ensemble. Express $\langle f \rangle$.

Problem 2 : Distinguishable Ideal Gas under Potential (30 points)

Consider a three-dimensional ideal gas that comprises N *distinguishable* and non-interacting molecules confined to a space of volume V. The molecules are subject to the potential $U_i = \alpha q_i^{2\gamma}$, where $i \in \{1, 2, \ldots, 3N\}$, $\alpha \geq 0$, and γ is positive integer.

a) (2 points) Write down the dimensionless Hamiltonian $\beta\mathcal{H}(q,p)$ of the system.

b) For $\alpha = 0$,
(i) (2 points) Calculate the partition function.
(ii) (2 points) Calculate the Helmholtz free energy $\mathcal{F}_{\text{dist}}$. Express the free energy $\mathcal{F}_{\text{indist}}$ of the *indistinguishable* ideal gas for large N, in terms of $\mathcal{F}_{\text{dist}}$, N and $k_B T$.
(iii) (2 points) Calculate the entropy $\mathcal{S}_{\text{dist}}$. Express the entropy $\mathcal{S}_{\text{indist}}$ of the *indistinguishable* ideal gas for large N, in terms of $\mathcal{S}_{\text{dist}}$, N and $k_B T$.
(iv) (2 points) Calculate the average energy.
(v) (2 points) Calculate the pressure.

c) For $\alpha > 0$,
(i) (5 points) Calculate and express the partition function in terms of $h \equiv (2\pi)\hbar$, α, β, γ, Γ, m and N. For the calculation, assuming that integral over q-space can be taken within the range of $[-\infty, \infty]$, use

$$\int_{-\infty}^{\infty} e^{-ax^{2b}} dx = 2a^{-\frac{1}{2b}} \Gamma\left(\frac{2b+1}{2b}\right), \tag{2}$$

where Γ is the gamma function, and $\{a, b\} \in$ positive real number.
(ii) (5 points) Calculate and express the average energy in terms of $k_B T$, γ, and N.
(iii) (5 points) Find the partition function for $\alpha = m\omega^2/2$ and $\gamma = 1$. Use the value of $\Gamma(3/2) = \sqrt{\pi}/2$.
(iv) (5 points) Find the partition function Z_N^{class} of the one-dimensional N distinguishable classical harmonic oscillators.

Problem 3 : Harmonic Oscillators (20 points)

Consider N quantum harmonic oscillators in one-dimension. They are non-interacting, distinguishable, and have the energy eigenvalues $\epsilon_k = (k + 1/2)\hbar\omega$ per one oscillator, where k is non-negative integer. The number of the oscillators that occupy the energy level ϵ_k is denoted by n_k.

a) (5 points) Calculate the partition function Z_N.

b) (5 points) Calculate the population of energy levels n_k/N.

c) (5 points) Sketch n_0/N, n_1/N and n_{10}/N as functions of β^{-1} in one plot, with $\hbar\omega$ put to unity.

d) (5 points) Compare Z_N in a) with the partition function Z_N^{class} in Problem 2-c)-(iv). Find the condition for $Z_N = Z_N^{\text{class}}$.

(see next page for Problem 4.)

Problem 4 : The N Spins (20 points)

Consider a system of N spins subject to a magnetic field B. The spins are non-interacting with the spin number $s = 1$, distinguishable, and have the non-degenerated energy eigenvalues $\epsilon_m = -\mu B m$ per one spin, where μ is the magnetic moment per one spin, and $m = -1, 0, 1$.

a) (2 points) Calculate the partition function Z_N.

b) (3 points) Calculate the average energy E.

c) (4 points) Calculate the heat capacity $C_B \equiv \left[\frac{\partial E}{\partial T}\right]_B$ at constant B. Plot C_B/k_B vs. $k_B T$, using values of $\mu B = 1$, and $N = 10$.

d) (3 points) Calculate the Helmholtz free energy.

e) (4 points) Calculate the entropy $\mathcal{S}$. Plot $\mathcal{S}/k_B$ vs. $k_B T$, using values of $\mu B = 1$, and $N = 10$.

f) (4 points) Calculate the magnetization $\mathcal{M}$ (the average of total magnetic moment). Plot $\mathcal{M}/\mu$ vs. $k_B T$, using values of $\mu B = 1$, and $N = 10$.