**SAMPLE QUESTIONS FOR DISCUSSION IN WEEK 7 (19 October 2016) and Week 8 EXERCISE CLASSES (24 October 2016)**

You may want to think about it before attending exercise class.

SQ17: Doing all of statistical physics using the microcanonical ensemble and the most probable distribution - The case of classical particles

SQ18: Evaluating $z$ for classical particles again - (a) integral treated by spherical coordinates and (b) integrating over energies of single-particle states

SQ17 **(Related to Problem 4.4) Doing statistical physics of classical particles using the microcanonical ensemble and the most probable distribution**

In Ch.VII, we counted the number of microstates for a given distribution $\{n_i\}$ for fermions and for bosons. In the classical limit where $n_i \ll g_i$ in every cell $i$, which is realized when we don't have that many particles in the system (dilute limit) or the temperature is high that many single-particle states become available for occupation (the high-temperature limit), both microstate numbers $W_{FD}$ and $W_{BE}$ approach the same form of $W_{classical}$ given by

$$W_{classical}(\{n_i\}) = \prod_i \frac{g_i^{n_i}}{n_i!} \tag{1}$$

where the subscript stresses that it is the "classical" particle limit or the Maxwell-Boltzmann limit. [Recall: All particles are either fermions or bosons formally.] The procedure is then to maximize $W_{classical}$ or $\ln W_{classical}$ under the constraints of a fixed number $N$ (thus $N = \sum_i n_i$) of such classical particles with a fixed total energy $E$ (thus $E = \sum_i n_i \epsilon_i$). The result is the most probable distribution $\{n_i\}$ and it follows that $W^{(mp)}$ is also known. Details are given in class notes.

Back to Ch.III, we emphasized that the most probable distribution $W^{(mp)}$ dominates all the other distributions and thus $S = k \ln W$ can be very accurately approximated by $S = k \ln W^{(mp)}$. Here, we illustrate that one can work out all the physics starting from $W^{(mp)}$. [In Problem 4.4, you will work out the physics of bosons in a similar way.]

Using the result of $n_i$ after applying the Lagrange multiplier methods, show that the entropy is given by

$$S_{classical} = \frac{E}{T} + Nk\left[1 + \ln\left(\frac{\sum_i g_i e^{-\epsilon_i/kT}}{N}\right)\right] \tag{2}$$

This is a general expression. Starting with the entropy $S(E, V, N)$ with $V$ hidden in the single-particle energies, everything can be found.

In particular, obtain an expression for the Helmholtz free energy $F_{classical} = E - TS_{classical}$. Hence, show that the result can be written as:

$$F = -kT \ln Z_{classical} \tag{3}$$

such that

$$Z_{classical} = \frac{z^N}{N!}\ , \tag{4}$$

and identify an expression for the single-particle partition function $z$.

**Important Remarks: What we did here is to start with the mircocanonical ensemble approach, find the most probable distribution and then get at the general expressions for canonical ensemble approach, for the case of classical non-interacting indistinguishable particles. It is a short cut in doing statistical mechanics. It is a very practical approach. Some undergraduate textbooks introduce this approach only. However, the method begins with single-particle states and therefore is applicable only to non-interacting particles. Our canonical ensemble formalism (Ch.V and Ch.VI) is general and can be applied even to interacting $N$-particle systems.**

SQ18 **Single-particle partition function for a free non-relativistic particle - Again!**

You should have calculated this quantity twice before in Problem Sets. The single-particle partition function for a free non-relativistic particle is given by (see Problem Set 1 and Set 3, Ch.VII classical limit or SQ17)

$$z = \sum_{all\ cells\ \ i} g_i\, e^{-\beta\epsilon_i} \tag{5}$$

$$= \sum_{all\ s.p.\ states\ i} e^{-\beta\epsilon_i} \tag{6}$$

where the sum in Eq. (5) is over the cells labelled $i$ where there are $g_i$ s.p. states (single-particle states) in the cell $i$, and the sum in Eq. (6) is over all single- particle states one-by-one.

We can evaluate $z$ by turning the sum into an integral in the phase space (6-dimension) of a single particle and the end result is (you did it before)

$$z = \frac{1}{h^3}\int d^3x \int d^3p\ e^{-\frac{p_x^2+p_y^2+p_z^2}{2mkT}} = \frac{V}{\lambda_{th}^3} \tag{7}$$

where $\lambda_{th} = h/\sqrt{2\pi mkT}$ is the thermal de Broglie wavelength. Previously, you did the integrals in Cartesian coordinates, i.e., integrated over $p_x$, $p_y$ and $p_z$.

Here, TA will illustrate that $z$ can be evaluated in other ways. The result, of course, will be the same.

(a) Noting that the integrand in Eq. (7) is actually $e^{-p^2/2m}$, where $p^2$ is the magnitude of the momentum squared, it is spherically symmetrical, i.e., the integrand takes on the same value for different $(p_x, p_y, p_y)$ with the same $|\mathbf{p}|$. Therefore, we could also carry out the integral $\int d^3p\,(\cdots)$ by **spherical coordinates**. Do it and show that the same result pops out, as it should be.

(b) Let's inspect Eq. (5) again. The sum can also be done by classifying the single-particle states according to their energies. Turning the discrete version of Eq. (5) into a continuum version, we introduce the quantity $g(\epsilon)$ (called the single-particle density of states, see Ch.VIII) such that $g(\epsilon)\,d\epsilon$ is the number of s.p. states in the interval $\epsilon$ to $\epsilon + d\epsilon$. Using $g(\epsilon)\,d\epsilon$, the single-particle partition function can be written as

$$z = \sum_{all\ cells\ \ i} g_i\, e^{-\beta\epsilon_i} = \int_0^\infty g(\epsilon)\, e^{-\beta\epsilon}\, d\epsilon = \int_0^\infty g(\epsilon)\, e^{-\epsilon/kT}\, d\epsilon\ . \tag{8}$$

Here, the lower end of the single-particle spectrum is taken to be zero.

Very soon (in Ch.VIII), we will show that for non-interacting particles in 3D, the density of states is given by

$$g(\epsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2}\ . \tag{9}$$

Here, the spin degeneracy $G_s = 2s+1$ is ignored. TA: Evaluate $z$ by integrating over $\epsilon$. You may make use of $\Gamma$ functions.