Department of Physics, The Chinese University of Hong Kong
PHYS 5130 Principles of Thermal and Statistical Physics (M.Sc. in Physics)

Problem Set 6
Due: 23 November 2020 (Monday); "T+2" = 25 November 2020 (Wednesday) (20% discount)

You should **submit your work in one PDF file via Blackboard** to the appropriate folder no later than 23:59 on the due date. Late submission before the T+2 due date will be marked with a 20% discount on the score. Follow Blackboard → Course Contents → Problem Set → **Problem Set 6 Submission Folder**.

Please work out the steps of the calculations in detail. Discussions among students are highly encouraged, yet it is expected that we do your homework independently.

This Problem Set is technically closely related to those used in Ch.X in obtaining the Fermi-Dirac and Bose-Einstein distributions and the density of single-particle states. The results of Problems 6.2 and 6.3, however, supplement those in Ch.IX. Total 110 Points.

6.0 **Reading Assignment.** This is a guide to our progress. **No need to hand in anything**. By the end of Week 10, we derived the governing equations for quantum gases. In Ch.X, we went back to the idea of finding the most probable distribution. Non-interacting particles are assumed, and the approach leads us to the Fermi-Dirac and Bose-Einstein distributions. It is important to realize that the "distributions" $f_{FD}(\epsilon)$ and $f_{BE}(\epsilon)$ actually mean *the number of the particles per single-particle state* at the energy ϵ. Technically, we discussed the method of Lagrange multipliers for constrained optimization. To proceed, we need to know how many single-particle states there are at the energy ϵ, as specified by the density of single-particle states $g(\epsilon)$. We derived $g(\epsilon)$ for 1D, 2D, 3D nonrelativistic free particles, and emphasized that $g(\epsilon)$ carries the information of the dimensionality and the energy dispersion relation. Technically, it is about fitting waves to boundary conditions and counting states in the k-space. Putting together $g(\epsilon)$ and the distributions, we found the equations that give N and E. The "N-equation" serves to fix the chemical potential $\mu(T)$ as a function of the temperature T, and the "E-equation" serves to give the dependence $E(T)$ of the energy of the system on the temperature. A third equation follows from finding the entropy using the most probable distributions and it gives pV directly. We are ready to study Ideal Fermi Gas and Ideal Bose Gas in any spatial dimensions. This Problem Set takes you through all these concepts and techniques. Ch.XI discusses the physics of 3D Ideal Fermi Gas.

6.1 (15 points) **Method of Lagrange Multipliers**

Read the pages on the Method Lagrange Multipliers under Essential Math Skills in class notes. We used the method to obtain the Fermi-Dirac and Bose-Einstein distributions in Ch.X.

There is a surface defined by $x^2 + y^2 - 2xz = 4$. **Find the shortest distance** from the origin to the surface. [Hint: The distance squared from the origin to a point (x, y, z) is $d^2 = x^2 + y^2 + z^2$.]

6.2 (32 points) **Re-deriving the probability of a system of fixed $T(T, V, N)$ to be found in an N-particle state of energy E_i is $exp(-\beta E_i)/Z$**

Background: We derived the result $P_i = \frac{1}{Z} e^{-E_i/kT}$, which is the probability of finding a system (in equilibrium with a heat bath at temperature T) to be **in a N-particle state of energy E_i** in Ch.IX. The partition function $Z(T, V, N)$ becomes the key quantity in the canonical ensemble theory. Here, you will derive the result again, but in a different way using the Lagrange multipliers method. Although there will be no new results, I would ask you to pay attention. The reasons are: it is a classic problem and it also justifies the Gibbs' entropy formula (see Problem 6.3).

The system we are interested in has N particles in a volume V. It doesn't matter whether the particles are interacting or not. In Ch.IX, we learned that the system does not have a fixed energy when it is in equilibrium at a temperature T, i.e., the system can be in different N-particle states but the probability is governed by $P_i = \frac{1}{Z}e^{-E_i/kT}$. This "system" is what we are interested in.

Collection of N-particle systems forming a composite system with fixed energy – Consider a huge number $\mathcal{N}$ of systems, with each system being an N-particle system (the one that we are interested in). Note that the symbol $\mathcal{N}$ is different from N. [Behind the scene: We already know that we can only talk about the mean energy $\langle E\rangle$ of a system, we therefore fix the total energy of the collection of $\mathcal{N}$ systems to be $\mathcal{E} = \mathcal{N}\langle E\rangle$. But you don't need this idea to move on.] We put these $\mathcal{N}$ systems together to form a big composite system, with a fixed energy $\mathcal{E}$. **The $\mathcal{N}$ systems can exchange energy among themselves** (so the systems will be in different states of different energies). The situation is that the $\mathcal{N}$ systems collectively form an isolated system with fixed total energy $\mathcal{E}$. We want to know, after allowing the systems to exchange energy among themselves and waiting long enough for the whole collection to reach equilibrium, how many of the $\mathcal{N}$ systems are in an N-particle states of energy E_1,..., how many are in an N-particle states of energy E_i, and so on. To proceed, we invoke a string of numbers $\{\mathcal{N}_1, \mathcal{N}_2, \cdots, \mathcal{N}_i, \cdots\}$, where $\mathcal{N}_i$ is the number of systems in the collection that are in the N-particle state i of energy E_i. Such a string of numbers must satisfy the two constraints:

$$\sum_i \mathcal{N}_i = \mathcal{N} \tag{1}$$

$$\sum_i E_i \mathcal{N}_i = \mathcal{E} \tag{2}$$

Approach – We will look for the most probable distribution, i.e., the way that the $\mathcal{N}$ N-particle systems share the total energy $\mathcal{E}$ so as the number of microstates is maximized. This is a situation perfectly set up for using the Lagrange multipliers method. The quantity to maximize is therefore

$$\ln W(\{\mathcal{N}_i\}) = \ln\left(\frac{\mathcal{N}!}{\mathcal{N}_1!\mathcal{N}_2!\cdots}\right) \tag{3}$$

Your Action – Apply the Lagrange multipliers method (using α as the multiplier for the constraint Eq. (1) and β as the multiplier for the constraint Eq. (2)),

(a) **derive** an expression for the optimal $\mathcal{N}_i$, in terms of the multipliers,

(b) **determine** the multiplier α using the constraint Eq. (1),

(c) **identify** the multiplier β by comparing results with those in Ch.IX, and hence **identify** the partition function that appeared as a part of your answer,

(d) **obtain** an expression for the mean energy per system $\langle E\rangle = \mathcal{E}/\mathcal{N}$ using the constraint Eq. (2). [Hint: The result should look familiar.]

6.3 (18 points) **Gibbs Entropy Formula - Problem 6.2 cont'd**

In Problem 6.2, you obtained the optimal values of $\mathcal{N}_i$. You saw that $\mathcal{N}_i/\mathcal{N} = P_i$ with $P_i = \frac{1}{Z}e^{-E_i/kT}$, as found in Ch.IX by a different method. Therefore, $\mathcal{N}_i = \mathcal{N}P_i$.

Obtain an expression for the Entropy of the whole collection of systems by $S_{collection} = k \ln W$. Hence, **show that** the **entropy per system** (actually mean entropy per system) $S = S_{collection}/\mathcal{N}$ is given by

$$S = -k \sum_i P_i \ln P_i \tag{4}$$

Here is an alternative path to see $F = -kT \ln Z$. Substituting $P_i = \frac{1}{Z} e^{-E_i/kT}$ into Eq. (4), **obtain** an expression for $\langle E \rangle - TS$ and hence **identify** that $F = -kT \ln Z$. [Hint: Substitute P_i into $\ln P_i$.]

[Remarks: (a) Eq. (4) is the famous Gibbs Entropy Formula. (b) Without the factor k, it gives the Shannon Entropy, which is *the* central quantity in Information Theory. Claude Shannon single-handedly established the information theory. (c) We saw that the formula is also valid in the microcanonical ensemble (see Ch.VIII). (d) Problems 6.2 and 6.3 form an appendix to Ch.IX. They give an alternative way to derive all the results in Ch.IX.]

6.4 (20 points) **Density of single-particle states in d dimensions**

For a non-relativistic particle confirmed in a d-dimensional box of size L^d, **find the density of single-particle states** $g_d(\epsilon)$. **Demonstrate** that your answer can be reduced to the $g_{3D}(\epsilon)$ discussed in class for $d = 3$.

Hence, **write down three governing equations** for studying the physics of Ideal Fermi Gas in d-dimension.

[Hint: Earlier in Ch.VIII, we had a formula for the volume of a d-dimensional sphere.]

6.5 (25 points) **Equation for the Entropy and pV of an Ideal Bose Gas**

In Section H of Ch.X, we derived a general equation for the entropy of an ideal Fermi gas using the Fermi-Dirac distribution as the most probable distribution and then obtained an equation of pV. These are Eq. (36) and Eq. (38) in Ch.X.

Derive the analogous equations for a ideal Bose gas.