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

Problem Set 4
Due: 31 October 2020 (Saturday); "T+2" = 2 November 2020 (Monday) (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 4 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 related to the microcanonical ensemble approach in statistical mechanics. The problems are closely related to the discussions in Ch.VIII of class notes. Total 120 Points.

4.0 **Reading Assignment.** This is a guide to our progress. **No need to hand in anything**. By the end of Week 7, we are close to finishing the discussion on the Boltzmann's formula $S = k \ln W$. We covered the conditions when it is valid, the idea behind replacing a time average by an ensemble average (and thus the idea of a microcanonical ensemble), and illustrated the ideas with three standard applications. The heat capacity of solids problem is related to each particle having an unbounded energy spectrum. The defect formation problem is related to each particle having a bounded energy spectrum. The classical ideal gas problem illustrates the idea of working in the 6N-dimensional phase space and how the breaking down of the result leads to the necessity of considering quantum gases. Ch.VIII ends with sections making connections to thermodynamics and opening new directions for developments. The entropy formula written into the Gibbs form turned out to be the foundation of information science. Irreversible processes and time arrows are related to the huge number of accessible microstates associated with a dominating type of distribution. This leads to the formalism of finding the Most Probable Distribution under some constraints. This method can readily be applied to obtain the Fermi-Dirac and Bose-Einstein distributions for non-interacting particles. The zeroth law of thermodynamics emerges when we put two systems in thermal contact and take the two systems as a composite system. This idea will be extended to the canonical ensemble formalism. Finally the third law of thermodynamics is related to the unique ground state.

Go through all sections of Ch.VIII. It gives all the principles of equilibrium statistical mechanics.

4.1 (15 points) **Frenkel defects or interstitial defects**

The physical picture is that some atoms will leave their equilibrium atomic sites in a solid and move into places somewhere in between the equilibrium atomic sites in a solid. In contrast, the Schottky defects discussed in Ch.VIII are atoms that leave the equilibrium sites and move to the surface sites. Here, you will do a similar calculation but with one additional complication. [For physicists – this completes the statement of the problem. The question is then work out the number of defects as a function of temperature, and what signal there will be in the heat capacity. And you can use whatever methods to get it done.]

As students, I set up the problem for you using only what we have learned so far. Let N be the number of atoms in the system. Let N' be the number of interstitial sites that an atom can move into. The energy required to create one defect (moves away from equilibrium site and go into one interstitial site) is ϵ, which is typically higher than kT at room temperature.

Do a counting of $W(E)$ for a given energy E of creating n such Frenkel defects. [Hint: The counting is related to how many ways that n atoms can be taken out from N atoms **and** placed them into N' sites.] Hence, **find the entropy** $S(E)$ and **derive** an expression for $1/T$. **Turn our result** into an expression giving the number of Frenkel defects $n(T)$ generated as a function of temperature T.

[Remark: For an introduction to the physics of point defects, see Kittel, *Introduction to Solid State Physics* (8th edition) Ch.20.]

4.2 (40 points) **Collection of independent and distinguishable "two-level" particles**

This is also related to the defect formation problem discussed in Ch.VIII, but in a more general situation and in a different context.

Physics Background: We have a collection of identical but distinguishable particles, each has a magnetic dipole moment that can only take on two components along a direction (thus spin-1/2 particles, don't worry if this piece of quantum mechanics is not with you). These dipole moments do not interact with each other and they only respond to an external magnetic field (should say magnetic induction $\vec{B}$). Each particle can therefore be in one of two states with energies $\epsilon_{low} = -\mu B$ and $\epsilon_{up} = +\mu B$, where μ is the standard magnetic dipole moment called the Bohr magneton usually represented by μ_B (I used μ there to save a symbol). Given B, the lowest energy of the whole system is $-N\mu B$, when all particles are in the ϵ_{low} energy state, i.e., ordered by the B-field. There is only one microstate corresponding to $E = -N\mu B$. We would expect this to be the situation at $T = 0$ K. Your task is to consider other values of E, count W, and how the thermal energy kT works to randomize what B wants to order.

We will consider the total energy being in the range $-N\mu B \leq E < 0$. [I will ask you why later.]

(a) For a total energy $E = -N\mu B + n(2\mu B)$ within the range stated above, **count** the number of microstates compatible with the given energy E.

(b) **Obtain** the entropy S. [Optional (no bonus): It will be educational to **sketch** $S(E)$.]

(c) Hence, **obtain** $1/T$ and **turn the answer** into an expression for $E(T)$. **Find** the heat capacity $C(T)$. **Sketch** the two results as a function of T. **What does it mean** by high temperature and low temperature in this problem? **Discuss** the low temperature and high temperature behavior of $E(T)$ and $C(T)$.

(d) With the answer in part (c), **discuss why** we don't consider $E > 0$. **What's wrong** if we do so?

(e) For magnetic field problems, it is more important to look at the total magnetic dipole moment $\mathcal{M}$ of the system. The convention is tricky and so be careful. When a particle is in lower energy ϵ_{low} state, its magnetic dipole moment is aligned with the B-field (this is EM idea) and so it contributes $+\mu$ to $\mathcal{M}$. Similarly, when a particle is in the upper energy ϵ_{up} state, its magnetic dipole moment is anti-aligned with the B-field and so it contributes $-\mu$ to $\mathcal{M}$. For example, at $T = 0$ K, $\mathcal{M} = N\mu$. Analyzing what you already did in the problem, **translate your answers (explain how)** into an expression that gives $\mathcal{M}(T)$, i.e., the total magnetic dipole moment of the system as a function of temperature.

(f) **Find** the high temperature behavior of $\mathcal{M}$.

(g) More formally, the expression of $\mathcal{M}(T)$ in part (e) can be regarded as $\mathcal{M}(T, B)$, as B also appears in the answer. **Obtain** $\partial\mathcal{M}/\partial B$, which is the magnetic susceptibility χ apart from a constant (probably off by μ_0 (the vacuum permeability)). Hence, **analyze** the high temperature behavior of χ.

[Remarks: If you carry the parts through, you have done/learned for yourself an important section in statistical mechanics and solid state physics about paramagnetic materials. The answer in part (g) is the Curie's law. For those who like to work more things out, you may also try the same problem with 3-level particles, e.g. $+\epsilon, 0, -\epsilon$ are the possible states for each particle. No bonus, of course.]

4.3 (25 points) **Microcanonical Ensemble approach for a collection of Distinguishable Classical Oscillators**

[Remarks: For Problems 4.3 and 4.4, I will not break the problems down into smaller parts. Instead, I will let you work out the problems as much as you like/can. They are closely related to sections in class notes. It is hoped that this will also build up your maturity in doing physics.]

Introduction: In Application A of Ch.XIII, we did the correct calculation of a collection of identical but distinguishable oscillators. By correct we meant that you took into account of the quantized energy spectrum of each oscillator. In Application C, we discussed the classical ideal gas by doing integrals in the 6N-dimensional phase space. And it works! Here is your turn to apply the techniques in the classical ideal gas calculation to a collection of **distinguishable classical oscillators**, i.e., the quantized nature of the energy levels in an oscillator is ignored in the calculation.

Consider a collection of $3N$ distinguishable (1D) oscillators, each with the same angular frequency ω. The Hamiltonian of each oscillator is

$$h(p, x) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \ .$$

The total Hamiltonian is given by summing over all the $3N$ oscillators.

Read Application C in Ch.VIII carefully. Your task is to repeat the calculation for $3N$ classical oscillators, find $E(T)$ and the heat capacity $C(T)$. [Basically, it is like writing another application for the class notes.]

You may start with the following expressions for **the number of microstates with energies less than or equal to a given energy** E,

$$W^{<}(E, N) = \frac{1}{h^{3N}} \underbrace{\int dp_1 \int dp_2 \cdots \int dp_{3N} \int dx_1 \int dx_2 \cdots \int dx_{3N}}_{\sum_{i=1}^{3N}\left(\frac{p_i^2}{2m} + \frac{1}{2}m\omega^2 x_i^2\right) \leq E} \ .$$

There is no $1/N!$ here because the oscillators are distinguishable (by their locations). The question is: **Obtain** all results and **discuss** the physics.

Hints: You may want to follow this path. Evaluate $W^{<}(E, N)$ (high-dimensional sphere?); obtain $\mathcal{W}(E, N)$; evaluate the entropy $S(E, N)$; evaluate the temperature; turn the result into $E(T, N)$; and then obtain the heat capacity $C(T)$; and compare results with the full quantum calculation in Application A of Ch.VIII.

4.4 (40 points) **Write a new section of notes on putting two subsystems of different particle numbers into thermal contact**

This is similar to Sec. J of Ch.VIII. There we illustrated how the zeroth law of thermodynamics emerges from our stat mech technique. We used two subsystems with the same particle numbers $N = 4$ and $N_2 = 4$ in Sec. J. Here, you will consider two subsystems with $N_1 \neq N_2$.

Let $N_1 = 3$ and $N_2 = 5$. Initially $E_1 = 2\epsilon$ and $E_2 = 14\epsilon$. The set up is exactly that in Sec. J.

Discuss all the physics when we start from two subsystems not exchanging anything between each other to putting them together into thermal contact (only energy can be exchanged) and reaching equilibrium. The physics includes (not limited to): the change in the accessible microstate numbers after systems are in thermal contact, entropy change, all energy distributions between the two subsystems when they are in thermal contact and the number of microstates for each distribution, the dominating distribution, irreversible processes, time of arrow, zero law, etc.