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

Problem Set 5
Due: 9 November 2020 (Monday); "T+2" = 11 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 5 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 closed related to discussions in Ch.IX of class notes on the calculation and applications of the Partition Function. Total 110 Points.

5.0 **Reading Assignment.** This is a guide to our progress. **No need to hand in anything**. By the end of Week 8, we introduced the second method in statistical mechanics. Namely, we consider a system with fixed N and V, and also with a temperature T that is fixed by a heat bath. There is no new physics and no new principles. Treating the composite system consisting of the heat bath and the system as an isolated system and that all microstates are equally probable for an isolated system at equilibrium, we derived that the probability of finding the system to be in **a state** of energy E_i is $e^{-\beta E_i}/Z(T,V,N)$, where $Z(T,V,N)$ is the **partition function**. We then show that the microscopic quantity $Z(T,V,N)$ is related to the macroscopic thermodynamic Helmholtz free energy $F(T,V,N)$ through $F(T,V,N) = -kT \ln Z(T,V,N)$. From thermodynamics, we know that by taking partial differentiations of F, we get S, P, and μ. This calculation scheme is called the canonical ensemble theory. We set up the theory in its general form, i.e., all the formulas are applicable to interacting N-particle systems. Of course, we (you) will do examples (problems) on non-interacting N-particle systems because Z can be evaluated exactly in these cases.

5.1 (36 points) **Be very careful about what are being summed up in getting Z**

The Partition Function $Z(T,V,N)$ enters the scene of statistical mechanics humbly as a normalization factor. However, it is related to the Helmholtz free energy $F(T,V,N)$ in one step and then every thermodynamic variable follows. The partition function is given by:

$$\begin{aligned} Z(T,V,N) &= \sum_{\text{all } N\text{-particle states } i} e^{-\beta E_i} & (1) \\ &= \sum_{\text{all } N\text{-particle levels } i} W(E_i,V,N)\, e^{-\beta E_i} & (2) \\ &= \int \mathcal{W}(E,V,N)\, e^{-\beta E} dE & (3) \end{aligned}$$

To apply Eq. (1) and Eq. (2), it is important to understand what are being summed up. A way (not the cleverest way perhaps, but works) is to list clearly the N-particle states (then use Eq. (1)) or list all the energy levels together with the degeneracies that are to be summed over (then use Eq. (2)). Eq. (3) makes use of the density of N-particle states $\mathcal{W}(E,V,N)$ as the energies of a N-particle system are usually densely packed and a continuum description is necessary and convenient.

You must have heard of fermions and bosons, as well as balls of different colors (an example of distinguishable particles). This problem serves to illustrate that Z will depend on the nature of the particles, using the simplest possible system of only **two particles**. The point is that the list of states to sum over will **depend on** whether the particles are distinguishable particles, identical fermions or bosons, i.e., the quantum nature of the particles really matters!

Consider a system of **two non-interacting particles**. The temperature is T. For such a system, the standard steps (similar to how atoms are treated approximately in quantum mechanics) are: solve for the single-particle states and then fill the two particles into the single-particle states according to some restrictions based on the nature of the particles. Let's say someone has solved the allowed energies and wavefunctions of the single-particle problem. Your task is to do the second step (how to fill the two particles in) and write down the Partition Function. It turned out that **there are only 5 single-particle states and their energies are** 0**,** 0**,** ϵ**,** ϵ**, and** 2ϵ. That is to say, there are two different single-particle wavefunctions with energy 0, two different wavefunctions with energy ϵ and one wavefunction with energy 2ϵ.

Find the partition function Z for each of the following cases.

(a) Two **distinguishable particles**. **Make a list of all the two-particle states** that are to be summed up in Eq. (1) and **find** $Z_{distinct}$. This case can be thought of having a red particle and a blue particle. Next, **demonstrate** how Eq. (2) can be used to obtain the result. **Show** explicitly that $Z_{distinct}$ can be factorized into a product of single-particle partition functions.

(b) Two **identical fermions** (don't worry about spin in this problem, the only restriction is the Pauli exclusion rule, i.e., two identical fermions cannot occupy the same single-particle state). **Find** $Z_{fermion}$. [Here, identical means indistinguishable.]

(c) Two **identical bosons**. The point here is that the Pauli exclusion rule does not work for bosons. **Find** Z_{boson}.

(d) Look at your results in (a)-(c). One would naturally think that $Z_{fermion} \neq Z_{distinct}$ because the Pauli exclusion rule and it is indeed the case. However, as the Pauli exclusion rule does not apply to bosons and therefore it is **not too obvious** why Z_{boson} is different from $Z_{distinct}$. From your calculations, **explain why** Z_{boson} **and** $Z_{distinct}$ **are different**.

Intermission-what's next: The following two parts serve to illustrate why (sometimes) a correction factor $1/N!$ could turn the distinguishable particles result in part (a) into a useful result for **indistinguishable but classical particles**. Part (e) shows that **the correction factor does not always work**. Part (f) shows that sometimes it works and why we have the idea of *classical particles.*

(e) Many tried to **make a correction** to the counting of states for distinguishable particles (as in part (a)) and use the modified result for indistinguishable particles (and hopefully for bosons and fermions). A standard (and lazy) way is to introduce a factor $1/N!$ and thus $1/2! = 1/2$ to our two-particle problem. The idea is to *correct for the over-counting* in 2-particle states in the distinguishable case. **Explain what** "over-counting" refers to? **Examine whether** a factor 1/2 works in correcting $Z_{distinct}$ into Z_{boson} or $Z_{fermion}$? If not, **why not**?

(f) Sometimes, the correction factor $1/N!$ does work! Let's say we impose an additional condition that the two particles cannot occupy the same single-particle state into the counting in each of the three cases in (a)-(c). **Show** that the correction factor $1/2!$ works in correcting the over-counting of states in the distinguishable particle case.

Important remark: This is exactly the $1/N!$ that we included in the counting of states for the classical ideal gas problem (see microcanonical ensemble approach). "*Classical*" here means that we don't need to worry about the particles are bosons or fermions at all (as they will not occupy the same state anyway). Thus, the correction factor $1/N!$ is also included in doing classical statistical mechanics within the canonical ensemble.

5.2 (22 points) **An alternative way to write down Z for the Fermion and Boson cases in Problem 5.1.**

The physical situation is exactly that in Problem 5.1. We will re-do the two-fermion case and the two-boson case, but using the *occupation number representation.* Let's label the five single-particle states by 1,2,3,4,5; which have energies $0, 0, \epsilon, \epsilon, 2\epsilon$. Let n_1 be the number of particles in the state number 1, n_2 be the number of particles in state number 2, and so on. Thus, what you considered in Problem 5.1 as a 2-particle state can be represented by a string of five occupation numbers $\{n_1, n_2, n_3, n_4, n_5\}$.

(a) The two particles are **two identical fermions** (don't worry about spin, the only restriction is the Pauli exclusion rule).

The Pauli exclusion rule imposes a restriction on the possible value of the occupation numbers, i.e., $n_i = 0$ or 1. We only have two particles in total, i.e., we also have the condition $\sum_{i=1}^{5} n_i = 2$ to satisfy. Explicitly, a list $\{n_1, n_2, n_3, n_4, n_5\}$ with $n_i = 0$ or 1 AND $\sum_{i=1}^{5} n_i = 2$ represents one possible 2-fermion state. [Pause: Understand this description?]

Your action: **Make a table that gives the occupation numbers** $\{n_1, n_2, n_3, n_4, n_5\}$ **for all possible 2-fermion states**. For each state, also give the corresponding energy E. Using your table, **evaluate** $Z_{fermion}$ for two identical fermions using Eq. (1).

(b) The two particles are **two identical bosons**.

For boson, an occupation number n_i can be any integer because the Pauli exclusion rule doesn't work. But we still have the condition $\sum_{i=1}^{5} n_i = 2$ as there are two particles in total. Explicitly, a list $\{n_1, n_2, n_3, n_4, n_5\}$ with n_i being integers AND $\sum_{i=1}^{5} n_i = 2$ represents one possible 2-boson state. **Make a table that gives the occupation numbers** $\{n_1, n_2, n_3, n_4, n_5\}$ **for all possible 2-boson states**. For each state, also give the corresponding energy E. Using your table, **evaluate** Z_{boson} for two identical bosons using Eq. (1).

[Remarks: Imagine now there are 10^{23} fermions/bosons to be filled into densely packed (say) 10^{30} states (should be infinitely many in principle). Writing down what to be summed up in Z is troublesome, if not impossible! Should we give up? At least we need to find some ways out. We could go back to the way formulated in Ch.XIII Sec I (the most probable distribution). Another way out is to relax the restriction on $\sum_i n_i = N$ (thus allowing for fluctuations in the total number of particles in the system), which is exploited in the Grand Canonical Ensemble theory.]

5.3 (28 points) $J = 1$ **case of the paramagnetic problem: three-level particles**

The case of $J = 1/2$ paramagnetism is discussed in class. It is a realization of two-level systems. Here you will do the $J = 1$ case. Here, J is the angular momentum quantum number in atomic physics. The sequence of arguments is that: (i) the electrons are orbiting around the nucleus (orbital angular momentum) and they themselves carry an intrinsic spin angular momentum; (ii) the spin angular momentum and orbital angular momentum will couple through the spin-orbit interaction, (iii) therefore the combined total angular momentum $\vec{J}$ of all the electrons in an atom is important, (iv) the magnitude is $|\vec{J}| = \sqrt{J(J+1)}\,\hbar$ in quantum mechanics with J can possibly take on values of an integer or a half-integer, (v) the z-component of $\vec{J}$ can only take on limited discrete values $J_z = m_J\hbar$ with $m_J = J, J-1, \ldots, -J$ for a given value of J, (vi) there is a magnetic dipole moment $\vec{\mu}$ associated with the total angular momentum $\vec{J}$ because the electrons are charged, (vii) so each particle/atom becomes a tiny magnet interacting with an external magnetic field. You do not need this background to work out this problem though.

Consider N particles/magnetic dipole moments. They are $J = 1$ particles. Therefore, $m_J = 1, 0, -1$ and each magnetic dipole moment becomes a three-level particle in the presence of a external field $\vec{B} = B\hat{z}$. Formally, the energies are $-g\mu_B B, 0, +g\mu_B B$, where g is called the g-factor. We may call them $-\epsilon, 0, +\epsilon$ in carrying out the calculation and at the end referring back to $\epsilon = g\mu_B B$ to extract the physical results.

(a) **Show** that $Z = z^N$ for N magnetic moments in a uniform B-field, and **calculate** the single particle partition function z, when the system is in equilibrium at a temperature T.

(b) **Calculate** the mean energy $\langle E \rangle$.

(c) **Identify** the average z-component of a magnetic moment $\langle \mu_z \rangle$.

(d) **Write down** an expression for the magnetization M (defined as the magnetic dipole moment per unit volume in electromagnetic theory). **Discuss** the physics in the two limits (what limits?). In particular, work out **how M depends on the temperature** in the limit of low applied field and high temperature and **relate** your result to the Curie's law.

5.4 (24 points) **Heat capacity of two-dimensional solids due to lattice vibrations**

Background: We did the Debye model of heat capacity for three-dimensional solids. The model is that of N atoms forming a 3D lattice. Since each atom is bonded to its neighbors, the classical mechanical normal-mode problem is that of balls connected by springs. With each atom oscillating in three directions, there are $3N$ normal modes. Each normal mode corresponds to an independent harmonic oscillator. Therefore, there are $3N$ oscillators with a spread in the angular frequencies. The number of normal mode frequencies in the interval ω to $\omega + d\omega$ is $D(\omega)d\omega$. Debye took $D(\omega) \propto \omega^2$ up to a cutoff Debye frequency ω_D and obtained the correct low temperature behavior of $C(T) \sim T^3$, as observed in experiments.

Here, you are asked to repeat the argument and find out how $C(T)$ behaves for a strictly two-dimensional solid. Consider N atoms in a 2D solid. The atoms can only vibrate within the 2D plane. It is given that in 2D, $D(\omega) \propto \omega$ for the low-frequency normal modes.

[Hint: You need NOT re-do the partition function calculation. You may take an appropriate starting point that can be applied to a collection of oscillators problem as suggested below.]

(a) **Debye model in 2D.** We will use the expression of the energy of a collection of oscillators:

$$\langle E \rangle = E_{GS} + \int D(\omega) \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \, d\omega \tag{4}$$

to explore how $C(T)$ behaves in 2D.

To do that, you need to **develop the Debye model** in 2D. Writing $D(\omega)$ within the Debye approximation as

$$D^{(2D)}_{Debye}(\omega) = \mathcal{A}\omega \ , \tag{5}$$

determine the prefactor $\mathcal{A}$ and the cutoff ω_D Debye frequency below which Eq (5) is valid.

(b) Work out how $\langle E \rangle$ depends on T at low temperatures in 2D. You may look up from integration tables or on the web a definite integral that appears in the calculation. Hence, **find** the temperature dependence of the heat capacity of a 2D solid at low temperatures.

(c) **Debye model in d-dimensions.** Without going into the details of a d-dimensional solid but to claim that $D(\omega) \propto \omega^{d-1}$ for the low-frequency normal modes, **extract how $C(T)$ behaves at low temperatures** for general dimension d. [Hint: The prefactor and integral are not important for getting $C(T)$ at low temperatures.]