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

**Problem Set 7**
**Due: 9 December 2020 (Wednesday); "T+2" = 11 December 2020 (Friday) (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 7 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 discussed in Ch.XI and Ch.XII on Ideal Fermi Gas and Ideal Bose Gas. Basic ideas in handling interacting systems are also involved. Total 110 Points.**

7.0 **Reading Assignment.** This is a guide to our progress. **No need to hand in anything**. By the end of Week 12, we studied ideal Fermi Gas and ideal Bose Gas, using 3D free particles as the system. We set up the set of general equations governing the physics in any dimensions and for particles obeying different dispersion relations (embedded in the DOS $g(\epsilon)$) for both cases. In Ch.XI, we did the 3D Fermi Gas. The $T = 0$ physics is the most important, as the Pauli exclusion rule forces the fermions to fill up single-particle (s.p.) states high up in energy. The $T = 0$ physics defines the Fermi Energy $E_F$, which is a high energy scale. Associated with $E_F$ are $T_F$ (the Fermi temperature), $k_F$, and $v_F$. We illustrated that for the conduction electrons in a metal, which was a successful attempt by Sommerfeld to explain much metal physics using the Fermi Gas idea, the number density $N/V \sim 10^{22}\ cm^{-3}$ gives a $E_F \sim$ a few $eV$. Noting that room temperature corresponds to $1/40\ eV$, making metal physics in ordinary temperatures (all the way to its melting) **low-temperature physics**. We also discussed the low-temperature physics. The integrals can be done by using the Sommerfeld expansion (which we didn't provide a proof). At high temperature, we also found that there is a quantum signature in $B_2$ with its sign signalling an effective repulsion between the fermions (even they are non-interacting).

In Ch.XII, we did the 3D Bose Gas. For the Bose Gas, the $T = 0$ physics is trivial but indicative. We were led to the idea that the form of the DOS $g(\epsilon) \sim \epsilon^{1/2}$ in 3D does not account for the boson in the lowest $\epsilon = 0$ s.p. state. But this particular state is especially important for bosons, because all bosons can go into it at $T = 0$. Therefore, we need to single out the $N_0$ term. We then discuss the physical picture behind the Bose-Einstein condensation and derived a formula for $T_c$. Below $T_c$, there is a macroscopic population $N_0 \sim N$ in the s.p. $\epsilon = 0$ state. This is called the condensate. At high temperature, we also found that there is a quantum signature in $B_2$ with its sign signalling an effective attraction between the bosons (even they are non-interacting). We also discussed the very clever physics behind the cooling of atoms and first experiments achieving BEC. The field has developed into a hot area covering several frontiers in physics.

In Ch.XIII, we outlined how statistical mechanics can systematically handle interaction between particles. We obtained the first correction term $B_2(T)$ for an interacting gas. It serves the purposes: (i) that the stat mech formalism is valid for non-interacting and interacting systems, (ii) interacting systems are hard to handle analytically but approximations can be developed, (iii) the results backed up the discussions on the high-temperature behavior in ideal Fermi and Bose gases. The calculation of $B_2$ is also in line with what we get from the van der Waals equation of state. We also discussed the physics near the critical point within the vdW equation.

In Ch.XIV, we use ferromagnetism as another example of interacting systems. The Ising model, including interactions between magnetic dipole moments (often called spin-spin interaction) and the effect of an external applied magnetic field, serves as the simplest model problem. We develop the simplest mean-field theory by copying results from paramagnetism, after decoupling the interaction terms into an unknown internal magnetic field acting on individual dipole moments. The idea of self-consistency is discussed. Critical exponents are obtained within the mean-field theory. At the end, a clever twist on the mean-field theory leads to some profound ideas in physics.

7.1 (24 points) **Fermi energy and Fermi temperature.**

It was found that the Fermi energy $E_F \sim n^{2/3}$ for 3D non- relativistic Fermi Gas, where $n = N/V$ is the particle number density. For metals, $n \sim 10^{22}/cm^3 = 10^{28}/m^3$, giving the Fermi energy $E_F$ being a few $eV$ and therefore room temperature metal physics is low-temperature Fermi gas physics.

(a) Data books say that sodium has a conduction-electron number density of $2.65 \times 10^{22}\ cm^{-3}$. Taking the conduction electron mass to be the bare electron mass (sometimes in a solid the mass of an electron is different from the bare electron mass), **evaluate** the Fermi energy $E_F$ and convert the answer to the Fermi temperature $T_F$.

(b) Given $N/V$ as in part (a), **evaluate** an average separation between two conduction electrons in sodium. Also **evaluate the temperature** $T_0$ such as the thermal de Broglie wavelength $\lambda_{th}(T_0)$ equals the average separation between two electrons. Comment on the orders of magnitude of $T_F$ and $T_0$.

(c) For astronomical purposes, a typical neutron number density is $n \sim 10^{44}\ m^{-3}$. [Note: use neutron mass.] Assuming a neutron gas to be a 3D non-relativistic Fermi gas, **evaluate** the Fermi energy $E_F$ (in $eV$), the Fermi wavevector $k_F$ (in Å$^{-1}$), and the Fermi temperature $T_F$ (in Kelvin).

(d) Let's get back to some solid state physics. In a clean (intrinsic) semiconductor, the valence band is completely full and the conduction band is completely empty at $T = 0$. An important part of the semiconductor industry is to fabricate extremely clean semiconductors and then make them dirty (called doping) in a controlled way for device applications. In $n$-type doping, some electrons are put into the conduction band. Through doping, it becomes possible to **control the number of conduction electrons** in the conduction band. This should be contrasted with the fixed $N/V$ for a given metal (e.g. sodium has a certain number). In semiconductors, it is possible to get at an electron number density of $10^{15}/cm^3$ to $10^{16}/cm^3$, which is a factor $10^{-6}$ to $10^{-7}$ of that of metals. It will change the Fermi energy and Fermi temperature. **Estimate** the Fermi energy and the Fermi temperature $T_F$ for $N/V = 10^{16}/cm^3$.

[Remark: This result is important. For such a very dilute sea of conduction electrons, room temperature could be high temperature! This actually makes life easier for semiconductor scientists and engineers, as the gas at high temperature behaves very much like a classical gas. Technically, $\mu$ becomes negative (below the bottom of the conduction band) and it is only the tail of the Fermi-Dirac distribution at positive energies matters and the tail looks just like the Maxwell-Boltzmann distribution. Got it! The statistical mechanics we learned is necessary for doing semiconductor physics.]

7.2 (27 points) $T = 0$ **physics for an ultra-relativistic Fermi gas**

We saw the even at $T = 0$, a 3D non-relativistic Fermi gas has a pressure $p \sim (N/V)^{5/3}$ due to the Pauli exclusion rule. This pressure, called the degenerate pressure, is argued to be the pressure due to electrons in dying stars that works against the collapse due to gravity. This is an important part of astrophysics concerning the life of a star. Its "success" immediately led to the question of whether the electrons in a star are non-relativistic. Intuition says that they are not. So, a proper way is to use the dispersion relation $\epsilon(p) = \sqrt{c^2p^2 + m^2c^4}$, obtain the s.p. density of states $g(\epsilon)$ and re-do the relativistic Fermi gas physics. It is not easy due to the complicated form of $\epsilon(p)$. For those astrophysics fans, see Greiner *et al.*, *Thermodynamics and Statistical Mechanics*, Ch.14 for a discussion.

Here, you will take on the easier task of an ultra-relativistic Fermi Gas. By that we meant using the dispersion relation of $\epsilon(k) = cp = c\hbar k \sim k$. Thus, we have $\epsilon(k) \sim k$ instead of $\epsilon(k) \sim k^2$ for non-relativistic particles.

(a) Using the idea of fitting waves into a $L \times L \times L = V$ volume, **show that** the density of states $g_{ultra}(\epsilon)$ is given by

$$g_{ultra}(\epsilon) = \frac{V}{\pi^2} \frac{1}{(c\hbar)^3} \epsilon^2, \tag{1}$$

where a spin-degeneracy factor of 2 has been included.

(b) At $T = 0$, the Fermi-Dirac distribution is a step function, where the step is adjusted to account for the number $N$ of fermions in the volume $V$. **Derive** an expression for the Fermi energy $E_F$. Hence, **find the total energy** $E$ at $T = 0$ and **find the energy per particle** at $T = 0$.

(c) **Derive** a relationship between $pV$ and the total energy $E$ for the ultra-relativistic Fermi gas. [Hint: It is different from that of a non-relativistic Fermi gas.]

(d) Hence, **derive** an expression for the pressure at $T = 0$ and **extract** how the pressure depends on the number density $N/V$.

[Hint: You will find that $p \sim (N/V)^?$ with "?" not being 5/3 as for a non-relativistic Fermi gas. For those who want to move forward, consider the gravitational pull in a uniform sphere (star) of volume $V$ and total mass $M$. In particular, the gravitational pull tends to lower the volume, but in doing so $N/V$ will increase and thus the pressure will go up to oppose the gravitational pull. Can you derive an effect from gravity that can be compared with the fermionic pressure? If so, the question becomes whether there is a critical mass of the star such that the gravitational pull will win over the fermionic pressure and eventually the star will collapse.]

7.3 (27 points) **Ideal Bose Gas in a 3D harmonic trap**

We considered 3D Ideal Bose Gas in which the density of states is calculated from particle-in-a-box of volume $V$. We saw that the experimental setup in trapping atoms in magneto-optical traps usually have a harmonic potential energy form at the place where atoms are trapped. Your task here is to examine Bose-Einstein condensation for non-interacting bosons trapped in a 3D isotropic harmonic potential.

[Technically, this is similar to Problem 7.2, i.e., changing the density of states $g(\epsilon)$ and then you can re-do a problem.]

For non-interacting bosons trapped in a potential energy function of the form

$$U(x, y, z) = \frac{1}{2} m\omega^2 (x^2 + y^2 + z^2) , \tag{2}$$

the single-particle states (after solving the 3D Schrödinger equation) are $\psi_{n_x,n_y,n_z}(x, y, z)$ with energies given by

$$\epsilon_{n_x,n_y,n_z} = (n_x + n_y + n_z)\hbar\omega + \frac{3}{2}\hbar\omega \tag{3}$$

where $n_x, n_y, n_z = 0, 1, 2, \ldots$ and the last term $3/2\hbar\omega$ is the ground state energy.

For simplicity, we may ignore the ground state energy and write

$$\epsilon_{n_x,n_y,n_z} = (n_x + n_y + n_z)\hbar\omega \tag{4}$$

instead, so that when all the boson go into the s.p. ground state, we regard them to go into the state of energy $\epsilon = 0$ instead of $\epsilon = 3/2\hbar\omega$.

(a) **Derive** an expression for the density of states $g(\epsilon)$. [Hint: Note that the allowed values of $(n_x, n_y, n_z)$ form a uniformly spaced array of dots. Therefore, the tricky part here is to consider what is the shape of the volume defined by a constant $\epsilon$ in this space formed by $n_x$, $n_y$, and $n_z$.]

(b) Let there be $N$ bosons in the trap. **Obtain an equation** that can be solved for the Bose-Einstein transition temperature $T_c$ for bosons in a 3D harmonic trap. **Examine** whether an integral exists or not, and hence **derive** an expression for $T_c$. [You may leave an integral unevaluated in the answer.]

(c) **Derive** an expression for $N_0(T)$, the number of bosons in the s.p. ground state for $T < T_c$.

7.4 (16 points) **The second virial coefficient $B_2(T)$ for the simplified Lennard-Jones potential**

The second virial coefficient describes the leading term in the deviation from ideal gas behavior. We introduced it as

$$\frac{p}{kT} = \frac{N}{V} + B_2(T)\left(\frac{N}{V}\right)^2 + \cdots \tag{5}$$

In class, we showed that $B_2(T)$ is related to an integral of the inter-particle potential energy function $U(r)$, i.e.,

$$B_2(T) = -2\pi \int_0^\infty [e^{-U(r)/kT} - 1] r^2 dr \tag{6}$$

Let's consider a model potential. The Lennard-Jones (or 6-12) potential is a popular inter-particle potential. The interaction is not strong. In full, it has the form of

$$U(r) = \frac{c_{12}}{r^{12}} - \frac{c_6}{r^6} \tag{7}$$

The first term is the very steep repulsive part that two particles don't want to get too close to each other. The second term is a softer attractive part crucial for condensation. This full form is not easy to handle. So we model the repulsive "12"-part by a hard core and keep the "6"-part. This leads us to **consider a model potential** of a hard sphere plus a Lennard-Jones attractive part, i.e., $U(r) = \infty$ for $r < r_c$, and $U(r) = -c_6/r^6$ for $r > r_c$.

**Evaluate** $B_2$ in terms of $c_6$ and $r_c$. Hence, identify the expressions of $a$ and $b$ that go into the van der Waals equation of state. [Hint: See class notes on how the positive and negative terms in $B_2$ get into the van der Waals equation.]

7.5 (16 points) **Behavior near the critical point of the van der Waals equation of state**

When the temperature, volume and pressure are expressed in units of the critical temperature $T_c$, critical volume per mole $v_c$, and critical pressure $P_c$, i.e., using the reduced quantities $P_R \equiv P/P_c$, $v_R \equiv v/v_c$, and $T_R = T/T_c$, the van der Waals equation becomes

$$\left(P_R + \frac{3}{v_R^2}\right)\left(v_R - \frac{1}{3}\right) = \frac{8}{3}T_R \tag{8}$$

In this form, the critical point is at $T_R = 1$, $P_R = 1$ and $v_R = 1$.

By studying the behavior of the van der Waals equation about the critical point, **extract** the critical behavior relating (a) $\delta v_R$ and $\delta T_R$, and (b) $\delta p_R$ and $\delta v_R$, where the quantities are tiny deviations from the critical point. That is to say, **extract** the critical exponents $\beta$ and $\delta$.