Physics 112 - Intro to Statistical and Thermal Physics - Spring 2023
Problem Set 09

Due Friday, April 14 at 11:59 PM (PDT)
Last Update: April 18, 2023

- **Highlighted/Most Relevant Reading for the material on this week's problem set:**
  - Schroeder, Sections 7.2
- **Reading for next week:**
  - Schroeder, 7.4, 7.5

Problem 9.1 - Permutations

In this problem set we will explore some of our different quantum statistics and systems. We start with the different possible states and number of states available in our different system types.

A set of $N = 5$ particles of mass m are in the same 1D simple harmonic oscillator potential of frequency ω. Consider the lowest-energy $N = 5$-particle microstate(s) for this system in the following cases:

- The particles are all distinguishable.
- The particles are identical spin-0 bosons.
- The particles are identical spin-1/2 fermions. (Don't forget to account for the spin!)
- **Extra Part** (*Not for Credit*) The particles are identical spin-1 bosons. (Don't forget to account for the spin!)

(a) For each of the cases, determine the energy of the lowest-energy $N = 5$-particle microstate, the degeneracy/multiplicity of that state, and describe the state by its occupation numbers (e.g. how many particles are in the $n = 0$ state, how many are in the $n = 1$ state, etc.)
Hint (highlight to reveal): [For a spin-1/2 particle, there are two different "ground states" available, $\{|0, \uparrow\rangle, |0, \downarrow\rangle\}$.]

When we have indistinguishable particles we only care about the ***permutation classes***. For example, in lecture we looked at the permutation classes in the cases when we had $N = 2$ particles in an $A = 2$-level system and then $N = 3$ particles in an $A = 3$-level system. Next let's look at a system of $N = 3$ identical particles with $A = 4$ available states $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$. We can list these states either using the "balls and bins" notation I used in class or by giving the four occupation numbers $\{n1, n2, n3, n4\}$ for each of the four states.

(b) How many permutation classes do we have in this system? How many bosonic states are in this system? How many fermionic states? Describe each of the possible fermionic states (using either the "balls and bins" notation or the occupation numbers).
[*Note: We can assume that our four states include spin - e.g. if we are looking at spin-1/2 fermions these four states could be two different energy levels with the two different spin values. If we are looking at spin-0 bosons these four states could just be four different energy levels or two different energy levels with some other source of a factor of two degeneracy. In the high-temperature limit we don't really care about the energies - the important point is that for a single particle a total of four states are available.*]

In the high-energy limit, each available state has equal probability of occurring. But different states are available based on whether our particles are bosons or fermions.

(c) Consider both fermions and bosons in this $N = 3$ particles in an $A = 4$-level system in the high-energy limit and determine the probability of finding exactly one particle in the one-particle ground state. That is, for both fermions and bosons determine the probability that $n_1 = 1$.

Even though most systems we will look at (like the harmonic oscillator or particle-in-a-box) have an infinite number of states, the finite energy of the system means in practice only a finite number of states are *actually* available to be populated. Consider a system with a set of A available one-particle quantum states. Each of the N particles can be in any one of the A states so if the particles were distinguishable there are $\mathscr{N}_D = A^N$ different available N-particle microstates. In class, we claimed that when we have identical bosons or fermions then the number of N-particle microstates is given by

$$\mathscr{N}_B = \binom{A+N-1}{N}; \qquad \mathscr{N}_F = \binom{A}{N}.$$

(d) **Extra Part** (*Not for Credit*) Argue why these expressions for the counting of bosonic and fermionic states are correct.
Hint (highlight to reveal): [Remember that there is one totally symmetric state per permutation class and we only have a totally antisymmetric state in a permutation class if none of the A states contain more than one particle.]

We call the system ***non-degenerate***[1] if the accessible one-particle states have average occupancies much less that 1. We basically want to ensure that $A \gg N$. This occurs when, for example, the concentration of a gas is much less than the quantum concentration or if the temperature is large. If the temperature/available energy of the system is too low, the number of available states will shrink and eventually start violating these conditions and the gas will become ***degenerate*** and our distinction between fermions and bosons will become extremely relevant. This non-degenerate case is what we call our ***classical limit***.

(e) Show that in the classical limit, the total number of fermionic states $\mathscr{N}_F$ approximates as,

$$\mathscr{N}_F \approx \frac{A^N}{N!}\left(1 - \frac{N^2}{2A}\right).$$

[*Supplementary Part (Not for Credit): Also show that the number of bosonic states approximates to*

[1] Note that this is the statistical mechanics definition of "degenerate" rather than the quantum mechanics definition (where a degeneracy just means more than one state has the same eigenvalue for a given operator). The linguistics of physics and math has always fascinated me. For fun, how many distinct definitions of the word "normal" have you run across? How about "degenerate"?

$\mathscr{N}_B \approx \frac{A^N}{N!}\left(1+\frac{N^2}{2A}\right)$.]
[*Note: You may also assume* $N^2/A \gg 1$ *and* $N \gg 1$ *as needed.*]
Hint (highlight to reveal): [There are a few different valid approaches! One is to use Stirling's approximation - though you won't need the square root term. If you do this you will need the approximation $\left(1+\frac{x}{n}\right)^n \approx e^{x-\frac{x^2}{2n}} \approx e^x\left(1-\frac{x^2}{2n}\right)$ which is valid when $n \gg 1$. Note that this reproduces the familiar limit $\lim_{n\to\infty}(1+\frac{x}{n})^n = e^x$.]

Commentary: *In the "classical statistical mechanics" part of the course when we dealt with "classical" identical particles, like in the ideal gas, we had to include an "over-counting factor" of* $1/N!$ *in our partition functions. We may define the "classically indistinguishable" number of states as*

$$\mathscr{N}_C \equiv \frac{1}{N!}\mathscr{N}_D = \frac{A^N}{N!}.$$

First we can see that this means $\mathscr{N}_F < \mathscr{N}_C < \mathscr{N}_B$*, where the subscripts F, C, and B stand for identical fermions, the classical limit, and identical bosons, respectively. if we add the further restriction that* $N^2 \ll A$ *then this means in the classical limit we have*

$$\mathscr{N}_F \approx \mathscr{N}_C = \tfrac{1}{N!}\mathscr{N}_D \approx \mathscr{N}_B.$$

Similar sorts of analyses can be used to show that these limits behave the same way for the microcanonical and canonical partition functions,

$$\textit{Classical limit:} \qquad \Omega_F \approx \Omega_C = \tfrac{1}{N!}\Omega_D \approx \Omega_B; \qquad Z_F \approx Z_C = \tfrac{1}{N!}Z_D \approx Z_B.$$

Problem 9.2 - A Distribution of Distribution Functions

Recall that the ***distribution function*** $\bar{n}(E,T)$ is a function that tells us the average occupancy for a state of energy E when our multi-particle system is at temperature T. That is, if $|\alpha\rangle$ is a one-particle state of energy E_α, then the average number of particles in state $|\alpha\rangle$ is $\langle n_\alpha\rangle = \bar{n}(E_\alpha,T)$. These distribution functions also depend on the chemical potential μ which we interpret as being fixed by the number of particles N in the system and the temperature of the system.

In class we found the ***Fermi-Dirac*** distribution function $\bar{n}_F$, classical limit/***Boltzmann*** distribution function $\bar{n}_C$, and ***Bose-Einstein*** distribution function $\bar{n}_B$,

$$\bar{n}_F = \frac{1}{e^{\beta(E-\mu)}+1}; \qquad \bar{n}_C = \frac{1}{e^{\beta(E-\mu)}}; \qquad \bar{n}_B = \frac{1}{e^{\beta(E-\mu)}-1}$$

(a) At room temperature, what is the average occupation of a state where E is 0.01 eV greater than the chemical potential μ in each of the three cases of identical fermions, the classical limit, and identical bosons?

Consider a one-particle state $|\alpha\rangle$ if energy E_α. Following the approach taken in Problem 8.2, we will consider this state as its own open subsystem (particles can enter and leave the state, e.g. by going to other states) and let Ξ_α be the grand canonical partition function for the state.

(b) **Extra Part** (*Not for Credit*) Show the following two relations,

$$\langle n_\alpha\rangle = k_BT\left(\frac{\partial \ln \Xi_\alpha}{\partial\mu}\right)_T; \qquad \sigma^2_{n_\alpha} = (k_BT)^2\left(\frac{\partial^2 \ln \Xi_\alpha}{\partial\mu^2}\right)_T = k_BT\frac{\partial\langle n_\alpha\rangle}{\partial\mu}.$$

(c) **Extra Part** (*Not for Credit*) Starting with $\Xi_{\alpha,B} = \frac{1}{1-e^{-\beta(E_\alpha-\mu)}}$, show that $\langle n_\alpha \rangle_B$ reproduces the expression for the Bose-Einstein distribution function.

(d) Use the result from part (b) to show that for identical bosons/fermions, $\sigma^2_{n_\alpha} = \langle n_\alpha \rangle \left(1 \pm \langle n_\alpha \rangle\right)$, with the plus sign for bosons and the minus sign for fermions.
[*Supplementary Part (Not for Credit): Also show* $\sigma^2_C = \langle n_\alpha \rangle$*.*]
[*Note: This part shows that* $\sigma_{n_\alpha,F} \leq \sigma_{n_\alpha,C} \leq \sigma_{n_\alpha,B}$].

There is a very useful symmetry feature of the Fermi-Dirac distribution function. Suppose we are at some fixed temperature and that the chemical potential of our fermionic system is a known value μ. Let's look at two one-particle states whose energies are some amount ε below and above the chemical potential, $|\alpha\rangle$ and $|\beta\rangle$ with energies $E_\alpha = \mu - \varepsilon$ and $E_\beta = \mu + \varepsilon$.

(e) Show that the probability of $|\beta\rangle$ being filled/occupied is the same as the probability of $|\alpha\rangle$ being empty/unoccupied.[2]
Hint (highlight to reveal): [This is equivalent to showing $\bar{n}_F(\mu+\varepsilon) = 1 - \bar{n}_F(\mu-\varepsilon)$, but please be sure to explain why this is so if you use it.]

There is one last important distribution function we will use in this class, the ***Planck distribution function*** $\bar{n}_P$. Let's build a special system that will be applicable to "wave-like systems" where we don't necessarily start with a well-defined concept of a particle. We can still talk about the energy of our system (e.g. for a given standing wave mode we can have different oscillation amplitudes and thus different energies in our waves). Suppose that the oscillation amplitudes are *quantized* in such a way that the possible wave energies are $E = n\varepsilon$ for some constant ε and some non-negative integer n. We interpret $\bar{n}_P = \langle E \rangle/\varepsilon$ as the expectation value for the quantum number n the system as a function of temperature.

(f) Find the canonical partition function for the system and from that the expectation value of the energy $\langle E \rangle$ and thus the Planck distribution function $\bar{n}_P$.

It turns out we can interpret Planck distribution function in terms of particles - or at least particle-like objects. Consider each of the quanta of energy we can put in a given mode as a "particle", in which case the quantum number n is interpreted as the numbers of these identical particles in a one-particle state of energy ε.

(g) Given the form of the Planck distribution function $\bar{n}_P$ you found in (f), would we interpret these particle-like objects as bosons or fermions? What would the chemical potential have to be?
[*Supplementary Part (Not for Credit): In one of our bonus lectures we interpreted the chemical potential as a Lagrange multiplier enforcing a constraint for having a fixed average number of particles in the system or, equivalently, enforcing conservation of particle number. Given the chemical potential for this part, what does that imply about our particle-like objects?*]

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[2] An unoccupied state below the Fermi energy in a fermionic system is sometimes referred to as a ***hole***. It turns out we can also approach these fermionic systems at low temperatures by treating holes as a species of particle with the same mass and opposite charge as the original fermionic particle.

Problem 9.3 - You Are My Density (of States)

The final key piece to analyzing quantum statistical mechanics is the ***density of states***, $g(E)$. This is interpreted so that $g(E)dE$ is the total number of one-particle states within infinitesimal energy dE of E. The density of states allows us to approximate the sums over states as integrals. In this problem we will construct the densities of states for a few different systems of interest. A key fact that will help us construct these is the way we change variables in densities. Given two variables a and b, the density in variable a is related to the density in variable b via[3]

$$g_a(a)\,da = g_b(b)\,db \quad \Longrightarrow \quad g_a(a) = g_b(b)\left|\frac{db}{da}\right|.$$

In lecture we derived the density of states for a 3D gas in a cube of side-length L (volume $V = L^3$),

$$g(E) = g_s 2\pi V \left(\frac{2m}{h^2}\right)^{3/2} \sqrt{E}, \tag{1}$$

where $g_s = 2s + 1$ is the spin-degeneracy.

Consider instead the density of states for a gas of particles in flatland! That is, consider a 2D gas in a box of side-length L (area $A = L^2$).

(a) Find the density of states for this 2D system.
Hint (highlight to reveal): [You should find that the answer is independent of energy in this case.]
[*Note: Fun fact, if we were to do the 1D case, we would find* $g(E) \propto E^{-1/2}$.]

Next, let's consider a (3D) gas of *massless* particles in a cube of side-length L (volume $V = L^3$). Alternatively, we can consider a (3D) gas of particles with mass m in the ***hyper-relativistic energy regime*** $E \gg mc^2$. In these cases the energy is related to the momentum via

$$E = |\vec{p}|\,c.$$

(b) Find the density of states $g(E)$ for this massless/hyper-relativistic 3D system.
Hint (highlight to reveal): [The quantization condition for the momentum remains the same in this case, $\vec{p} = h\vec{n}/2L$.]

(c) Using $E = hc/\lambda$, determine the density of states for this system in the wavelength variable, $g_\lambda(\lambda)$.

If we know the average number of particles then we can determine the chemical potential using

$$\langle N \rangle = \int_{E_g}^{\infty} g(E)\bar{n}(E)\,dE, \tag{2}$$

where E_g is the one-particle ground-state energy. Recall that in the $T \to 0$ limit, we define the ***Fermi energy*** as $E_F \equiv \mu(T = 0)$ and the Fermi-Dirac distribution becomes

$$\lim_{T\to 0} \bar{n}_F(E) = \begin{cases} 0, & E > E_F \\ 1, & E < E_F \end{cases}.$$

Consider a 3D gas of spin-1/2 fermions in a cube of volume V. The appropriate density of states is given by Eq. 1. Recall that in this system $E_g = \frac{h^2}{8mL^2}|\vec{n}|^2 = \frac{3h^2}{8mL^2}$. We will approximate this energy as $E_g = 0$ for the purposes of this problem (it will be much smaller than all of the other relevant energies).

[3] Note that if our density of states is in any variable besides energy, we will use a subscript on g to indicate which variable the function is a density is with respect to.

(d) Use Eq. 2 to determine the Fermi energy E_F as a function of particle number N.

In terms of $\hbar$ (instead of h), you should have found $E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$. At finite but low temperatures $T \ll E_F/k_B$ we can approximate the chemical potential as

$$\mu(T \ll E_F/k_B) \approx \left(1 - \frac{\pi^2}{12}\left(\frac{k_B T}{E_F}\right)^2\right) E_F.$$

For this problem we will fix the temperature at $k_B T = 0.02 E_F$. We may define dimensionless energy $\varepsilon \equiv E/E_F$.

(e) Evaluate $\beta\mu$ at this temperature. Setting $N = 10$, find and plot $g_\varepsilon(\varepsilon) = g(\varepsilon E_F)E_F$. On this graph superimpose a graph of $g_\varepsilon \bar{n}_F$.
[*Note: You should find a pair of graphs very similar to what is found in Figure 7.14 of Schroeder. We interpret the area under the graph of* $g(\varepsilon)\bar{n}(F)$ *gives us the number of particles in a given energy range!*]

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