Phys 7230

Sample final exam problems

1 Classical Harmonic Oscillator

Calculate the classical partition function of an oscillator whose energy is given by $E = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$. Use it to calculate its heat capacity.

Solution

The partition function is given by

$$Z = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{-\frac{p^2}{2mT} - \frac{m\omega^2 x^2}{2T}}.$$

Changing variables $x = \sqrt{T}u$, $p = \sqrt{T}v$, we find

$$Z = T \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} \frac{dv}{2\pi\hbar}\, e^{-\frac{u^2}{2m} - \frac{m\omega^2 v^2}{2}}.$$

The free energy is then

$$F = -T \log Z = -T \log T - T \log \left[\int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} \frac{dv}{2\pi\hbar}\, e^{-\frac{u^2}{2m} - \frac{m\omega^2 v^2}{2}} \right].$$

The heat capacity is

$$c = -T \frac{d^2 F}{dT^2} = 1,$$

in accordance with the equipartition theorem.

2 Ideal gas

Classical ideal monoatomic gas with N atoms is kept in a cylinder of height H, as shown in the figure 1, at temperature T and in the presence of gravity force mg acting on each atom.

Determine its pressure on the bottom of the cylinder, as well as its pressure on the top of the cylinder. Discuss the behavior of both pressures as $H \gg T/(mg)$ (or $H \ll T/(mg)$).

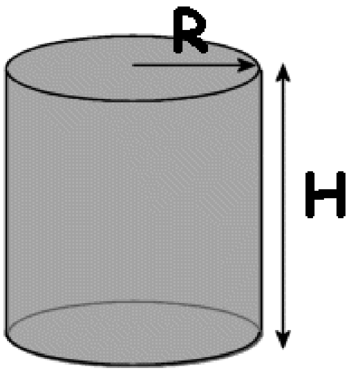

Figure 1: Cylinder with a gas.

<u>Solution</u>

The partition function is given by

$$Z = \frac{1}{N!}\left[\int_{H_0}^{H} \pi R^2 dx\, e^{-\frac{mgx}{T}} \int_0^{\infty} \frac{p^2 dp}{2\pi^2 \hbar^3} e^{-\frac{p^2}{2mT}}\right]^N .$$

Here $H_0 = 0$, however, we keep it as H_0 for convenience. Doing the integrals gives

$$F = -TN \log\left[\frac{R^2\sqrt{mT^5}}{\hbar^3 g N\sqrt{8\pi}}\left(e^{-\frac{mgH_0}{T}} - e^{-\frac{mgH}{T}}\right)\right] + TN.$$

Pressure on top of the cylinder is calculated by means of

$$P_{\text{top}} = -\frac{1}{\pi R^2}\frac{\partial F}{\partial H} = \frac{Nmg}{\pi R^2}\frac{1}{e^{\frac{mgH}{T}} - 1},$$

where $H_0 = 0$ was substituted. We see that if $H \gg T/(mg)$, then P_{top} vanishes. If, on the other hand, $H \ll T/(mg)$, then $P_{\text{top}} = NT/V$, where $V = \pi R^2 H$, as it should in the standard ideal gas.

Pressure on the base of the cylinder is calculated by means of

$$P_{\text{bottom}} = \frac{1}{\pi R^2}\frac{\partial F}{\partial H_0} = \frac{Nmg}{\pi R^2}\frac{1}{1 - e^{-\frac{mgH}{T}}},$$

where again $H_0 = 0$ was substituted. Notice the positive sign in front of the derivative over H_0, resulting from the fact that increasing H_0 compresses the gas. This is where introducing H_0 at the very beginning pays off.

Notice that if $H \gg T/(mg)$, $P_{\text{bottom}} = mgN/(\pi R^2)$. In other words, it is the entire weight of all the atoms in gas applied to the bottom of the cylinder. If $H \ll T/(mg)$, then $P_{\text{bottom}} = NT/V$.

Finally, we observe that

$$(P_{\rm bottom} - P_{\rm top})\,\pi R^2 = Nmg,$$

as it should simply because of mechanical equilibrium (otherwise, the container would fly away).

3 Ultrarelativistic electron gas

When an electron gas at zero temperature (or at low temperature where $T \ll mc^2$) is compressed so that its density goes over some critical value n_c, its chemical potential becomes so high, $\mu \gg mc^2$, that the electrons become ultrarelativistic. In this regime, their energy is proportional to their momentum $E = cp$. Calculate the pressure of this gas of density $n \gg n_c$ kept at at zero temperature. Estimate n_c.

Solution

We first calculate the grand canonical potential of this gas

$$\Omega = -2T \int \frac{Vp^2dp}{2\pi^2\hbar^3} \log\left(1 + e^{\frac{\mu}{T} - \frac{cp}{T}}\right).$$

The factor of 2 appears because of the spin-1/2 of the electrons.

Taking this integral by parts, as is standard here, gives

$$\Omega = -\frac{V}{3\pi^2\hbar^3} \int \frac{cp^3dp}{e^{\frac{cp}{T} - \frac{\mu}{T}} + 1} = -\frac{E}{3}.$$

Here E is the energy of the system, given by

$$E = \frac{V}{\pi^2\hbar^3} \int \frac{cp^3dp}{e^{\frac{cp}{T} - \frac{\mu}{T}} + 1}.$$

Thus the pressure is given by

$$P = -\frac{\Omega}{V} = \frac{E}{3V},$$

which is in fact a standard expression for a relativistic gas.

Since we work at zero temperature, the energy is given by

$$E = \frac{V}{\pi^2\hbar^3} \int_0^{p_f} cp^3dp = \frac{V}{4\pi^2\hbar^3} cp_f^4,$$

where $\mu = cp_f$. The particle number is

$$n = \int_0^{p_f} \frac{p^2dp}{\pi^2\hbar^3} = \frac{p_f^3}{3\pi^2\hbar^3}.$$

Solving for p_f and substituting into E we find

$$E = \frac{3^{\frac{4}{3}}\pi^{\frac{2}{3}}\hbar c n^{\frac{4}{3}}}{4}V.$$

This gives

$$P = \frac{(3\pi^2)^{\frac{1}{3}}\hbar c n^{\frac{4}{3}}}{4}.$$

In order for the gas to be relativistic, we need $p_f \gg mc$. This gives

$$n \gg \frac{m^3c^3}{3\pi^2\hbar^3} = n_c.$$

4 Bose-Einstein condensation in a Bose-Fermi mixture

In the experiments done at JILA, a number noninteracting fermionic atoms of mass m are kept in equilibrium with a number of noninteracting bosonic molecules of mass $2m$. Each fermionic atom has spin 1/2 and can thus be in one of two possible states, with spin $+1/2$ and $-1/2$. Two fermionic atoms of opposite spin, when they collide, can bind together to form one bosonic molecule, which has no spin. The binding energy of the molecule is ϵ_0, in other words, this is the energy which gets absorbed during the formation of the molecule. ϵ_0 can be either positive or negative, and can be easily controlled experimentally. The bosonic molecule can freely decay back into two fermionic atoms with opposite spins.

The experiment begins when $N/2$ spin-up atoms and $N/2$ spin down atoms (so that their total number $N_f = N/2 + N/2 = N$) are put into a box of volume V. Then some of the atoms combine to form molecules until the system reaches equilibrium.

(In truth, the atoms and molecules reside inside a harmonic trap instead of a box, but let's ignore it for the sake of this problem. In truth, they are also *not* noninteracting, but we will ignore this as well).

(a) Treat the fermionic and bosonic atoms as two independent systems in equilibrium, with fermionic system having entropy $S_f(N_f)$, where N_f is the total number of fermions, and bosonic system having entropy $S_b(N_b)$. Prove that at equilibrium

$$2\mu_f = \mu_b, \tag{4.1}$$

where μ_f and μ_b are fermionic and bosonic chemical potentials, respectively. *Hint:* Use the fact that at equilibrium the total entropy takes the maximum possible value.

(b) The energy of fermions and bosons is given by

$$E_f = \frac{p^2}{2m}, \; E_b = \epsilon_0 + \frac{p^2}{4m}.$$

Calculate the number of bosons N_b at zero temperature $T = 0$ as a function of ϵ_0, N, and V. Note that all the bosons will be Bose condensed under these conditions. Treat bosons and fermions as two independent systems whose chemical potentials satisfy the condition Eq. (4.1).

(c) Determine the temperature T_c at which the Bose condensate disappears. Note that you won't be able to find it explicitly, but you will be able to write down an equation for T_c, which cannot be solved analytically but can in principle be analyzed numerically.

<u>Solution</u>

(a) The total entropy is

$$S = S_f(N_f) + S_b(N_b).$$

As atoms convert into molecules and back, a decrease of the atomic number by 2 is accompanied by the increase of the molecular number by 1. Therefore, the number of molecules is given by $N_b = (N - N_f)/2$. This gives

$$S(N_f) = S_f(N_f) + S_b((N - N_f)/2).$$

Maximizing S with respect to N_f, we find

$$\frac{\partial S}{\partial N_f} = \frac{\partial S_f}{\partial N_f} - \frac{1}{2}\frac{\partial S_b}{\partial N_b} = 0.$$

Introducing $\mu = -T\frac{\partial S}{\partial N}$, we find

$$\mu_f = \frac{\mu_b}{2}.$$

(b) The molecules obey Bose-Einstein distribution,

$$n_b(p) = \frac{1}{e^{\frac{p^2+\epsilon_0}{4mT} - \frac{\mu_b}{T}} - 1}.$$

Bose-Einstein distribution ensures the following basic condition

$$\mu_b \le \epsilon_0.$$

Since we work at zero temperature, $n_b(p)$ becomes especially simple: $n_b(p) = 0$ for all $|p| > 0$. $n_b(0)$ is also equal to zero if $\mu_b < \epsilon_0$. Finally, if $\mu_b = \epsilon_0$ all the bosons are Bose condensed. That means, $n_b(0)$ coincides with the total number of molecules N_b. Alternatively, we could say that if $N_b \neq 0$, then $\mu_b = \epsilon_0$, and if $N_b = 0$, then $\mu_b < \epsilon_0$.

The atoms obey Fermi-Dirac distribution which, at zero temperature, demands that all the states with $p < p_f$ are occupied, where $\sqrt{2m\mu_f} = p_f$. Thus the total number of fermions is given by

$$N_f = 2V\int_0^{p_f} \frac{p^2 dp}{2\pi^2\hbar^3} = V\frac{p_f^3}{3\pi^2\hbar^3},\ \mu_f > 0,$$

where the factor of 2 accounts for spin. On the other hand, the following is obvious

$$N_f = 0,\ \mu_f < 0.$$

Combining all this together, and using $\mu_f = \mu_b/2$, we write down the particle number equation

$$N = N_f + 2N_b = V\frac{p_f^3}{3\pi^2\hbar^3}\theta(\mu_b) + 2N_b = V\frac{(m\mu_b)^{\frac{3}{2}}}{3\pi^2\hbar^3}\theta(\mu_b) + 2N_b, \tag{4.2}$$

combined with the Bose-Einstein condensation condition

$$N_b \ge 0, \mu_b = \epsilon_0;\ N_b = 0, \mu_b < \epsilon_0.$$

In (4.2), $\theta(x) = 1$ if $x > 0$. If $x \le 0$, then $\theta(x) = 0$. This allows us to find the number of bosons in the following three regimes.

1. If

$$0 < \epsilon_0 < \frac{1}{m}\left(\frac{3\pi^2\hbar^3 N}{V}\right)^{\frac{2}{3}},$$

we find

$$N_b = \frac{1}{2}\left(N - V\frac{(m\epsilon_0)^{\frac{3}{2}}}{3\pi^2\hbar^3}\right).$$

Indeed, in this case, $N_b > 0$, so $\epsilon_0 = \mu_b$.

2. If

$$\epsilon_0 > \frac{1}{m}\left(\frac{3\pi^2\hbar^3 N}{V}\right)^{\frac{2}{3}},$$

then $\mu_b < \epsilon_0$, which gives

$$N_b = 0.$$

Indeed, if μ_b were to be equal to ϵ_0, then the application of (4.2) would immediately give $N_b < 0$, which does not make sense. Thus we conclude that there are no bosons at all. All the particles are fermions, which occupy all the states up to the energy $\mu_f = \frac{\mu_b}{2} = \frac{1}{2m}\left(\frac{3\pi^2\hbar^3 N}{V}\right)^{\frac{2}{3}}$.

3. Finally, if $\epsilon_0 < 0$, then

$$N_b = N/2.$$

Here $\mu_b = \epsilon_0 = 2\mu_f$. All particles are Bose-condensed bosons. There are no fermions.

(c) Turning our attention to nonzero temperature, we find the following generalization of the particle number equation (4.2)

$$2V\int \frac{d^3p}{(2\pi\hbar)^3}\frac{1}{e^{\frac{p^2}{2mT}-\frac{\mu_b}{2T}}+1} + 2V\int \frac{d^3p}{(2\pi\hbar)^3}\frac{1}{e^{\frac{p^2+\epsilon_0}{4mT}-\frac{\mu_b}{T}}-1} + N_0 = N.$$

Here N_0 is the number of Bose-Condensed bosons, and it is only nonzero if $\mu_b = \epsilon_0$. The condition for the onset of Bose-Einstein condensation is $N_0 = 0$ while $\epsilon_0 = \mu_b$. This gives

$$2V\int \frac{d^3p}{(2\pi\hbar)^3}\frac{1}{e^{\frac{p^2}{2mT_c}-\frac{\epsilon_0}{2T_c}}+1} + 2V\int \frac{d^3p}{(2\pi\hbar)^3}\frac{1}{e^{\frac{p^2}{4mT_c}}-1} = N. \tag{4.3}$$

This equation must be solved for T_c.

While this is generally hard to do analytically, it is easy to observe that if

$$\epsilon_0 \ll -\frac{1}{m}\left(\frac{3\pi^2\hbar^3 N}{V}\right)^{\frac{2}{3}},$$

the Fermi-Dirac factor in (4.3) can be completely neglected (there are almost no fermionic atoms left). This reduces (4.2) to the usual Bose-Einstein condensation condition

$$T_c = \frac{\pi}{m}\left(\frac{N}{2V\zeta\left(\frac{3}{2}\right)}\right)^{\frac{2}{3}}.$$

As ϵ_0 is increased, T_c decreases and finally reaches zero when

$$\epsilon_0 = \frac{1}{m}\left(\frac{3\pi^2\hbar^3 N}{V}\right)^{\frac{2}{3}}.$$

At ϵ_0 above this value, there are no Bose-Einstein condensate of molecules at any temperature.