Problem Set 10

1 Bose-Einstein condensation temperature in atomic hydrogen

Schroeder

Problem 7.67. For the numbers given, equation 7.126 predicts a condensation temperature of

$$T_c = \frac{(0.527)h^2}{2\pi mk}\left(\frac{N}{V}\right)^{2/3} = \frac{(0.527)(6.63\times10^{-34}\ \mathrm{J\cdot s})^2}{2\pi(1.67\times10^{-27}\ \mathrm{kg})(1.38\times10^{-23}\ \mathrm{J/K})}(1.8\times10^{20}\ \mathrm{m^{-3}})^{2/3}$$
$$= 5.1\times10^{-5}\ \mathrm{K} = 51\ \mu\mathrm{K},$$

almost exactly equal to the measured value.

2 Bose-Einstein condensation of ^{87}Rb atoms

(a) For a rubidium-87 atom in a cube-shaped box of with 10^{-5} m, the ground-state energy is

$$\epsilon_0 = \frac{h^2}{8mL^2}(1^2+1^2+1^2) = \frac{3}{8}\frac{(6.63\times10^{-34}\ \mathrm{J{\cdot}s})^2}{(87)(1.66\times10^{-27}\ \mathrm{kg})(10^{-5}\ \mathrm{m})^2}$$
$$= 1.14\times10^{-32}\ \mathrm{J} = 7.1\times10^{-14}\ \mathrm{eV}.$$

This is a tiny energy indeed.

(b) According to equation 7.126, the condensation temperature is

$$kT_c = (0.527)\Big(\frac{h^2}{2\pi mL^2}\Big)N^{2/3} = (0.224)N^{2/3}\epsilon_0,$$

where the coefficient 0.224 comes from comparing this expression to the previous one. If there are 10,000 atoms in our box, then the kT_c is greater than ϵ_0 by a factor of $(0.224)(10,000)^{2/3} = 104 \approx 100$, that is, $kT_c = 7.4\times10^{-12}$ eV or $T_c = 8.6\times10^{-8}$ K. This is in rough agreement with the value 10^{-7} K quoted on page 319.

(c) At $T = 0.9T_c$, the number of atoms in the ground state is

$$N_0 = \Big[1-\Big(\frac{T}{T_c}\Big)^{3/2}\Big]N = [1-(0.9)^{3/2}]N = (0.146)N.$$

For $N = 10,000$, this is 1460. Therefore, by equation 7.120,

$$\epsilon_0 - \mu = \frac{kT}{N_0} = \frac{(0.9)(7.4\times10^{-12}\ \mathrm{eV})}{1460} = 4.6\times10^{-15}\ \mathrm{eV}.$$

That is, the chemical potential lies below the ground-state energy by about $(0.065)\epsilon_0$. The energy of the first excited states is

$$\epsilon_1 = \frac{h^2}{8mL^2}(2^2+1^2+1^2) = \frac{6h^2}{8mL^2} = 2\epsilon_0,$$

so the expected number of particles in any one of these states is

$$N_1 = \frac{1}{e^{(\epsilon_1-\mu)/kT}-1} = \frac{1}{e^{(1.065)\epsilon_0/kT}-1} = \frac{1}{e^{1.065/(0.9)(104)}-1} = 87,$$

and the number of particles in all three of these states is about 260. This less than the number of particles in the ground state by a factor of 5.6—significant, but not enormous.

3 Boson gas in one and two dimensions

(a) - same as in Problem 1, Problem set 8, with $s=0$

(b) $$N_e(T) = \int_{\Delta E}^{\infty} dE\, D(E)\, f_B(E,T) \approx \int_0^{\infty} dE\, D(E) f_B(E,T)$$
(where $\Delta E = E_2 - E_1 \to 0$)

$$= \begin{cases} \dfrac{L}{2\pi}\left(\dfrac{2m}{\hbar^2}\right)^{1/2} \displaystyle\int_0^{\infty} dE \, \dfrac{1}{\sqrt{E}\,\left(e^{(E-\mu)/k_BT} - 1\right)} & \text{- in 1D} \\ \dfrac{L^2 m}{2\pi \hbar^2} \displaystyle\int_0^{\infty} dE \, \dfrac{1}{e^{(E-\mu)/k_BT} - 1} & \text{- in 2D} \end{cases}$$

[Take $D(E)$ for 1D and 2D from Problem 1, Problem Set 6, with $s=0$]

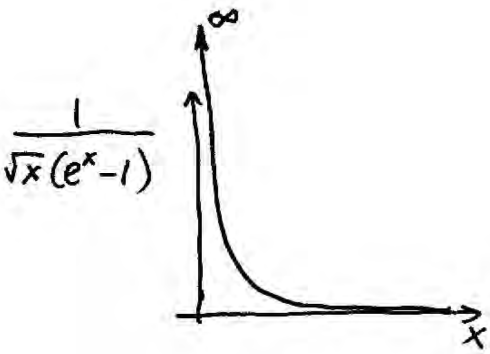
If we put $\lambda = e^{\mu/k_BT} = 1$ and define $x \equiv \frac{E}{k_BT}$, the we get

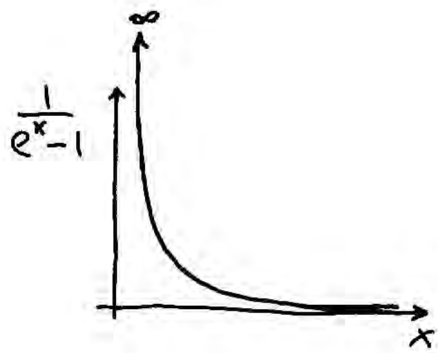
$$N_e(T) \propto \begin{cases} \displaystyle\int_0^{\infty} \frac{dx}{\sqrt{x}\,(e^x - 1)} & \text{- in 1D} \\ \displaystyle\int_0^{\infty} \frac{dx}{e^x - 1} & \text{- in 2D} \end{cases}$$

In both cases, the integrands

$\dfrac{1}{\sqrt{x}\,(e^x-1)}$ and $\dfrac{1}{e^x-1}$ diverge as $x \to 0$

(in the lower limit of the integrals)





Because of this divergence, both integrals do NOT converge (are infinite), while N_e has to be finite.

Therefore, replacing λ by $\lambda = 1$ is not valid here.
From lecture notes (Lecture 16) the reason for approximating $\lambda \simeq 1$ was that

$$N_0 = \frac{1}{\lambda^{-1} - 1}$$
↳ ground state occupation

In order that $N_0 \gg 1$ (macroscopic, as required for condensate formation)
we have to have

$$\lambda \simeq 1 \quad \left(\text{then} \quad \lambda = \frac{1}{1 + 1/N_0} \simeq 1 - \frac{1}{N_0} + \ldots \simeq 1\right)$$

So the fact that the integrals diverge, suggests that the approximation of $\lambda \simeq 1$ is not valid, and therefore N_0 is no longer macroscopic → no condensate formation.

For comparison, in 3D: $N_e(T) \propto \int_0^\infty \frac{\sqrt{x}\, dx}{e^x - 1}$ — converges!
with $\lambda = 1$

Another approximation involved here is the replacement of the lower limit ΔE in the integral

$$N_e(T) = \int_{\Delta E}^{\infty} dE\, D(E)\, f_B(E,T)$$

by 0 $(\Delta E \to 0)$, so that $N_e(T)$ is evaluated as

$$N_e(T) \simeq \int_{0}^{\infty} dE\, D(E)\, f_B(E,T)$$

With $N_e(T) = \int_{\Delta E}^{\infty} dE\, D(E)\, f_B(E,T)$ – would have to be calculated numerically, and would be finite (the divergence of the integrand as $E \to 0$ would not be relevant as the integration region starts from $\Delta E > 0$, not from 0)

Still, the condensation in 1D and 2D box potentials does not occur because N_0 does not become of the order of N.

[many particles remain in the excited states $N_e(T)$]

– but this is beyond what was asked in the question.

4 Energy, heat capacity, entropy, free energy amd pressure of a degenerate boson gas.

(a) $$U = (\overset{\to s=0}{2s+1}) \sum_{\underline{n}} E_{\underline{n}} f_B(E_{\underline{n}}) \longrightarrow \frac{1}{8} 4\pi \int_0^\infty dn\, n^2 E_{\underline{n}} f_B(E_{\underline{n}})$$

$$= \int_0^\infty dE\, \underbrace{D(E)}\, E\, f_B(E)$$

$$D(E) = (\underset{s=0}{2s+1}) \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E}$$ – from Problem 1, Problem Set 6

$$= \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty dE \frac{E^{3/2}}{e^{(E-\mu)/k_BT} - 1}$$

put $\lambda = e^{\mu/k_BT} = 1$

$$= \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty dE \frac{E^{3/2}}{e^{E/k_BT} - 1}$$

define $x \equiv \frac{E}{k_BT}$

$$= \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} (k_BT)^{5/2} \int_0^\infty dx \frac{x^{3/2}}{e^x - 1}$$

$\Rightarrow$ def $J \equiv \int_0^\infty dx \frac{x^{3/2}}{e^x - 1}$

$\simeq 1.006\sqrt{\pi}$

Thus:

$$\boxed{U = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} (k_B T)^{5/2} \cdot J}$$

(b) $C_V = \left(\frac{\partial U}{\partial T}\right)_V = \frac{5V}{8\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} k_B (k_B T)^{3/2} \cdot J$

$$= \frac{5U}{2T}$$

(c) From $C_V = T\left(\frac{\partial S}{\partial T}\right)_V$

$$\Rightarrow \quad S = \int_0^T \frac{C_V}{T}\, dT = \frac{5V}{8\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} (k_B)^{5/2} \cdot J \cdot \int_0^T T^{1/2}\, dT$$

$$= \frac{5V}{8\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} k_B^{5/2} \cdot J \cdot \frac{2}{3} T^{3/2}$$

$$= \frac{5V}{12\pi^2}\left(\frac{2m}{\hbar^2}\right) k_B^{5/2} \cdot T^{3/2} \cdot J = \frac{5U}{3T}$$

(d) $F = U - TS = U - T \cdot \frac{5U}{3T} = U - \frac{5}{3}U = -\frac{2}{3}U$

$$= -\frac{V}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} k_B^{5/2}\, T^{5/2} \cdot J$$

(e) $\boxed{p = -\left(\frac{\partial F}{\partial V}\right)_T = \frac{1}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} (k_B T)^{5/2} \cdot J}$

$$\therefore \quad pV = \frac{V}{6\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} (k_B T)^{5/2} \cdot J$$

$$= \frac{2}{3}U \qquad \boxed{pV = \frac{2}{3}U}$$ equation of state

(f) $C_V = \frac{5U}{2T}$, $S = \frac{5U}{3T}$, $F = -\frac{2}{3}U$, $p = \frac{2U}{3V}$

5 Bose-Einstein condensation (BEC) in a harmonic trap.

(a) n quanta ("balls") among 3 harmonic oscillators ("boxes")

[one harmonic oscillator per each spatial dimension]

$$g(n) = \frac{[n+(3-1)]!}{n!\ (3-1)!} = \frac{(n+2)!}{n!\ 2!} =$$

$$= \frac{\cancel{n!}\,(n+1)(n+2)}{\cancel{n!}\ 2} = \frac{(n+1)(n+2)}{2}$$

For $n \gg 1$ $\boxed{g(n) \simeq n^2/2}$

(b) $$N_e(T) = \sum_{n=1}^{\infty} g(n)\, f_B(E_n) \simeq \int_0^\infty dn\, g(n)\, \frac{1}{e^{E_n/k_BT}-1}$$

here $\lambda = e^{\mu/k_BT}$ has been replaced by 1 (same arguments as in lecture notes, lecture 16, apply)

$$= \int_0^\infty dn\, \frac{n^2}{2}\, \frac{1}{e^{\hbar\omega n/k_BT}-1}$$

define $x \equiv \frac{\hbar\omega n}{k_BT}$

$$= \frac{1}{2}\left(\frac{k_BT}{\hbar\omega}\right)^3 \underbrace{\int_0^\infty dx\, \frac{x^2}{e^x-1}}_{\simeq 2.404} = 1.202\left(\frac{k_BT}{\hbar\omega}\right)^3$$

Thus

$$\boxed{N_e(T) = 1.202\left(\frac{k_B T}{\hbar\omega}\right)^3}$$

T_c is defined as the temperature for which $N_e(T_c) \simeq N$

$$\therefore \quad 1.202\left(\frac{k_B T_c}{\hbar\omega}\right)^3 = N$$

$$\therefore \quad \boxed{T_c = \frac{\hbar\omega}{k_B}\left(\frac{N}{1.202}\right)^{1/3}}$$

(c) At $T \gtrsim T_c$ the potential energy of the spring can be set to

$$\frac{1}{2}k_s a^2 \simeq k_B T_c$$

The amplitude a sets an equivalnt volume of $V \simeq a^3 \implies a \simeq V^{1/3}$
(of the equivalent cubic box)

In addition, with k_s corresponding to $m\omega^2$, we can rewrite $\frac{1}{2}k_s a^2 = k_B T_c$ as

$$\frac{1}{2}m\omega^2 \cdot V^{2/3} = k_B T_c$$

$$\text{or} \quad \omega \simeq \left(\frac{k_B T_c}{m}\right)^{1/2}\frac{1}{V^{1/3}}$$

Eliminating ω from $T_c = \frac{\hbar\omega}{k_B}\left(\frac{N}{1.202}\right)^{1/3}$
we obtain :

$$T_c = \frac{\hbar}{k_B} \cdot \left(\frac{k_B T_c}{m}\right)^{1/2} \cdot \frac{1}{V^{1/3}} \cdot N^{1/3}$$

Solving for T_c we get

$$T_c^{1/2} = \frac{\hbar}{k_B^{1/2}\ m^{1/2}} \left(\frac{N}{V}\right)^{1/3}$$

or

$$\boxed{T_c \simeq \frac{\hbar^2}{m k_B} \left(\frac{N}{V}\right)^{2/3}}$$

This is approximately the same
as $T_c = \frac{2\pi\hbar^2}{m k_B}\left(\frac{N}{2.612\,V}\right)^{2/3}$ derived
in lecture notes for the condensation
transition temperature for a gas in
a cubic box.