Bose-Einstein Condensation in 1, 2 and 3 dimensions for massive and massless bosons in a box

I. MASSIVE BOSONS

Consider a gas of massive, non-interacting, non-relativistic, identical, spin-0 bosons. The total number of bosons in a given state with energy ϵ is given by

$$N=\int_0^\infty \bar{n}(\epsilon)dN=\int_0^\infty \bar{n}(\epsilon)D(\epsilon)d\epsilon \tag{1}$$

where

$$\bar{n}(\epsilon)=\frac{1}{e^{\beta(\epsilon-\mu)}-1} \tag{2}$$

is the quantum distribution function for bosons, and

$$D(\epsilon)=\frac{dN}{d\epsilon} \tag{3}$$

is the "density of states" function. For a particle in a box of side length L, the contained modes are quantized by the condition that the wave function vanish at the walls, Ψ(x,y,z=0)=Ψ(x,y,z=L)=0. Thus for each spatial dimension i, we have the condition

$$k_i=\frac{n_i\pi}{L} \tag{4}$$

In **3D**:

$$D_{3D}(\epsilon)=\frac{dN}{d\epsilon}=\frac{dN}{dn}\frac{dn}{d\epsilon}=4\pi n^2\frac{dn}{d\epsilon} \tag{5}$$

For a massive particle in the box the energy is quadratic in the momentum,

$$\epsilon=\frac{1}{2m}({p_x}^2+{p_y}^2+{p_z}^2)=\frac{\hbar^2}{2m}({k_x}^2+{k_y}^2+{k_z}^2)=\frac{\hbar^2\pi^2}{2mL^2}({n_x}^2+{n_y}^2+{n_z}^2)=\frac{\hbar^2\pi^2}{2mL^2}n^2 \tag{6}$$

thus

$$n=\frac{L}{\hbar\pi}\sqrt{2m\epsilon},\qquad and\qquad dn=\frac{L}{2\hbar\pi}\sqrt{\frac{2m}{\epsilon}}d\epsilon \tag{7}$$

Combining terms into the density of states,

$$D_{3D}(\epsilon)=4\pi\frac{2mL^2}{\hbar^2\pi^2}\epsilon\Big(\frac{L}{2\hbar\pi}\sqrt{\frac{2m}{\epsilon}}\Big)=2\pi\Big(\frac{L}{\hbar\pi}\Big)^3(2m)^{\frac{3}{2}}\sqrt{\epsilon} \tag{8}$$

The total number of particles can now be expressed as

$$\begin{aligned}
N_{3D}&=\frac{2\pi}{8}\Big(\frac{L}{\hbar\pi}\Big)^3(2m)^{\frac{3}{2}}\int_0^\infty\frac{\sqrt{\epsilon}}{e^{\beta(\epsilon-\mu)}-1}d\epsilon\\
&=\frac{2\pi V}{h^3}(2m)^{\frac{3}{2}}\int_0^\infty\frac{\sqrt{\epsilon}}{e^{\beta(\epsilon-\mu)}}\frac{1}{1-e^{-\beta(\epsilon-\mu)}}d\epsilon\\
&=\frac{2\pi V}{h^3}(2m)^{\frac{3}{2}}\int_0^\infty\frac{\sqrt{\epsilon}}{e^{\beta(\epsilon-\mu)}}\Big(\sum_{l=0}^\infty e^{-\beta l(\epsilon-\mu)}\Big)d\epsilon\\
&=\frac{2\pi V}{h^3}(2m)^{\frac{3}{2}}\int_0^\infty\sqrt{\epsilon}\Big(\sum_{l=1}^\infty e^{-\beta l(\epsilon-\mu)}\Big)d\epsilon\\
&=\frac{2\pi V}{h^3}(2m)^{\frac{3}{2}}\int_0^\infty\sqrt{\epsilon}\Big(\sum_{l=1}^\infty e^{-\beta l\epsilon}e^{\beta l\mu}\Big)d\epsilon\\
&=\frac{V}{h^3}\Big(\frac{2m\pi}{\beta}\Big)^{\frac{3}{2}}\sum_{l=1}^\infty\frac{e^{\beta l\mu}}{l^{\frac{3}{2}}}
\end{aligned} \tag{9}$$

where the factor of 8 has been introduced since we are including only the positive values of n, and thus only the first quadrant of the 3D sphere in n-space. The last sum on the right is a polylogarithm function, also called the the weighted Zeta function (weighted by the exponential factor). We have used the expansion condition $e^{-\beta(\epsilon-\mu)} < 1$, which is validated by the physical mandate that we do not obtain negative values for $\bar{n}(\epsilon)$. It follows then that we posit the restriction $\epsilon > \mu$.

From the expression it can be seen that N_{3D} is a maximum at μ=0, which is therefore when the condensate occurs. The sum can be evaluated and we arrive at the condensate phase transition temperature,

$$N_{3D} = \frac{V}{h^3}\Big(\frac{2m\pi}{\beta}\Big)^{\frac{3}{2}} \underbrace{\sum_{l=1}^{\infty} \frac{1}{l^{\frac{3}{2}}}}_{\zeta(\frac{3}{2})} \approx \frac{V}{h^3}\Big(\frac{2m\pi}{\beta}\Big)^{\frac{3}{2}}(2.612) \qquad \Longrightarrow \qquad T_c \approx \frac{h^2}{2m\pi k_b}\Big(\frac{N_{3D}}{2.612V}\Big)^{\frac{2}{3}} \tag{10}$$

For massive bosons in **2D** we follow the same procedure. The density of states is

$$D_{2D}(\epsilon) = \frac{dN}{d\epsilon} = \frac{dN}{dn}\frac{dn}{d\epsilon} = 2\pi n \frac{dn}{d\epsilon}. \tag{11}$$

The energy has a similar form as previously

$$\epsilon = \frac{1}{2m}({p_x}^2 + {p_y}^2) = \frac{\hbar^2\pi^2}{2mL^2}n^2 \tag{12}$$

Plugging into the integral for N_{2D}, we note that the density of states here does not depend on the energy. Consequently the integral is over only the distribution function, with a factor of 1/4 that comes from dealing with only the first quadrant of the 2D sphere in n-space.

$$N_{2D} = \frac{2\pi}{4}\Big(\frac{L}{\hbar\pi}\Big)^2 \frac{2m}{2} \int_0^\infty \frac{1}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = \frac{2\pi m A}{h^2\beta} \sum_{l=1}^{\infty} \frac{e^{\beta l \mu}}{l} \tag{13}$$

For the condensate to occur, μ=0 and the above expression diverges, $\zeta(1) \to \infty$. Hence, the condensate does not occur for massive bosons in 2D.

Lastly for the **1D** case, the density of states is simply

$$D_{1D}(\epsilon) = \frac{dN}{d\epsilon} = \frac{dN}{dn}\frac{dn}{d\epsilon} = (1)\frac{dn}{d\epsilon} \tag{14}$$

The energy is, again, the same as above

$$\epsilon = \frac{1}{2m}({p_x}^2) = \frac{\hbar^2\pi^2}{2mL^2}n^2 \tag{15}$$

So the total number is

$$N_{1D} = \frac{L}{2h}\sqrt{2m} \int_0^\infty \frac{1/\sqrt{\epsilon}}{e^{\beta(\epsilon-\mu)} - 1} d\epsilon = \frac{L}{2h}\sqrt{\frac{2\pi m}{\beta}} \sum_{l=1}^{\infty} \frac{e^{\beta l \mu}}{l^{\frac{1}{2}}} \tag{16}$$

There is a factor of 1/2 from dealing with only positive n values. Again, this expression is non-physical for μ=0, so the condensate for massive bosons in 1D does not occur.

II. MASSLESS BOSONS

For massless bosons by contrast, we must express their energy relativistically. Thus from the relation

$$\epsilon = c|p| \tag{17}$$

it is evident that the energy is linear in momentum. This alters the conditions for the BEC to occur. In every case the energy is given as

$$\epsilon = c\hbar|k| = c\hbar\frac{n\pi}{L} \qquad \Longrightarrow \qquad n = \frac{\epsilon L}{c\hbar\pi} \tag{18}$$

For **3D** the density of states is

$$D_{3D}(\epsilon) = 4\pi n^2 \frac{dn}{d\epsilon} = 4\pi \Big(\frac{L}{c\hbar\pi}\Big)^3 \epsilon^2 \tag{19}$$

so the total number is

$$N_{3D} = \frac{4\pi}{8}\Big(\frac{L}{c\hbar\pi}\Big)^3 \int_0^\infty \frac{\epsilon^2}{e^{\beta(\epsilon-\mu)}-1} d\epsilon = \frac{8\pi V}{(ch\beta)^3}\sum_{l=1}^{\infty}\frac{e^{\beta l\mu}}{l^3} \underset{\mu\to 0}{=} \frac{8\pi V}{(ch\beta)^3}\zeta(3) \approx \frac{8\pi V}{(ch\beta)^3}1.1202 \tag{20}$$

Now we can calculate the phase transition temperature for massless bosons in **3D**:

$$T_c \approx \Big(\frac{N_{3D}}{8\pi V(1.1202)}\Big)^{\frac{1}{3}}\frac{ch}{k_b}. \tag{21}$$

In **2D** the density of states is

$$D_{2D}(\epsilon) = 2\pi n \frac{dn}{d\epsilon} = 2\pi\Big(\frac{L}{c\hbar\pi}\Big)^2 \epsilon \tag{22}$$

Note that now the 2D density of states *does* depend on the energy. The total number of particles is

$$N_{2D} = \frac{2\pi}{4}\Big(\frac{L}{c\hbar\pi}\Big)^2 \int_0^\infty \frac{\epsilon}{e^{\beta(\epsilon-\mu)}-1} d\epsilon = \frac{2\pi A}{(ch\beta)^2}\sum_{l=1}^{\infty}\frac{e^{\beta l\mu}}{l^2} \underset{\mu\to 0}{=} \frac{2\pi A}{(ch\beta)^2}\zeta(2) = \frac{2\pi A}{(ch\beta)^2}\big(\frac{\pi^2}{6}\big) \tag{23}$$

This result shows that massless bosons in 2D do indeed form a condensate, whereas massive bosons in 2D do not. The temperature of condensation here is

$$T_c = \Big(\frac{3N_{2D}}{A\pi^3}\Big)^{\frac{1}{2}}\frac{ch}{k_b} \tag{24}$$

Finally, for the 1D system of massless bosons we have a density of states that is independent of energy, just like the 2D massive boson system.

$$D_{1D}(\epsilon) = \frac{dn}{d\epsilon} = \frac{L}{c\hbar\pi}. \tag{25}$$

Again, the integral diverges for μ=0,

$$N_{1D} = \frac{L}{2c\hbar\pi}\int_0^\infty \frac{1}{e^{\beta(\epsilon-\mu)}-1} d\epsilon = \frac{L}{ch}\sum_{l=1}^{\infty}\frac{e^{\beta l\mu}}{l} \underset{\mu\to 0}{\Rightarrow} \frac{L}{ch\beta}\zeta(1) \Rightarrow \infty \tag{26}$$

and thus in the 1D massless case we find the same condition as the massive bosons in 1D, i.e., the condensate is forbidden in this geometry.

III. CONCLUSION

For the particle-in-a-box model, BEC's occur for both massive and massless bosons in 3D. They occur only in the massless case for 2D, and never for 1D. This model can in principle be applied to higher spatial dimensions whereupon evaluation of the total number of particles would be an integral of the form

$$\begin{aligned} N_{qD} &\sim \int_0^\infty \frac{\epsilon^{(q-2)/2}}{e^{\beta(\epsilon-\mu)}-1} d\epsilon \underset{\mu\to 0}{\sim} \zeta(\frac{q}{2}) \qquad (Massive) \\ N_{qD} &\sim \int_0^\infty \frac{\epsilon^{(q-1)}}{e^{\beta(\epsilon-\mu)}-1} d\epsilon \underset{\mu\to 0}{\sim} \zeta(q) \qquad (Massless) \end{aligned} \tag{27}$$

where q is the dimension of the space.