Ideal Bose Gas

Bose Einstein Condensation

Bose occupation function

$$n(\epsilon) = \frac{1}{z^{-1}e^{\beta\epsilon}-1}$$

We had for the density of an ideal (non-interacting) bose gas

$$\frac{N}{V} = \frac{1}{V}\sum_k \frac{1}{z^{-1}e^{\beta\epsilon(k)}-1} = \frac{1}{(2\pi)^3}\int_0^\infty dk\, 4\pi k^2 \frac{1}{z^{-1}e^{\beta\hbar^2k^2/2m}-1}$$

spin zero bosons $g_s=1$

recall, we need $z \leq 1$ for the occupation number at $\epsilon(k=0)=0$ to remain positive $n(0) \geq 0$

$$n(0) = \frac{1}{z^{-1}-1} = \frac{z}{1-z} \Rightarrow z \leq 1, \quad z = e^{\beta\mu} \Rightarrow \mu \leq 0$$

substitute variables $y = \frac{\beta\hbar^2k^2}{2m} \Rightarrow k = \sqrt{\frac{2my}{\beta\hbar^2}}$

$$dk = \sqrt{\frac{2my}{\beta\hbar^2}}\,\frac{dy}{2y}$$

$$\Rightarrow \frac{N}{V} = \left(\frac{2m}{\beta\hbar^2}\right)^{3/2}\frac{4\pi}{(2\pi)^3}\frac{1}{2}\int_0 dy\,\frac{y^{1/2}}{z^{-1}e^y-1}$$

$$\frac{N}{V} = \frac{1}{\lambda^3}\, g_{3/2}(z) \qquad \text{where } \lambda = \left(\frac{h^2}{2\pi m k_B T}\right)^{1/2} \text{ thermal wavelength}$$

$$g_{3/2}(z) \equiv \frac{2}{\sqrt{\pi}}\int_0^\infty dy\,\frac{y^{1/2}}{z^{-1}e^y-1}$$

Consider the function

$$g_{3/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty dy \, \frac{y^{1/2}}{z^{-1} e^{y} - 1} = z + \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \cdots$$

$g_{3/2}(z)$ is monotonic increasing function of z for $z \le 1$

as $z \to 1$, $g_{3/2}(z)$ approaches a <u>finite</u> constant

$$g_{3/2}(1) = 1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}} + \cdots \equiv \zeta(3/2) \simeq 2.612$$

Reimann zeta function

We can see that $g_{3/2}(1)$ is finite as follows:

$$g_{3/2}(1) = \frac{2}{\sqrt{\pi}} \int_0^\infty dy \, \frac{y^{1/2}}{e^{y} - 1}$$

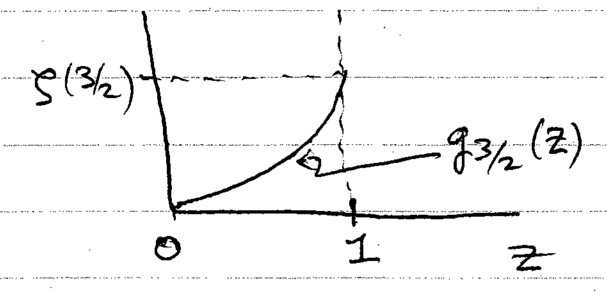
as $y \to \infty$ the integral converges. Integral is largest at small y

(recall small y corresponds to low energy where $n(\epsilon)$ is largest)

For small y we can approx $\frac{1}{e^{y}-1} \simeq \frac{1}{y}$

$$\int_0^{y^*} dy \, \frac{y^{1/2}}{e^{y}-1} \simeq \int_0^{y^*} dy \, \frac{1}{y^{1/2}} = 2 \, y^{1/2} \Big|_0^{y^*}$$

So we see the integral also converges at its lower limit $y \to 0$.



So we conclude

$$n = \frac{N}{V} = \frac{g_{3/2}(z)}{\lambda^3} \leq \frac{g_{3/2}(1)}{\lambda^3} = \frac{2.612}{\lambda^3} = 2.612\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}$$

But we now have a contradiction!
For a system with fixed density of bosons n, as T decreases we will eventually get to a temperature below which the above inequality is violated!
This temperature is

$$T_c = \left(\frac{n}{2.16}\right)^{2/3} \frac{h^2}{2\pi m k_B}$$

Solution to the paradox:
when we made the approx $\frac{1}{V}\sum_k \rightarrow \frac{1}{(2\pi)^3}\int_0^\infty dk\, 4\pi k^2$

we gave a weight $\frac{4\pi k^2}{(2\pi)^3}$ to states with wavevector $|\vec{k}|$.

This gives zero weight to the state $\vec{k}=0$, ie to the ground state. But as T decreases, more and more bosons will occupy the ground state, as it has the lowest energy. Thus when we approx the sum by an integral, we should treat the ground state separately

$$\frac{1}{V}\sum_k n(\epsilon(k)) \cong \frac{n(0)}{V} + \frac{1}{(2\pi)^3}\int_0^\infty dk\, 4\pi k^2\, n(\epsilon(k))$$

ground state with occupation $n(0)$.
This term is important when $n(0)/V$ stays finite as $V \to \infty$, ie a macroscopic fraction of bosons occupy the ground state

Then we get

$$n = \frac{N}{V} = \frac{n(0)}{V} + \frac{g_{3/2}(z)}{\lambda^3}.$$

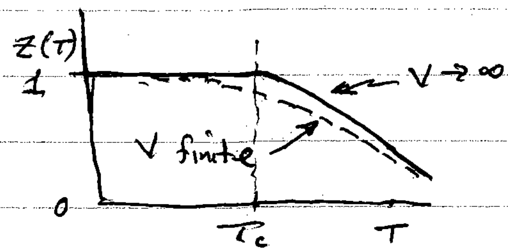
$$n = n_0 + \frac{g_{3/2}(z)}{\lambda^3}$$ where $n_0 = \frac{n(0)}{V}$ density of bosons in ground state

For a system with fixed n, at higher T one can always choose z so that $n = \frac{g_{3/2}(z)}{\lambda^3}$ and $n_0 = 0$.

But when $T < T_c$ it is necessary to have $n_0 > 0$.

Using $n(0) = \frac{z}{1-z}$ we can write above as

$$n = \frac{z}{1-z}\frac{1}{V} + \frac{g_{3/2}(z)}{\lambda^3}$$



For $T > T_c$ we will have a solution to the above for some fixed $z < 1$. In thermodynamic limit $V \to \infty$, the first term will then vanish, i.e. the density of bosons in the ground state vanishes.

As $T \to T_c$, $z \to 1$ and, as $V \to \infty$, the first term $\left(\frac{z}{1-z}\right)\left(\frac{1}{V}\right)$ stays finite to give the additional needed density at $T < T_c$:

diverges as $z \to 1$ vanishes as $V \to \infty$

$$\frac{z}{1-z}\frac{1}{V} = n_0 = n - \frac{g_{3/2}(1)}{\lambda^3}$$

T_c defines the Bose-Einstein transition temperature below which the system developes a finite density of particles in the ground state n_0.
n_0 is also called the condensate density.
The particles in the ground state are called the condensate

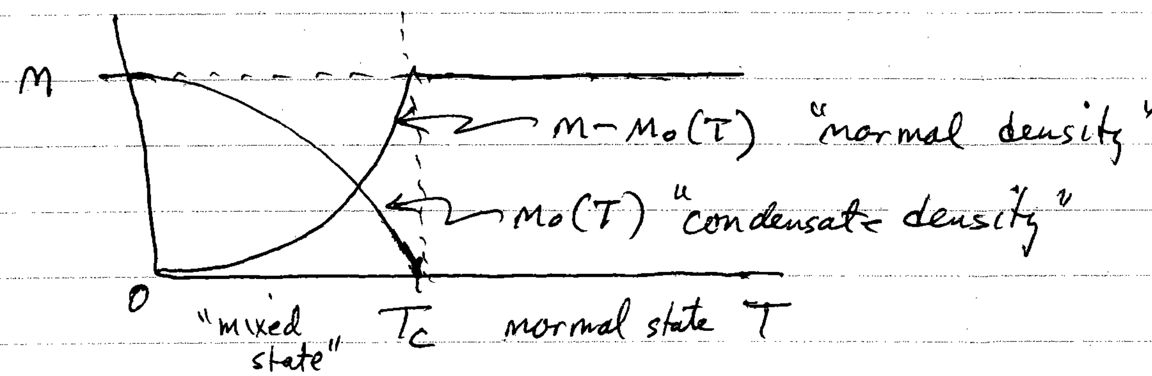
$$\left.\begin{array}{l} z(T) \to 1 \\ \mu(T) \to 0 \end{array}\right\} \text{as } T \to T_c \quad , \quad \left.\begin{array}{l} z(T) = 1 \\ \mu(T) = 0 \end{array}\right\} \text{ for } T \leq T_c$$

For $T \leq T_c$

$$n_0(T) = n - \frac{g_{3/2}(1)}{\lambda^3} = n - 2.612 \left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}$$

$$\boxed{n_0(T) = n\left(1 - \left(\frac{T}{T_c}\right)^{3/2}\right)}$$

condensate density vanishes continuously as $T \to T_c$ from below



At $T = 0$, all bosons are in condensate
At $T > T_c$, all bosons are in the "normal state"
At $0 < T < T_c$, a macroscopic fraction of bosons are in the condensate, while the remaining fraction are in the normal state – call it the "mixed state"