Ideal Bose Gas

Bose-Einstein Condensation

Bose occupation function

\[ n(\varepsilon) = \frac{1}{z^{-1} e^{\beta \varepsilon} - 1} \]

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

\[ \frac{N}{V} = \frac{1}{V} \sum_k \frac{1}{Z e^{\beta \varepsilon(k)} - 1} = \frac{1}{(2\pi)^3} \int_0^\infty \frac{dk}{4\pi} \frac{k^2}{\theta} \frac{1}{e^{\beta h^2 k^2 / 2m} - 1} \]

recall, we need \( z \leq 1 \) for the occupation number
at \( \varepsilon(k=0) = 0 \) to remain positive \( M(0) \geq 0 \)
\[ \frac{m(0)}{z^{-1} - 1} = \frac{z}{z - 1} \Rightarrow z \leq 1, \quad z = e^{\beta \mu} \Rightarrow M \leq 0 \]

Substitute variables \( y = \beta \hbar^2 k^2 \Rightarrow k = \sqrt{\frac{2my}{\beta \hbar^2}} \)
\[ dk = \frac{\sqrt{2my}}{\beta \hbar^2} \, dy, \quad d_k = \frac{\sqrt{2my}}{\beta \hbar^2} \frac{dy}{\sqrt{y}} \]

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

\[ \frac{N}{V} = \frac{1}{\lambda^3} g_{3/2}(z) \quad \text{where} \quad \lambda = \left( \frac{\hbar^2}{2\pi m k_B T} \right)^{1/2} \text{ thermal wavelength} \]

\[ g_{3/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty dy \frac{y^{1/2}}{z^{-1} e^{by} - 1} \]
Consider the function

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

\( g_{3/2}(z) \) is a monotonically increasing function of \( z \) for \( z \leq 1 \).

As \( z \to 1 \), \( g_{3/2}(z) \) approaches a finite constant

\[ g_{3/2}(1) = 1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}} + \cdots = \zeta(3/2) \approx 2.612 \]

\( \zeta \) is the Riemann zeta function.

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

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

as \( y \to \infty \) the integral converges. Integers correspond to low energy, while near 1 is largest.

(Recall small \( y \) corresponds to low energy while near 1 is largest.)

For small \( y \), we can approximate \( e^{\beta y} - 1 \approx \frac{1}{\beta y} \)

\[ \int_0^{y^*} dy \frac{y^{1/2}}{e^{\beta y} - 1} \approx \frac{1}{\beta} \int_0^{y^*} \frac{y^{1/2}}{y^{1/2}} = \frac{1}{\beta} \]

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

\[ n = \frac{N}{V} = \frac{9^{3/2}(2)}{\frac{V}{a^3}} \leq \frac{9^{3/2}(1)}{a^3} = \frac{2.613}{a^3} \left( \frac{2\pi m k_B T}{\hbar^2} \right)^{3/2} \]

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

\[ T_0 = \left( \frac{m}{2\pi \hbar^2} \right)^{2/3} \left( \frac{\hbar^2}{2\pi m k_B} \right) \]

**Solution to the paradox:**

When we made the approx \( \frac{1}{V} \sum_k \to \frac{1}{(2\pi)^3} \int_0^\infty dk \, 4\pi k^2 \)

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 \( \vec{k} = 0 \), i.e. 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 approximate the sum by an integral, we should treat the ground state separately.

\[ \frac{1}{V} \sum_k n(E(k)) \approx \frac{n(0)}{V} + \frac{1}{(2\pi)^3} \int_0^\infty dk \, 4\pi k^2 \, n(E(k)) \]

**ground state with occupation \( n(0) \).**

This term is important when \( n(0)/V \) stays finite as \( V \to \infty \), i.e. a macroscopic fraction of bosons occupy the ground state.
Then we get

\[ M = \frac{N}{V} = \frac{n(0)}{V} + \frac{g_{3/2}(z)}{\lambda^3} \]

\[ m = m_0 + \frac{g_{3/2}(z)}{\lambda^3} \]

where \( m_0 = \frac{n(0)}{V} \) density of bosons in ground state.

For a system with fixed \( m_0 \), at higher \( T \) one can always choose \( z \) so that \( m = \frac{g_{3/2}(z)}{\lambda^3} \) and \( m_0 = 0 \).

But when \( T < T_c \) it is necessary to have \( m_0 > 0 \).

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

\[ M = \frac{z}{1-z} \frac{1}{V} + \frac{g_{3/2}(z)}{\lambda^3} \]

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 the first term \( \left( \frac{z}{1-z} \right) \) stays finite to give the additional needed density at \( T < T_c \):

\[ \frac{z}{1-z} \frac{1}{V} = m_0 = m - \frac{g_{3/2}(1)}{\lambda^3} \]

As \( z \to 1 \) as \( V \to \infty \). Diverges vanishes as \( z \to 1 \) as \( V \to \infty \).
$T_c$ defines the Bose-Einstein transition temperature below which the system develops a finite density of particles in the ground state $M_0$. $M_0$ is also called the condensate density. The particles in the ground state are called the condensate.

\[ Z(T) \rightarrow 1 \quad \text{as} \quad T \rightarrow T_c \quad \text{for} \quad T \leq T_c \]
\[ \mu(T) \rightarrow 0 \quad \text{for} \quad T \leq T_c \]

For $T \leq T_c$

\[ m_0(T) = m - \frac{g_{3/2}}{\lambda^3} = m - 2.612 \left( \frac{2\pi m k_B T}{\hbar^2} \right)^{3/2} \]

\[ m_0(T) = m \left( 1 - \left( \frac{T}{T_c} \right)^{3/2} \right) \]

The condensate density vanishes continuously as $T \rightarrow T_c$ 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".
Pressure — separate out ground state from sum as we saw we needed to do in computing $N/V$

\[
\frac{P}{k_B T} = \frac{1}{V} \ln \xi = -\frac{1}{V} \sum_k \ln \left(1 - z e^{-\beta \epsilon_k}\right)
\]

\[
= -\frac{1}{V} \ln (1 - z) - \frac{4\pi}{(2\pi)^3} \int_0^\infty dk \ k^2 \ln \left(1 - z e^{-\beta \hbar^2 k^2/2m}\right)
\]

\[
\uparrow \quad \text{ground state} \quad \uparrow \quad \text{all other } |k| > 0 \text{ states}
\]

\[
= \frac{1}{V} \ln \left(\frac{1}{1 - z}\right) + \frac{9 \zeta_2(z)}{2^3 z^3}
\]

where $\zeta_2(z) = \frac{1}{\Gamma(z)} \int_0^\infty \frac{y^{3/2}}{z^4} e^{-y} \text{d}y$

as derived when we began our discussion of quantum gases

Also recall the number of bosons occupying the ground state is

\[
\xi(0) = \frac{1}{z^{-1} e^{-\beta \epsilon(0)} - 1} = \frac{1}{z^{-1} - 1} = \frac{z}{1 - z}
\]

So $\xi(0) + 1 = \frac{z}{1 - z} + 1 = \frac{1}{1 - z}$

\[
\frac{P}{k_B T} = \frac{\ln (\xi(0) + 1)}{V} + \frac{9 \zeta_2(z)}{2^3 z^3}
\]

In the thermodynamic limit of $V \to \infty$, the first term always vanishes as $\xi(0) \leq N = nV$ and $\lim_{V \to \infty} \left[ \frac{\ln (nV)}{V} \right] = 0$

So the condensate does not contribute to the pressure.

This is not surprising as particles in the condensate have $k = 0$ and hence carry no momentum. In the kinetic theory of gases, one sees that pressure arise from particles with finite momentum $|p| > 0$ hitting the walls of the container.
So \[ \frac{\Phi}{k_B T} = g_{5/2}(z) \left( \frac{2\pi m k_B T}{\hbar^2} \right)^{3/2} \]

\[ \Phi = g_{5/2}(z(T)) \left( \frac{2\pi m k_B T}{\hbar^2} \right)^{3/2} \left( k_B T \right)^{5/2} \quad \text{< equation of state} \]

for a system of fixed density \( m \), \( z \) must be chosen to be a function of \( T \) that gives the desired density \( m \).

\[ \begin{array}{c}
\text{Note: } g_{5/2}(z=1) = \xi(5/2) = 1.342 \\
\text{is finite}
\end{array} \]

In thermodynamic limit of \( N \to \infty \), \( z = 1 \) for \( T \leq T_c(m) \)

\[ \Rightarrow \Phi = g_{5/2}(1) \left( \frac{2\pi m}{\hbar^2} \right)^{3/2} \left( k_B T \right)^{5/2} \quad \text{for } T \leq T_c \]

\[ \text{Note: for } T \leq T_c, \text{ the pressure } p \propto T^{5/2} \text{ is independent of the system density.} \]

\[ \begin{array}{c}
p \propto T^{5/2} \\
m_1 < m_2 \\
T_c(m_1) < T_c(m_2) \\
T_c(m) = \left( \frac{m}{2.16} \right)^{2/3} \frac{\hbar^2}{2\pi m k_B}
\end{array} \]

\[ \text{Recall: } T_c(m) \propto m^{2/3} \]