Bose-Einstein Condensation

PHYS 301, Prof. Cyr-Racine

1 Introduction to the Boson Gas

Today, I would like to discuss a Nobel Prize winning topic: Bose-Einstein condensation. The 2001 Physics Nobel Prize was awarded for the experimental realization of a Bose-Einstein condensate (BEC): a strange state of matter in which all (bosonic) particles of a system occupy the exact same ground state. This state only occurs when the system when a bosonic system is cooled to extremely cold temperatures, hence the challenge to realize this experimentally. To see how this works, we first need to compute the grand partition function of a non-relativistic bosons gas. Consider a gas of non-interacting, non-relativistic bosons in a volume V. The energy-momentum relation for these particles is given by:

$$E = \frac{p^2}{2m} \tag{1}$$

where m is the mass of the particles.

Let the allowed energy states of the system be $E_0, E_1, E_2, \ldots$, where we define the ground state energy as $E_0 = 0$.

At a given temperature T and chemical potential μ, we can consider each energy state E_r as an independent subsystem exchanging particles with a reservoir. The grand partition function for a single energy state r is:

$$Z_r = \sum_{N=0}^{\infty} e^{-\beta N(E_r - \mu)} = \sum_{N=0}^{\infty} \left(e^{-\beta(E_r-\mu)}\right)^N \tag{2}$$

This is a geometric series which converges provided that $e^{-\beta(E_r-\mu)} < 1$, which requires $E_r > \mu$. Summing the series gives:

$$Z_r = \frac{1}{1 - e^{-\beta(E_r-\mu)}} \quad (\text{for } \mu < E_r) \tag{3}$$

Since the ground state energy is $E_0 = 0$, and the condition must hold for all states, this strictly implies that the chemical potential must be negative:

$$\mu < 0 \quad \text{always.} \tag{4}$$

Since the bosons are non-interacting, the occupancy of each state is independent of any other. The total grand partition function for the entire gas is simply the product of the individual partition functions:

$$Z = \prod_r Z_r = \prod_r \frac{1}{1 - e^{-\beta(E_r-\mu)}} \tag{5}$$

2 Average Particle Number

We can find the total average number of particles $\langle N \rangle$ in the system by using the standard thermodynamic relation:

$$\begin{aligned}
\langle N \rangle &= \frac{1}{\beta}\frac{\partial}{\partial \mu}\ln Z \\
&= \frac{1}{\beta}\frac{\partial}{\partial \mu}\ln\left[\prod_r \frac{1}{1-e^{-\beta(E_r-\mu)}}\right] \\
&= \frac{1}{\beta}\frac{\partial}{\partial \mu}\sum_r \ln\left(\frac{1}{1-e^{-\beta(E_r-\mu)}}\right) \\
&= -\frac{1}{\beta}\sum_r \frac{\partial}{\partial \mu}\ln\left(1-e^{-\beta(E_r-\mu)}\right) \\
&= -\frac{1}{\beta}\sum_r \frac{1}{1-e^{-\beta(E_r-\mu)}}\left(-e^{-\beta(E_r-\mu)}\right)(\beta)
\end{aligned}$$

Dividing the numerator and denominator by $e^{-\beta(E_r-\mu)}$, we recover the familiar Bose-Einstein distribution summed over all states:

$$\langle N \rangle = \sum_r \frac{1}{e^{\beta(E_r-\mu)}-1} \tag{6}$$

3 Continuous Approximation and the Density of States

For a macroscopic volume, the energy levels are very close together, allowing us to convert the discrete sum over states into an integral over phase space:

$$\sum_r \longrightarrow \frac{1}{h^3}\int d^3x \int d^3p \tag{7}$$

The spatial integral trivially evaluates to the volume V. For the momentum integral, we use spherical coordinates ($d^3p = 4\pi p^2 dp$):

$$\langle N \rangle = \frac{V}{h^3}\int_0^\infty \frac{4\pi p^2 dp}{e^{\beta(p^2/2m-\mu)}-1} \tag{8}$$

Let's change the integration variable from momentum p to energy $E = p^2/2m$. This implies $p = \sqrt{2mE}$ and $dp = \frac{m}{\sqrt{2mE}}dE$. Substituting these into the phase space factor:

$$4\pi p^2 dp = 4\pi(2mE)\frac{m}{\sqrt{2mE}}dE = 2\pi(2m)^{3/2}\sqrt{E}\,dE$$

Substituting this back into the integral for $\langle N \rangle$:

$$\langle N \rangle = \frac{2\pi V(2m)^{3/2}}{h^3}\int_0^\infty \frac{\sqrt{E}\,dE}{e^{\beta(E-\mu)}-1} \tag{9}$$

To make the constants match our definition of the thermal de Broglie wavelength ($\lambda_Q = \frac{h}{\sqrt{2\pi m k_B T}}$), we can multiply and divide by appropriate factors of π and $k_B T$. This allows us to rewrite the prefactor purely in terms of λ_Q:

$$\langle N \rangle = \frac{V}{\lambda_Q^3}\frac{2}{\sqrt{\pi}}\beta^{3/2}\int_0^\infty \frac{\sqrt{E}\,dE}{e^{\beta(E-\mu)}-1} \tag{10}$$

4 Fugacity and the Bose-Einstein Integral

To evaluate this integral, we introduce two new variables:

- **Fugacity:** $z = e^{\beta\mu}$. Since $\mu < 0$, the fugacity is bounded: $z \in (0, 1)$.
- **Dimensionless Energy:** $x = \beta E$, which implies $dx = \beta dE$.

Substituting x and z into our integral, the factors of β perfectly cancel out:

$$\begin{aligned}\langle N \rangle &= \frac{V}{\lambda_Q^3} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{x/\beta}\,(dx/\beta)}{e^x z^{-1} - 1} \beta^{3/2} \\ &= \frac{V}{\lambda_Q^3} \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{x}\,dx}{z^{-1} e^x - 1} \end{aligned} \tag{11}$$

To solve this integral, we expand the integrand into an infinite series. Note that:

$$\frac{1}{z^{-1}e^x - 1} = \frac{ze^{-x}}{1 - ze^{-x}}$$

Since $ze^{-x} < 1$, we can expand this as a geometric series:

$$\frac{ze^{-x}}{1 - ze^{-x}} = ze^{-x} \sum_{m=0}^{\infty} (ze^{-x})^m = \sum_{m=1}^{\infty} z^m e^{-mx}$$

Substitute this series back into the integral and interchange the order of integration and summation:

$$\begin{aligned}\frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{x}\,dx}{z^{-1}e^x - 1} &= \frac{2}{\sqrt{\pi}} \int_0^\infty \sqrt{x} \left(\sum_{m=1}^{\infty} z^m e^{-mx} \right) dx \\ &= \frac{2}{\sqrt{\pi}} \sum_{m=1}^{\infty} z^m \int_0^\infty \sqrt{x}\, e^{-mx}\, dx \end{aligned} \tag{12}$$

We can evaluate the integral using the substitution $u = mx$, which gives $dx = du/m$ and $\sqrt{x} = \sqrt{u/m}$:

$$\begin{aligned}\int_0^\infty \sqrt{x}\, e^{-mx}\, dx &= \int_0^\infty \sqrt{\frac{u}{m}}\, e^{-u} \frac{du}{m} \\ &= \frac{1}{m^{3/2}} \int_0^\infty u^{1/2} e^{-u}\, du \end{aligned}$$

The remaining integral is the definition of the Gamma function, $\Gamma(3/2) = \frac{\sqrt{\pi}}{2}$.

$$\int_0^\infty \sqrt{x}\, e^{-mx}\, dx = \frac{\sqrt{\pi}}{2} \frac{1}{m^{3/2}}$$

Substituting this back into our summation, the factors of $\frac{2}{\sqrt{\pi}}$ and $\frac{\sqrt{\pi}}{2}$ beautifully cancel:

$$\frac{2}{\sqrt{\pi}} \sum_{m=1}^{\infty} z^m \left(\frac{\sqrt{\pi}}{2} \frac{1}{m^{3/2}} \right) = \sum_{m=1}^{\infty} \frac{z^m}{m^{3/2}} \tag{13}$$

This specific infinite series appears so frequently in quantum statistics that it is given a special name, the **Bose-Einstein integral** (or Polylogarithm function), denoted as $g_{3/2}(z)$:

$$g_{3/2}(z) \equiv \sum_{m=1}^{\infty} \frac{z^m}{m^{3/2}} \tag{14}$$

Finally, substituting this back into our equation for the particle number, we get a highly compact and elegant equation of state for the ideal boson gas:

$$\boxed{\langle N \rangle = \frac{V}{\lambda_Q^3} g_{3/2}(z)} \tag{15}$$

5 Preparing a condensate

The above calculation was done in the grand canonical ensemble in which the system is in equilibrium with a reservoir at temperature T, and chemical potential μ. Now take this system, enclose it so it can no longer exchange particles with the reservoir. So N is now fixed. Now we start cooling the system. We still have

$$N = \frac{V}{\lambda_Q^3} g_{3/2}(z). \tag{16}$$

The left-hand side is a constant (N is now fixed), so the right-hand side must be constant too. But λ_Q increases at T is decreased, so $g_{3/2}(z)$ must also increase at T goes down. But this can't go on forever since z cannot exceed 1 and $g_{3/2}$ is a monotonically increasing function of z. So something special is happening when $z = 1$, which can be expressed in terms of a critical temperature T_c. You will solve for T_c in the worksheet. But the key question is what happens when $T < T_c$? Again, the worksheet will ask you to sort this out.