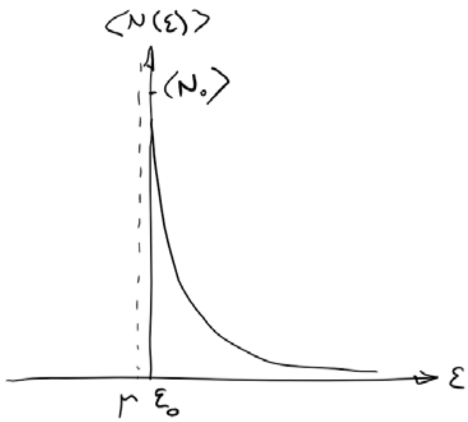
Lecture 18 – Bose-Einstein condensation

PREVIOUSLY: Recall that in contrast to fermionic systems, there is no Pauli exclusion principle for bosons, so particles can occupy the same energy levels in bosonic systems.

TODAY: Bose-Einstein condensation – phenomenon where macroscopic # of bosons fall into (or "condense" into) a single quantum state (e.g. superfluid ^{4}He, superconductivity, laser cooled boson gas)



The occupancy of a particular level is given by the Bose-Einstein distribution:

$$\langle N(\varepsilon,T)\rangle = f_{BE}(\varepsilon,T) = \frac{1}{e^{\beta(\varepsilon-\mu)}-1}$$

To ensure that $\langle N(\varepsilon,T)\rangle \geq 0$, we saw that $\mu(T) < \varepsilon$ for all energy levels, including the ground state ε_0, at all temperatures

Recall that the occupancies must sum to the total # of particles:

$$N = \langle N\rangle = \sum_n \langle N(\varepsilon_n,T)\rangle_{BE} = \sum_n f_{BE}(\varepsilon_n,T) = \sum_n \frac{1}{e^{\beta(\varepsilon_n-\mu)}-1}$$

As T approaches 0, we expect that eventually all the bosons occupy the ground state. So, at some sufficiently low T

$$\langle N(\varepsilon_0,T)\rangle_{BE} = N = \frac{1}{e^{\beta(\varepsilon_0-\mu)}-1}$$

Since N is always a very large number ~ 10^{22}, the denominator must be very small, i.e. $\beta(\varepsilon_0-\mu)$ must be very small

$$N \approx \frac{1}{\cancel{1}+\beta(\varepsilon_0-\mu)-\cancel{1}} = \frac{k_BT}{\varepsilon_0-\mu}$$

and

$$\mu(T\to 0) \approx \varepsilon_0 - \frac{k_BT}{N}$$

$\mu(T) < \varepsilon_0$, as expected, but also <u>extremely</u> close to the ground state energy ε_0 for small T and for N >> 1. How close? Let's put some numbers in:

Consider a cubic box of volume V = 1 cm^3 containing $N = 10^{22}$ ^{4}He atoms ($m = 6.6 \times 10^{-27}$ kg) at some very low temperature (e.g. T ~ 1 mK). Using the standard "particle in a box" approach:

$$\varepsilon_n = \frac{\hbar^2 k_n^2}{2m} \text{ with } k_n^2 = k_x^2 + k_y^2 + k_z^2 \text{ and}$$

$$k_x = \frac{n_x \pi}{L_x} \text{ with } n_x = 1,2,3\cdots$$

and the same for y, z

The ground state energy is

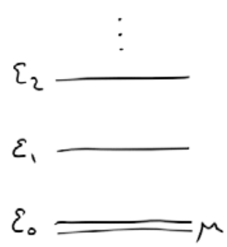
$$\varepsilon_0 = \frac{\hbar^2\pi^2}{2mL^2}(1^2+1^2+1^2) \sim 1.5\times 10^{-18}\,\text{eV} \quad (\text{i.e. } \varepsilon_0/k_B \sim 2\times 10^{-14}\,\text{K})$$

The first excited state energy is

$$\varepsilon_1 = \frac{\hbar^2\pi^2}{2mL^2}(2^2+1^2+1^2) \sim 3\times 10^{-18}\,\text{eV}, \quad \text{or } \Delta\varepsilon = \varepsilon_1 - \varepsilon_0 \sim 1.5\times 10^{-18}\,\text{eV}$$

On the other hand, the chemical potential at T is

$$\mu(T) \approx \varepsilon_0 - \frac{k_B T}{N} = \varepsilon_0 - \frac{8.6\times 10^{-5}\cdot 10^{-3}}{10^{22}} = \varepsilon_0 - \underset{\substack{\uparrow \\ \text{tiny!}}}{10^{-29}}\,\text{eV}$$



The conclusion is that μ is closer to ε_0 than ε_1 is to ε_0 by <u>many, many orders of magnitude</u>!

This means that the Gibbs factor $e^{\beta(\varepsilon_0-\mu)}$ is much closer to 1 than $e^{\beta(\varepsilon_1-\mu)}$ is to 1

What are the consequences of this?
Compare the occupancies of ground state vs. excited state at T = 1 mK.

If bosons obeyed Maxwell-Boltzmann statistics, we would predict:

$$\frac{\langle N(\varepsilon_1,T)\rangle_{MB}}{\langle N(\varepsilon_0,T)\rangle_{MB}} = \frac{e^{-\beta(\varepsilon_1-\mu)}}{e^{-\beta(\varepsilon_0-\mu)}} = e^{-\beta\Delta\varepsilon} = \exp\left(-\frac{1.5\times 10^{-18}}{8.6\times 10^{-5}\cdot 10^{-3}}\right)$$
$$= \exp(-1.8\times 10^{-11}) \approx 1 - 1.8\times 10^{-11} \approx 1$$

Basically, there is no difference in occupancy. Makes sense, since spacing between levels $\Delta\varepsilon = \varepsilon_1 - \varepsilon_0 \ll k_B T$ (~10^{-14} K vs. 10^{-3} K)

Question 1: Estimate the occupancy of the first excited state at *T* = 1 mK using correct statistics.

Using correct Bose-Einstein statistics:

$$\left\langle N(\varepsilon_1,T)\right\rangle_{BE} = \frac{1}{e^{\beta(\varepsilon_1-\mu)}-1} \approx \frac{1}{e^{\beta\Delta\varepsilon}-1}$$

In the last step we used $\beta(\varepsilon-\mu) \approx \beta\varepsilon_0 - \beta\varepsilon_1 + \dfrac{1}{N} \approx \beta\Delta\varepsilon = 1.8\times10^{-11}$ (since $1/N \sim 10^{-22}$). So,

$$\left\langle N(\varepsilon_1,T)\right\rangle_{BE} \approx \frac{1}{e^{1.8\times10^{-11}}-1} \approx \frac{1}{\cancel{1}+1.8\times10^{-11}-\cancel{1}} \approx 5\times10^{10}$$

Now compare to the ground state occupancy $\left\langle N(\varepsilon_0,T)\right\rangle_{BE} = N \approx 10^{22}$:

$$\frac{\left\langle N(\varepsilon_1,T)\right\rangle_{BE}}{\left\langle N(\varepsilon_0,T)\right\rangle_{BE}} \approx 5\times10^{-12}$$

Big difference! Only about 1 in a trillion particles are in the first excited level!

BE distribution is an unusual function, putting the great majority of the particles in the ground state at a sufficiently low temperature, much more than that expected from MB statistics.

This is called <u>Bose-Einstein condensation</u>

KEY CONCEPT: Condensation temperature
The next step is figuring out the temperature at which condensation starts to happen

Since the ground state is so important, we will treat it separately:

$$N = \sum_n f(\varepsilon_n,T) = \underbrace{\left\langle N_0(T)\right\rangle}_{\text{ground state}} + \underbrace{\left\langle N_e(T)\right\rangle}_{\text{all excited states}}$$

i.e. $\left\langle N_0(T)\right\rangle = \left\langle N(\varepsilon_0,T)\right\rangle$.
Since the spacing between energy levels is very small compared to k_BT, we can still write

$$N_e = \int_0^\infty d\varepsilon\, D(\varepsilon) f(\varepsilon,T)$$

(Technically the lower limit should be ε_1, but $\varepsilon_1 \approx 0 \approx \varepsilon_0$ at this level of description.)

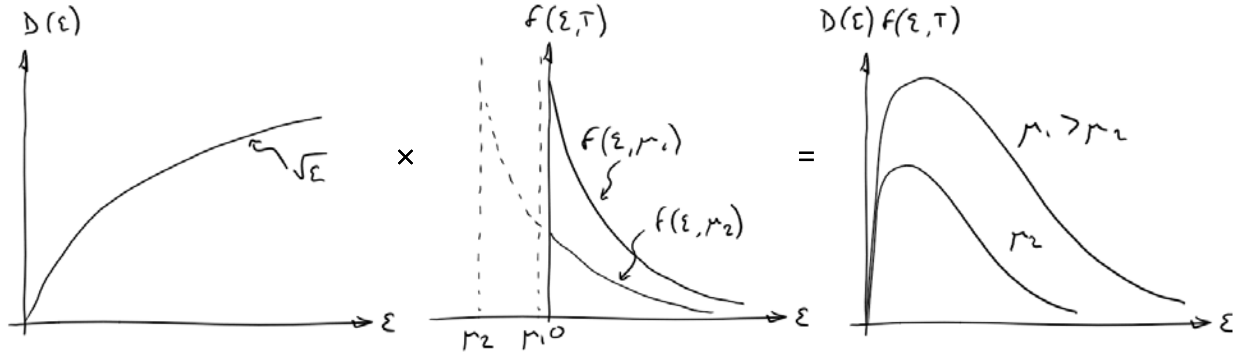
(Note: you may be worried that this integral also includes the ground state, but it does NOT because the density of states goes to 0 at ε = 0!)

$$D(\varepsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\varepsilon^{1/2}$$

(Note no factor of 2 as we saw for fermions because there is 1 spin state for a spin 0 particle.)

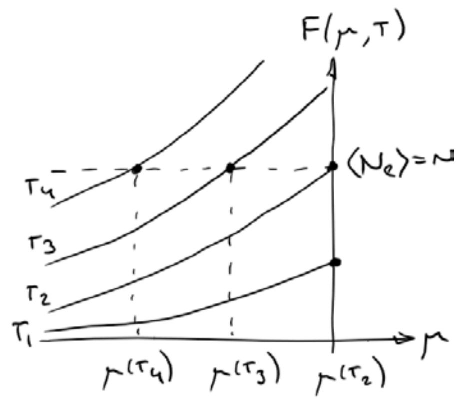
$$\left\langle N_e(T)\right\rangle = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^\infty d\varepsilon\,\frac{\varepsilon^{1/2}}{e^{\beta(\varepsilon-\mu)}-1} \equiv F(\mu,T)$$

where we've defined the function $F(\mu,T)$, treating μ and T as independent variables. We cannot solve this integral analytically, so we will do it graphically. Let's look at the integrand:



Since $\mu < \varepsilon_0$ and $\varepsilon_0 \approx 0$, μ is essentially negative for all T. The area under the curve is the integral, so $F(\mu,T)$ increases as μ increases from a negative value to ~0.

For fixed μ, $F(\mu,T)$ is also an increasing function of T (the function $(e^{E/k_BT}-1)^{-1}$ starts off increasing as $\sim e^{-E/k_BT}$ for small T, then as $\sim k_BT$ for larger T)



So, graphically $\left\langle N_e(T)\right\rangle = F(\mu,T)$ looks like this, plotted vs. μ for different temperatures: $T_4 > T_3 > T_2 > T_1$

We solve for $\mu(T)$ from the intersection of $F(\mu,T)$ with a horizontal line at $\left\langle N_e(T)\right\rangle$

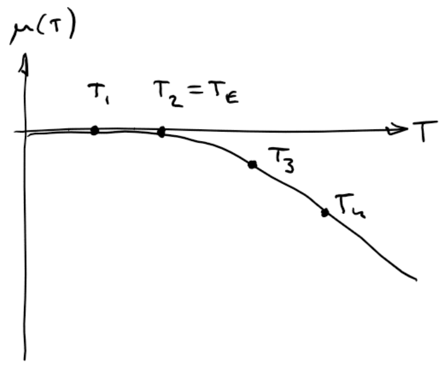
Let's imagine we start at a sufficiently high $T = T_4$, where the boson gas behaves classically, and cool down

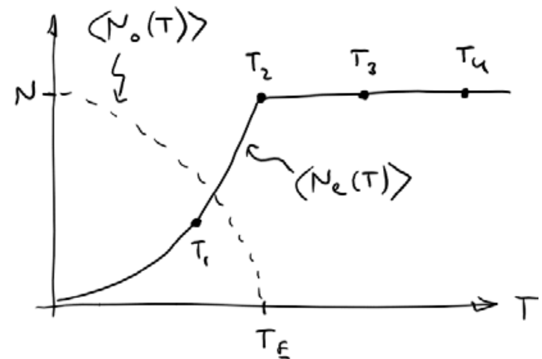
At T_4, μ is a negative number, since $\mu = k_B T \ln \frac{n}{n_Q}$ with $n \ll n_Q(T)$, so the occupancy of the ground state is negligibly small:

$$\langle N_0 \rangle = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1} \approx \frac{1}{e^{-\beta\mu} - 1} \approx e^{+\beta\mu} = \frac{n}{n_Q} \ll 1$$

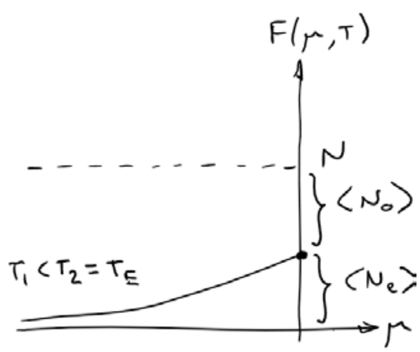
i.e. all bosons are in the excited states, $\langle N_e(T_4) \rangle \approx N$

Same is true for T_3, down to T_2. As we cool, μ approaches 0. What happens for $T < T_2$?
$F(\mu, T < T_2) < N$ and there is no way to satisfy the equation, unless $\langle N_e \rangle$ drops below N





Therefore $\langle N_e \rangle < N$ and $\langle N_0 \rangle$ must increase dramatically:



For $T_1 < T_2$, $\langle N_0 \rangle$ becomes a sizable fraction of N. Macroscopic # of bosons occupy the ground state – Bose-Einstein condensate.

The temperature at which this starts to happen is called the Einstein condensation temperature T_E.

Graphs tell us qualitatively what happens. Now let's calculate it.

Note that for $T \le T_E$, $\mu \approx 0$ (actually $\mu(T) \approx \varepsilon_0 - k_B T / N$ but this is a very small number), so:

$$\langle N_e(T \le T_E) \rangle = F(\mu \approx 0, T \le T_E)$$
$$= \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty d\varepsilon \, \frac{\varepsilon^{1/2}}{e^{\beta\varepsilon} - 1}$$

Question 2: How does the occupancy of the excited state depend on temperature for $T \leq T_E$?

Change integration variables to $x = \beta\varepsilon = \varepsilon / k_B T$

$$\left\langle N_e(T \leq T_E)\right\rangle = \frac{V}{4\pi^2}\left(\frac{2mk_B T}{\hbar^2}\right)^{3/2} \underbrace{\int_0^\infty dx\,\frac{x^{1/2}}{e^x - 1}}_{\text{number}}$$

So, the excited state occupancy decreases from N as $\left\langle N_e(T \leq T_E)\right\rangle \propto T^{3/2}$

Recall that we've encountered integrals of the form $\int_0^\infty dx\,\frac{x^n}{e^x - 1} = \Gamma(n+1)\varsigma(n+1)$, so

$$\int_0^\infty dx\,\frac{x^{1/2}}{e^x - 1} = \Gamma(\tfrac{3}{2})\varsigma(\tfrac{3}{2}) = \frac{\sqrt{\pi}}{2}2.612$$

Also, recall that the quantum density $n_Q(T) = \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3/2}$ so

$$\left\langle N_e(T)\right\rangle = \frac{V}{\cancel{4\pi^2}}\cancel{(4\pi)^{3/2}}\left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3/2}\frac{\cancel{\sqrt{\pi}}}{\cancel{2}}2.612 = 2.612\,n_Q(T)V$$

Note that at the onset of condensation, i.e. $T = T_E$, $\left\langle N_e(T = T_E)\right\rangle = N$ still, so:

Question 3: Derive an expression for T_E in terms of constants of the problem.

At T_E: $\left\langle N_e(T_E)\right\rangle = N = 2.612 n_Q(T_E)V$ (Notice how $n = N/V \sim n_Q(T)$)

Solving for T_E: $k_B T_E = \left(\frac{n}{2.612}\right)^{2/3}\frac{2\pi\hbar^2}{m}$

(For ^{4}He, this predicts T_E = 3.1 K. Actual superfluid transition temperature is 2.17 K. Not bad!)

Normalizing $\left\langle N_e(T)\right\rangle$ by $\left\langle N_e(T_E)\right\rangle = N$, we get the fraction of bosons in the excited states:

$$\frac{\left\langle N_e(T)\right\rangle}{N} = \frac{n_Q(T)}{n_Q(T_E)} = \left(\frac{T}{T_E}\right)^{3/2} \quad \text{for } T \leq T_E$$

Or:

$$\frac{\left\langle N_0(T)\right\rangle}{N} = 1 - \left(\frac{T}{T_E}\right)^{3/2} \quad \text{for } T \leq T_E$$

Even for T slightly less than T_E, a macroscopic number of bosons are in the ground state.