PHYS 427 - Thermal and Statistical Physics - Discussion 10 - Bose-Einstein Condensation

Apr. 8, 2025

In a system of trapped non-interacting identical bosons, there is no fundamental limit to how many particles can occupy the same single-particle state—no Pauli exclusion principle.

Let N be the total number of particles in the system, and let N_0 be the number of particles in the ground state. At low temperatures, we expect the system to minimize its energy by putting most of the particles in the ground state. That is, $N_0/N \to 1$ as $T \to 0$. We say that a macroscopic number of bosons *condense* into the ground state at low temperature—a *condensate* is formed. Despite the fancy terminology, there is nothing really remarkable or unexpected about this. It would happen even if bosons obeyed classical Boltzmann statistics, at low enough temperature.

What *is* remarkable is that the temperature doesn't need to be as low as you might expect. On the basis of classical Boltzmann statistics, you would expect that $k_B T$ would need to be on the order of $\Delta\varepsilon = \varepsilon_1 - \varepsilon_0$, the gap between the ground and first excited states, in order for a sizeable condensate to form. This would correspond to $T \approx 10^{-9}$ K for a typical dilute atomic gas. But in fact, you only need $T \approx 10^{-6} K$.

Even more remarkable is the fact that, as you cool down the system, $\frac{N_0}{N}$ doesn't increase smoothly like you would guess. Instead, it increases rather abruptly, and only after the temperature falls below a *critical temperature* T_c—see Figure 1. Some degree of "abruptness" is a generic feature of a *phase transition*, of which Bose-Einstein condensation is our first example. Our main question today is, "how does the condensate fraction N_0/N depend on temperature?" That is, we want to "prove" Figure 1.

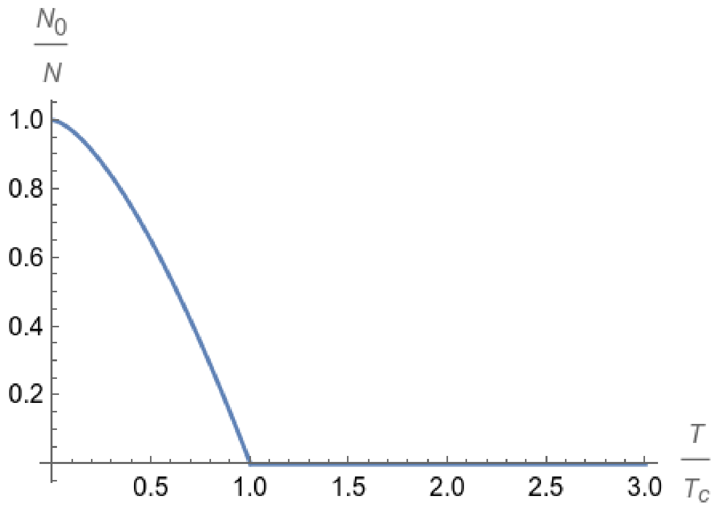

Figure 1

1. **Bose gas in a box**: Consider a gas of identical, non-interacting, non-relativistic spin–0 bosons of mass m trapped in a cubic box with volume $V = L^3$.

   (a) Compute the density of states $\mathcal{D}(\varepsilon)$ for this system by starting from its definition:

   $$\mathcal{D}(\varepsilon)d\varepsilon = \#\text{ of single-particle states with energy between } \varepsilon \text{ and } \varepsilon + d\epsilon. \tag{1}$$

   Answer: $\mathcal{D}(\varepsilon) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{\varepsilon}$.

   Now that we have $\mathcal{D}(\varepsilon)$, recall that for any function $F(\varepsilon)$,

   $$\sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \to \int_0^\infty d\varepsilon\, \mathcal{D}(\varepsilon)F(\varepsilon) \tag{2}$$

   as $L \to \infty$. This is why $\mathcal{D}(\varepsilon)$ is useful to know—it's the key to converting sums over quantum numbers into integrals over energy.

   (b) Now, using (2), we will compute $N = \sum_{\vec{k}} f(\varepsilon_{\vec{k}})$, where

   $$f(\varepsilon) \equiv \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} \tag{3}$$

   is the Bose-Einstein distribution. We expect something interesting to happen in the ground state, so we will treat it carefully—pull it out of the sum and leave it as a separate term. We get

   $$N = f(0) + \int_0^\infty d\varepsilon\ \mathcal{D}(\varepsilon)f(\varepsilon). \tag{4}$$

   In this expression, we used that the ground state energy $\varepsilon_0 = \frac{\hbar^2\pi^2}{2mL^2} \approx 0$ if the box is large enough.

   From (4), show that the total particle density $n = N/V$ can be written as

   $$n = \frac{1}{V}\frac{\lambda}{1-\lambda} + n_Q g(\lambda), \tag{5}$$

where $\lambda \equiv e^{\beta\mu}$ is the fugacity, $n_Q \equiv \left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}$ is the so-called "quantum concentration" and $g(\lambda) \equiv \frac{1}{\Gamma(3/2)}\int_0^\infty dx\ \frac{\sqrt{x}}{\lambda^{-1}e^x-1}$ is a function called the "polylogarithm of order 3/2".

You may need the following properties of the Gamma function: $x\Gamma(x) = \Gamma(x+1)$ and $\Gamma(1/2) = \sqrt{\pi}$. These are worth memorizing!

(c) We can write the total density (5) in terms of the condensate density n_0 and the density of excited particles n_e:

$$n = n_0 + n_e \qquad n_0 = \frac{1}{V}\frac{\lambda}{1-\lambda} \qquad n_e = CT^{3/2}g(\lambda), \tag{6}$$

where $C \equiv \left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2}$ is a constant. The densities n_0, n_e and $n_0 + n_e$ are visualized as functions of λ in Figures 2.

We will now pass to the *thermodynamic limit*. This is the limit in which all the extensive quantities (N and V) become very large, but in such a way that all intensive quantities (n, μ and T) remain the same. Strictly speaking, phase transitions only occur in the thermodynamic limit.

i. In the thermodynamic limit, what must happen to the fugacity λ in order for for a sizeable condensate to form (i.e. in order for n_0/n to be appreciably different from 0)? *Hint: examine Figure 2(a).*

ii. By examining Figures 2, argue that $n_0/n \approx 0$ until T drops below a certain *critical temperature* T_c. Convince yourself that

$$n = CT_c^{3/2}g(1) \tag{7}$$

and use this to solve for k_BT_c. You may use the result $g(1) = \zeta(3/2)$, where ζ is the Riemann zeta function. *Answer:* $k_BT_c = \left(\frac{n}{\zeta(3/2)}\right)^{2/3}\frac{2\pi\hbar^2}{m}$.

iii. Using (7) and $n_0 = n - n_e$, show that when $T < T_c$,

$$\frac{n_0(T)}{n} = 1 - \left(\frac{T}{T_c}\right)^{3/2}. \tag{8}$$

This, together with $n_0 \approx 0$ when $T > T_c$, establishes Fig. 1.

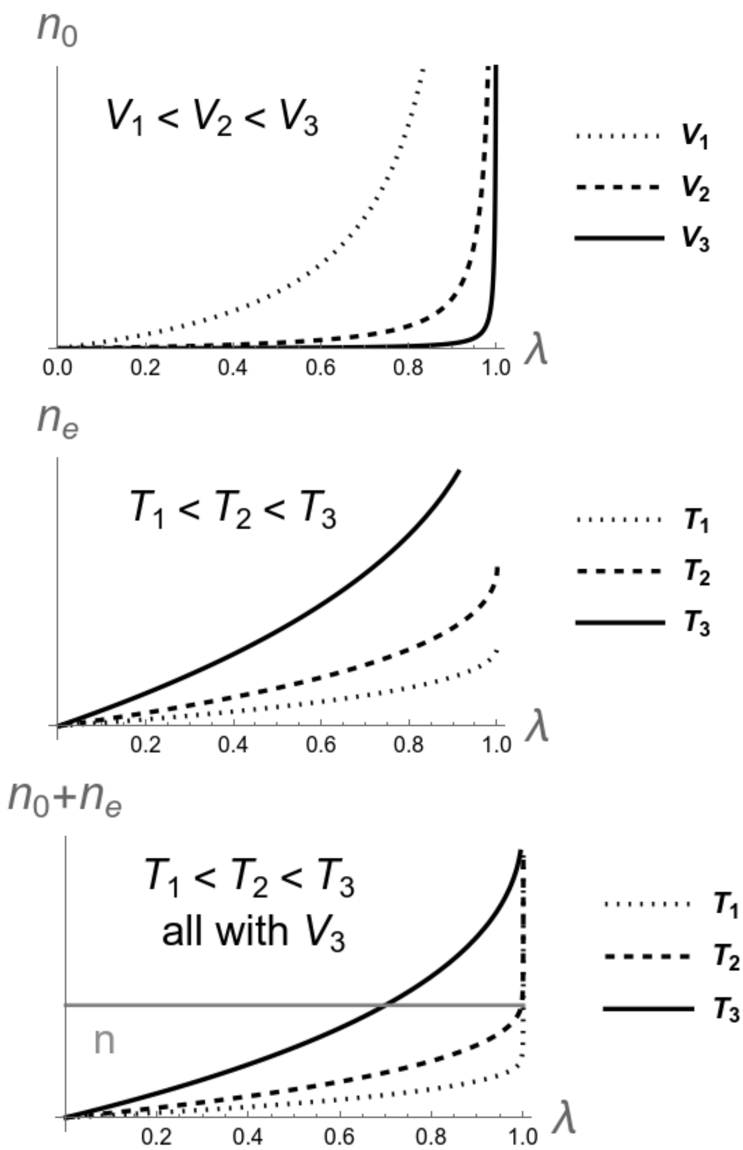

Figure 2

2. **2D Bose gas in harmonic trap**: Consider a gas of identical, non-interacting spin–0 bosons of mass m confined to the plane. They are trapped by a harmonic potential $V(x, y) = \frac{1}{2}m\omega^2(x^2 + y^2)$.

   The single-particle eigenstates are labeled by quantum numbers $n_x = 0, 1, \ldots, \infty$ and $n_y = 0, 1, \ldots, \infty$, and their energies are $\varepsilon_{n_x,n_y} = \hbar\omega(n_x + n_y)$. Notice that we have dropped the zero-point energy from this expression (i.e. we've shifted our reference energy).

   (a) Compute the density of states $\mathcal{D}(\varepsilon)$ for this system by starting from its definition:

   $$\mathcal{D}(\varepsilon)d\varepsilon = \#\text{ of single-particle states with energy between } \varepsilon \text{ and } \varepsilon + d\epsilon. \quad (9)$$

   Apply the approximation $\varepsilon/\hbar\omega \gg 1$, which is good for all but the lowest-lying states.

   Hint: First find the degeneracy[1] *of the energy level $\varepsilon = \hbar\omega n$. Then write down*

[1] i.e. count how many single-particle eigenstates have this energy.

the spacing $\Delta\varepsilon$ *between energy levels. Then write down the answer. Answer:* $\mathcal{D}(\varepsilon) = \varepsilon/(\hbar\omega)^2$.

(b) Just as in problem 1, the critical temperature for Bose-Einstein condensation is determined by the condition that $N_e = N$ when $\lambda = 1$. Using (2) to evaluate N_e, show that this condition becomes

$$\left(\frac{k_B T_c}{\hbar\omega}\right)^2 \zeta(2) = N, \tag{10}$$

which can be rearranged to obtain

$$k_B T_c = \hbar\omega\sqrt{\frac{N}{\zeta(2)}}. \tag{11}$$

Note: when $N \gg 1$*, we find* $k_B T/\hbar\omega \gg 1$*. That is, the Bose-Einstein condensation temperature is much larger than* $\Delta\varepsilon = \varepsilon_1 - \varepsilon_0$*, the gap between the ground and first excited states, when* N *is large. Bosons like to group together, in contrast to Fermions.*

(c) Using (10), show that when $T < T_c$,

$$\frac{N_0(T)}{N} = 1 - \left(\frac{T}{T_c}\right)^2. \tag{12}$$

This is similar to, but not quite the same as, Figure 1.