

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

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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, $N_0/N \rightarrow 1$ as $T \rightarrow 0$. 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.

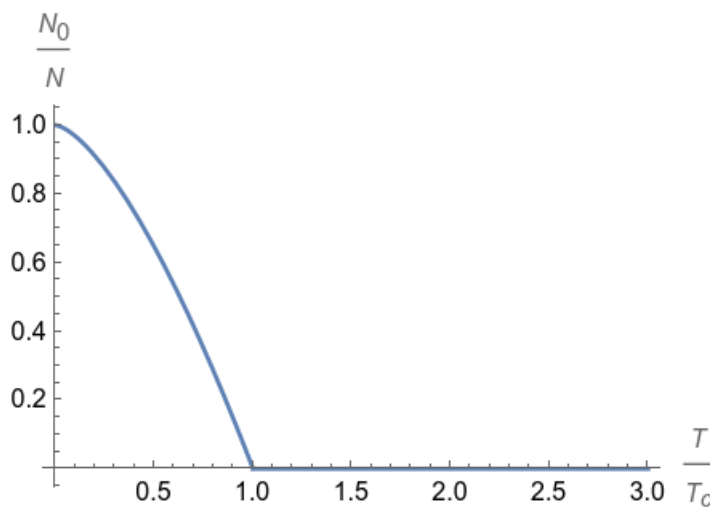


Figure 1

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:

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

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

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

$$\sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \rightarrow \int_0^\infty d\varepsilon \mathcal{D}(\varepsilon) F(\varepsilon) \quad (2)$$

as $L \rightarrow \infty$. 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

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

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

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

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

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

where $\lambda \equiv e^{\beta\mu}$ is the fugacity, $n_Q \equiv \left(\frac{mk_B T}{2\pi\hbar^2} \right)^{3/2}$ 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 :

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

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 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

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

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

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

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

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

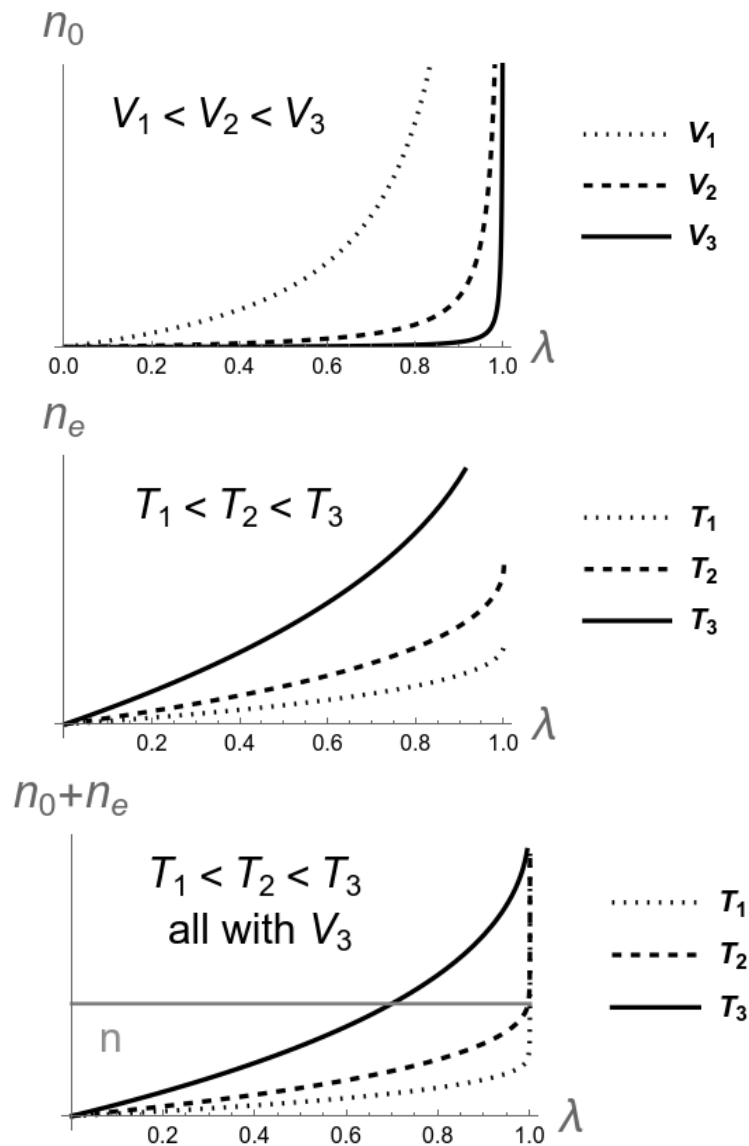


Figure 2

SOLUTION:

(a) Using the dispersion $\varepsilon = \hbar^2 k^2 / 2m$, the number of states with energy between ε and $\varepsilon + d\varepsilon$ is the number of states with wavevector magnitude between k and $k + dk$, where $k = \sqrt{2m\varepsilon/\hbar^2}$ and dk is related to $d\varepsilon$ by

$$d\varepsilon = \frac{\hbar^2 k}{m} dk. \quad (9)$$

The number of states with wavevector magnitude between k and $k + dk$ is the number of states in a thin spherical shell in k -space whose radius is k and whose thickness is dk . More precisely, because $k_x, k_y, k_z > 0$, it is only the part of this shell lying in the first octant. The k -space volume of this part of the shell is $\frac{1}{8}4\pi k^2 dk$.

From quantum mechanics, we know that $k_x = \pi n_x / L$, and similarly for k_y and k_z . Therefore, each state occupies a k -space volume $(\pi/L)^3$. Hence the total number of states in the shell is

$$\frac{\frac{1}{8}4\pi k^2 dk}{(\pi/L)^3}. \quad (10)$$

Note that the particles are spin-0, so there is no spin degeneracy factor to include out front. Finally, inserting the above relations between k and ε in this expression, we find

$$\mathcal{D}(\varepsilon)d\varepsilon = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon} d\varepsilon. \quad (11)$$

(b) Dividing (4) by V gives

$$n = N/V \quad (12)$$

$$= \frac{1}{V} f(0) + \frac{1}{V} \int_0^\infty d\varepsilon \mathcal{D}(\varepsilon) f(\varepsilon). \quad (13)$$

For the first term, note that the Bose-Einstein distribution with $\varepsilon = 0$ is

$$f(0) = \frac{1}{e^{-\beta\mu} - 1} = \frac{1}{\lambda^{-1} - 1} = \frac{\lambda}{1 - \lambda}, \quad (14)$$

where we identified the fugacity $\lambda = e^{\beta\mu}$.

For the second term, we insert the density of states and Bose-Einstein distribution to obtain

$$\frac{1}{V} \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^\infty d\varepsilon \frac{\sqrt{\varepsilon}}{e^{\beta(\varepsilon-\mu)} - 1}. \quad (15)$$

Making a variable substitution $x = \beta\varepsilon$, this becomes

$$\frac{1}{V} \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \beta^{-3/2} \int_0^\infty dx \frac{\sqrt{x}}{\lambda^{-1}e^x - 1}, \quad (16)$$

where we also identified $\lambda = e^{\beta\mu}$ here. Identifying the given definition of $g(\lambda)$, this becomes

$$\frac{1}{V} \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \beta^{-3/2} \Gamma(3/2) g(\lambda). \quad (17)$$

Finally we do some algebra. We can cancel the V s. We can also write $\beta^{-3/2} = (k_V T)^{3/2}$ and bring this underneath the existing $(2m/\hbar^2)^{3/2}$ as they share the same exponent. Also, using $y\Gamma(y) = \Gamma(y+1)$ with $y = 1/2$, we have $\Gamma(3/2) = \Gamma(1/2)/2 = \sqrt{\pi}/2$. After doing all this we get

$$\frac{1}{8\pi^{3/2}} \left(\frac{2mk_B T}{\hbar^2} \right)^{3/2} g(\lambda). \quad (18)$$

Finally, we bring the $1/8\pi^{3/2}$ into the other factor, obtaining

$$n_Q g(\lambda). \quad (19)$$

This proves the desired result,

$$n = \frac{1}{V} \frac{\lambda}{1 - \lambda} + n_Q g(\lambda). \quad (20)$$

(c)(i) Take a look at Figure 2a. This shows the curve $n_0(\lambda)$ at three different volumes. Notice that the curve becomes sharper as we pass to the thermodynamic limit (large V). In fact, we see that n_0 is basically zero unless λ is close to 1. So in order to have an appreciable condensate form in the thermodynamic limit, the fugacity λ must be close to 1. File that away.

(c)(ii) From now on, we will work in the thermodynamic limit. In particular, each of the three curves in Figure 2c are drawn for large V .

The way to interpret Figure 2c is as follows. Suppose we create a Bose gas in the laboratory with a certain density of particles per area n . So n is some specific number that we have measured, represented by the horizontal gray line in Figure 2c. This measured number must be correctly given by the right-hand side of (5). This places a condition on λ . In other words, at a given (measured) T , only one value of λ will satisfy (5) with our measured value of n . This is precisely what we talked about in problem 1(e) of discussion 8 and problem 1(e) of discussion 9 (see solutions). The only difference is we're talking in terms of the fugacity instead of the chemical potential. In terms of Figure 2c, this means λ is determined by the intersection of the horizontal line with the curve corresponding to the measured temperature T .

For example, if the measured temperature of the gas is $T = T_3$, then the intersection point appears to be at $\lambda \approx 0.7$. But, from Figure 2a, we see that n_0 is basically zero when $\lambda \approx 0.7$ (recall we are now working exclusively in the thermodynamic limit, so look at the V_2 curve in Figure 2a). Hence at $T = T_3$, there is no condensate.

As T decreases, Figure 2a passes through a series of curves between T_3 and T_2 . It is clear that the intersection point moves closer and closer to $\lambda = 1$. But, as observed in part (a), n_0/n remains very close to zero until λ gets very close to 1. When T reaches T_2 , there is still no condensate (all particles are in excited states), but if we lowered the temperature any further then λ would be sufficiently close to 1, and a condensate would form. This is the meaning of the critical temperature T_c . That is, in the figure, T_2 is the critical temperature T_c .

Unpacking the previous paragraph, we find that, when $T = T_c$, we have $n = n_c$ (all particles are in excited states) and $\lambda \approx 1$ (further decreasing the temperature would cause a condensate to form). From (6), this means

$$n = CT_c^{3/2} g(1). \quad (21)$$

Recall that we take n to be measured in the lab. So this relation can be inverted to obtain a prediction for the critical temperature. Using $g(1) = \zeta(3/2)$, we find

$$k_B T_c = \left(\frac{n}{\zeta(3/2)} \right)^{2/3} \frac{2\pi\hbar^2}{m}. \quad (22)$$

This is the critical temperature appearing in Figure 1, although we haven't quite proven that the curve should take that form. We'll do that in the next problem. But while we're here, let's notice something interesting.

The energy gap between the ground and first excited states is

$$\Delta\varepsilon \equiv \varepsilon_1 - \varepsilon_0 = \frac{\hbar^2\pi^2}{2mL^2}(2^2 + 1^2 + 1^2) - \frac{\hbar^2\pi^2}{2mL^2}(1^2 + 1^2 + 1^2) = \frac{3\hbar^2\pi^2}{2mL^2}. \quad (23)$$

If we only knew about classical Boltzmann statistics, we might have guessed that the critical temperature would be $k_B T_c^{\text{guess}} \approx \Delta\varepsilon$. Let's see how far off this guess is. From (22) and (23),

$$\frac{T_c}{T_c^{\text{guess}}} = \left(\frac{n}{\zeta(3/2)} \right)^{2/3} \frac{4L^2}{3\pi} = \left(\frac{N}{\zeta(3/2)} \right)^{2/3} \frac{4}{3\pi}, \quad (24)$$

where I used $nL^3 = N$ in the last step. Suppose we create a Bose gas consisting of $N \approx 10^5$ particles (this is routinely done in atomic physics labs). Then

$$\frac{T_c}{T_c^{\text{guess}}} \approx 500. \quad (25)$$

In other words, our classical guess for the critical temperature is too low by almost three orders of magnitude! Evidently, using the correct quantum statistics causes bosons to collect in the ground state earlier than expected. "Bosons like to be with other bosons", so the higher N is, the higher is T_c (easier to condense).

(c)(iii) We have

$$\frac{n_0}{n} = \frac{n - n_e}{n} = 1 - \frac{n_e}{n}. \quad (26)$$

Since we're at $T < T_c$, we have $\lambda \approx 1$, so from (6) we have $n_e \approx CT^{3/2}g(1)$. Using also (21), we have

$$\frac{n_0}{n} = 1 - \frac{CT^{3/2}g(1)}{CT_c^{3/2}g(1)} = 1 - \left(\frac{T}{T_c} \right)^{3/2}. \quad (27)$$

This "proves" Figure 1. Note that we have relied on the thermodynamic limit in this calculation. In fact, if we have a finite-sized system, Figure 1 will not look quite as "abrupt". Instead, the sharp part at $T = T_c$ will be smoothed out a bit. Strictly speaking, this is not considered to be a phase transition. Idealized phase transitions with abrupt behavior only occur in the thermodynamic limit.

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 $n_x = 0, 1, \dots, \infty$ and $n_y = 0, 1, \dots, \infty$, 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:

$$\mathcal{D}(\varepsilon)d\varepsilon = \# \text{ of single-particle states with energy between } \varepsilon \text{ and } \varepsilon + d\varepsilon. \quad (28)$$

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

Hint: First find the degeneracy¹ of the energy level $\varepsilon = \hbar\omega n$. Then write down 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

$$\left(\frac{k_B T_c}{\hbar\omega}\right)^2 \zeta(2) = N, \quad (29)$$

which can be rearranged to obtain

$$k_B T_c = \hbar\omega \sqrt{\frac{N}{\zeta(2)}}. \quad (30)$$

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 (29), show that when $T < T_c$,

$$\frac{N_0(T)}{N} = 1 - \left(\frac{T}{T_c}\right)^2. \quad (31)$$

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

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

SOLUTION: (a) The degeneracy of the level $\varepsilon = \hbar\omega n$ is the number of ways to have $n = n_x + n_y$. One way is to choose $n_x = 0$ and $n_y = n$. Another way is to choose $n_x = 1$ and $n_y = n - 1$. And so on. There are $n + 1$ ways, so the degeneracy of this level is $n + 1$, or $\frac{\varepsilon}{\hbar\omega} + 1$, which we approximate as $\frac{\varepsilon}{\hbar\omega}$.

The spacing between levels is $\hbar\omega$. We what we have found is that there are $\frac{\varepsilon}{\hbar\omega}$ number of states within an energy interval $\Delta\varepsilon = \hbar\omega$. That is,

$$\mathcal{D}(\varepsilon) = \frac{\varepsilon/\hbar\omega}{\hbar\omega}, \quad (32)$$

which is what we wanted to show.

(b) We have

$$N_e = \int_0^\infty d\varepsilon \mathcal{D}(\varepsilon) f(\varepsilon) \quad (33)$$

$$= \int_0^\infty d\varepsilon \frac{\varepsilon}{(\hbar\omega)^2} \frac{1}{e^{\beta(\varepsilon-\mu)} - 1} \quad (34)$$

$$= \left(\frac{k_B T}{\hbar\omega}\right)^2 \int_0^\infty dx \frac{x}{\lambda^{-1}e^x - 1}. \quad (35)$$

The condition that determines the critical temperature, as discussed in the previous problem, is that $N_e = N$ when $\lambda = 1$. That is,

$$N = \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \int_0^\infty dx \frac{x}{e^x - 1}. \quad (36)$$

The integral here is

$$\int_0^\infty dx \frac{x}{e^x - 1} = \Gamma(2)\zeta(2) = \zeta(2). \quad (37)$$

A proof can be found in the gamma function handout on the course schedule, and also in the lecture notes. Using this result, we have

$$N = \left(\frac{k_B T_c}{\hbar\omega}\right)^2 \zeta(2) \implies k_B T_c = \hbar\omega \left(\frac{N}{\zeta(2)}\right)^{1/2}. \quad (38)$$

(c) First,

$$\frac{N_0}{N} = \frac{N - N_e}{N} = 1 - \frac{N_e}{N}. \quad (39)$$

Since $T < T_c$, we have $\lambda \approx 1$, so from (33) we have

$$N_e = \left(\frac{k_B T}{\hbar\omega}\right)^2 \int_0^\infty dx \frac{x}{e^x - 1} \quad (40)$$

$$= \left(\frac{k_B T}{\hbar\omega}\right)^2 \zeta(2). \quad (41)$$

Inserting also (38) gives

$$\frac{N_0}{N} = 1 - \frac{\left(\frac{k_B T}{\hbar\omega}\right)^2 \zeta(2)}{\left(\frac{k_B T_c}{\hbar\omega}\right)^2 \zeta(2)} = 1 - \left(\frac{T}{T_c}\right)^2. \quad (42)$$