

Statistical Mechanics
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Lecture - 59
Bose - Einstein Condensation in a Harmonically Trapped Bose Gas

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Harmonically trapped Bose Gas ← $g(\epsilon) \sim \epsilon^{\alpha}$ (d=3)

3 Dimensional D=3 $d = \frac{3}{2}$

$$\mathcal{H} = \sum_{\vec{p}} \frac{p^2}{2m} + \frac{1}{2} \sum m \omega_x^2 x_i^2 + \frac{1}{2} \sum m \omega_y^2 y_i^2 + \frac{1}{2} \sum m \omega_z^2 z_i^2$$

Energy levels are discrete

$$\left. \begin{aligned} \epsilon_x &= \left(m_x + \frac{1}{2}\right) \hbar \omega_x \\ \epsilon_y &= \left(m_y + \frac{1}{2}\right) \hbar \omega_y \\ \epsilon_z &= \left(m_z + \frac{1}{2}\right) \hbar \omega_z \end{aligned} \right\}$$

$$\epsilon = \epsilon_x + \epsilon_y + \epsilon_z$$



So, we want to now look at a Harmonically Trapped Bose Gas and our motivation is that this is typically what is realized in experiments, but the second point is also that we will see that α is different, even though that this system is in 3 dimension. So, that D is equal to 3 your $g(\epsilon)$ has a different behavior as ϵ^{α} to the power α where α is equal to 3 for a free Bose gas we knew that α was 3 by sorry, α was 1 by 2, but here we want to look at it.

Now, the Hamiltonian is p^2 over twice m plus half $m \omega^2 x^2$ plus half $m \omega_y^2 y^2$ plus half $m \omega_z^2 z^2$. So, one can have an anisotropic harmonic potential. So, that you have $\omega_y^2 y^2$ plus half $m \omega_z^2 z^2$ the half factor should we not be missed, but the energy levels are discrete.

So, that we have $\epsilon_x = n_x + \frac{1}{2} \hbar \omega_x$, $\epsilon_y = n_y + \frac{1}{2} \hbar \omega_y$ and $\epsilon_z = n_z + \frac{1}{2} \hbar \omega_z$. So, the total energy is now $\epsilon_x + \epsilon_y + \epsilon_z$.

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$$n_x = 0, 1, 2, \dots$$

Energy levels are discrete

$$\left. \begin{aligned} \epsilon_x &= (n_x + \frac{1}{2}) \hbar \omega_x \\ \epsilon_y &= (n_y + \frac{1}{2}) \hbar \omega_y \\ \epsilon_z &= (n_z + \frac{1}{2}) \hbar \omega_z \end{aligned} \right\} g = 1$$

$$\epsilon = \epsilon_x + \epsilon_y + \epsilon_z \qquad g(\epsilon) = \frac{dG}{d\epsilon}$$

The total number of states $G(\epsilon)$ that lies between 0 and ϵ . $\epsilon_i = \hbar \omega_i n_i$

$$G(\epsilon) = \frac{1}{3! \hbar^3 \omega_x \omega_y \omega_z} \int d\epsilon_x \int d\epsilon_y \int d\epsilon_z$$



We will ignore the ground state energy and try to figure out the total number of state. The total number of states $G(\epsilon)$ that lies between 0 and ϵ . The idea is that once I know this number then $g(\epsilon)$ the density of state is given by $dG/d\epsilon$. Further we also consider particles which do not have internal degrees of freedom. So, that we will set the factor g is

equal to 1, if you do have particles which has internal degrees of freedom, then you need to multiply that factor.

Now, $g(\epsilon)$ of epsilon is then given by integral $d\epsilon_x \times d\epsilon_y$ and $d\epsilon_z$ divided by $h^3 \omega_x \omega_y \omega_z$ not much of a space here. So, $1/h^3 \omega_x \omega_y \omega_z$ is equal to $g(\epsilon)$.

Here, we have essentially is defined the variables or defined a coordinate system, if the variable $h \omega_i$ and this gives me the total density of total number of states between the energies 0 and epsilon, but one has to be careful about the integration limit.

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$\gamma(\epsilon) = \frac{dn}{d\epsilon}$

$\epsilon = \epsilon_x + \epsilon_y + \epsilon_z$

The total number of states $G(\epsilon)$ that lies between 0 and ϵ .

$$G(\epsilon) = \frac{1}{(h\omega_x\omega_y\omega_z)^3} \int_0^\epsilon d\epsilon_x \int_0^{\epsilon-\epsilon_x} d\epsilon_y \int_0^{\epsilon-\epsilon_x-\epsilon_y} d\epsilon_z$$

$\epsilon_i = h\omega_i \gamma_i$
 $\omega_x = \omega_y = \omega_z = \omega$

$$= \frac{1}{(h\omega)^3} \int_0^\epsilon d\epsilon_x \int_0^{\epsilon-\epsilon_x} d\epsilon_y \int_0^{\epsilon-\epsilon_x-\epsilon_y} d\epsilon_z$$



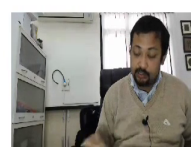
Clearly, ϵ_z can go from $\epsilon_x - \epsilon_y$ and ϵ_y can be from 0 to $\epsilon - \epsilon_x$ and ϵ_x will be from 0 to ϵ . Well, we want to carry forward this

cumbersome factor that sits outside, but here we make the assumption that ω_x equal to ω_y is equal to ω_z is equal to ω .

So, that I have $\hbar \omega$ whole cube and then the integral is 0 to ϵ $d\epsilon_x$, 0 to $\epsilon - \epsilon_x$ $d\epsilon_y$, if you carry out the integral over ϵ_z you will be left out with $\epsilon - \epsilon_x - \epsilon_y$ 0 to $\epsilon - \epsilon_x - \epsilon_y$.

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$$\begin{aligned}
 G(\epsilon) &= \frac{1}{(\hbar\omega)^3} \int_0^\epsilon d\epsilon_x \int_0^{\epsilon-\epsilon_x} d\epsilon_y \left[\frac{(\epsilon-\epsilon_x-\epsilon_y)^2}{2} \right] \\
 &= \frac{1}{(\hbar\omega)^3} \int_0^\epsilon d\epsilon_x \left[\frac{(\epsilon-\epsilon_x)\epsilon_y}{2} - \frac{\epsilon_y^2}{2} \right]_0^{\epsilon-\epsilon_x} = \frac{(\epsilon-\epsilon_x)^2}{2} - \frac{(\epsilon-\epsilon_x)^2}{2} \\
 &= \frac{1}{(\hbar\omega)^3} \int_0^\epsilon d\epsilon_x \frac{(\epsilon-\epsilon_x)^2}{2} = \frac{1}{2} \frac{1}{(\hbar\omega)^3} \int_0^\epsilon (\epsilon-\epsilon_x)^2 d\epsilon_x \\
 &= \frac{1}{6} \left(\frac{\epsilon}{\hbar\omega} \right)^3
 \end{aligned}$$



The first integral, let us now carry out the integration over ϵ_y .

So, at the first term is going to be $\epsilon - \epsilon_x - \epsilon_y$ 0 to $\epsilon - \epsilon_x - \epsilon_y$ minus ϵ_y square by 2 and then I have an integral over ϵ_x 0 to ϵ outside I have a factor $\hbar \omega$ whole cube and this is your total number of energy states that is available between the energies 0 and ϵ .

So, $\frac{1}{h^3} \int_0^\epsilon dx \left(\frac{\epsilon - \epsilon x}{2} \right)^2$ substitute this, this part can simplify to $\frac{\epsilon^3}{6} - \frac{\epsilon^3 x}{2} + \frac{\epsilon^3 x^2}{2}$ divided by 2 so, that I have $\frac{\epsilon^3}{6} - \frac{\epsilon^3 x}{2} + \frac{\epsilon^3 x^2}{2}$ divided by 2. So, $\frac{\epsilon^3}{6} - \frac{\epsilon^3 x}{2} + \frac{\epsilon^3 x^2}{2}$ divided by 2, which is going to be half $\frac{1}{h^3} \int_0^\epsilon dx \left(\frac{\epsilon - \epsilon x}{2} \right)^2$.

This integration is very easy to do, if you substitute $\epsilon - \epsilon x$ as u then essentially you have $\int_0^\epsilon u^2 du$ which is going to be $\frac{u^3}{3}$ from 0 to ϵ and that gives you $\frac{\epsilon^3}{3}$. So, that the total number of energy states lying between 0 and ϵ is going to be $\frac{1}{6} \frac{\epsilon^3}{h^3}$.

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Handwritten derivation:

$$G(\epsilon) = \frac{1}{6} \left(\frac{\epsilon}{h\nu_0} \right)^3$$

$$g(\epsilon) = \frac{dG}{d\epsilon} = \frac{1}{2} \frac{\epsilon^2}{(h\nu_0)^3} \leftarrow \text{Density of states}$$

Additional notes on the right side of the slide:

$$\sum_{\epsilon} \rightarrow \int g(\epsilon) d\epsilon$$

$$\int_0^\epsilon du u^2 = \frac{u^3}{3} \Big|_0^\epsilon = \frac{\epsilon^3}{3}$$

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So, this has a very nice x expression. The density of states is $g(\epsilon)$ and that is which is of primary importance to us is $\frac{dG}{d\epsilon}$, which is going to be half $\frac{\epsilon^2}{h^3}$.

divided by $\hbar \omega$ naught whole cube. We are going to work with this expression for the density of states why is it so, important to us? Because, I know that all the discrete sums over k I can replace by integration $g(\epsilon) d\epsilon$ and that is precisely what we plan to do.

The starting point then is going to be the particle number; well one can also look at the canonical grand.

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$$G(\epsilon) = \frac{1}{6} \left(\frac{\epsilon}{\hbar\omega_0} \right)^3$$

$$g(\epsilon) = \frac{dG}{d\epsilon} = \frac{1}{2} \frac{\epsilon^2}{(\hbar\omega_0)^3} \leftarrow \text{Density of states}$$

$$\sum_k \rightarrow \int g(\epsilon) d\epsilon$$

$$\ln Q_T = - \sum_k \ln(1 - z e^{-\beta\epsilon_k}) = - \int g(\epsilon) d\epsilon \ln(1 - z e^{-\beta\epsilon})$$



Let us look at the grand canonical partition function and the grand canonical partition function is given by minus sum of a $k \ln(1 - z e^{-\beta\epsilon_k})$ which is going to be minus integral $g(\epsilon) d\epsilon \ln(1 - z e^{-\beta\epsilon})$. Now, remember we also have to separate out the ground state that is the half $\hbar \omega$.

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$$g(\epsilon) = \frac{dG}{d\epsilon} = \frac{1}{2} \frac{\epsilon}{(\hbar v)^3}$$

$\{\mathbf{n}\} = \{n_1, n_2, n_3, \dots\}$

$$\Rightarrow \ln Q_+ = - \sum_{\{\mathbf{n}\}} \ln(1 - z e^{-\beta \epsilon_n}) = - \int g(\epsilon) d\epsilon \ln(1 - z e^{-\beta \epsilon})$$

$$N = \sum_n \frac{1}{z^{-1} e^{\beta \epsilon_n} - 1} = \int g(\epsilon) d\epsilon \frac{1}{z^{-1} e^{\beta \epsilon} - 1}$$

$g(\epsilon) = \frac{1}{2} \frac{\epsilon^2}{(\hbar v)^3}$

$$= \frac{1}{2} \frac{1}{(\hbar v)^3} \int d\epsilon \frac{\epsilon^2}{z^{-1} e^{\beta \epsilon} - 1}$$



So, here one has to be careful because, the sum over k is now going to be replaced by the sum over n , where this set is essentially equivalent to $n_1 \times n_2 \times n_3$ then I have $n_1 \times n_2 \times n_3$ so on and so forth right. But we will simply write down this and not separate out the ground state right now we will not worry about that. In fact, we in the calculation that we want to do later on, we do not need this grand canonical partition function we want to calculate the critical temperature first.

The critical temperature for that we need for the critical temperature for the Bose Einstein condenser to appear in such a system.

Now, for that I need the total particle number and the total particle number is given by sum over n_1 over z inverse e to the power $\beta \epsilon_n$ minus 1 and this is going to be integral $g(\epsilon) d\epsilon \frac{1}{z^{-1} e^{\beta \epsilon} - 1}$, that we plugin the

expression for g ϵ ϵ which was half 1 over h bar ω naught whole cube times ϵ ϵ square.

So, I have a half factor, 1 over h bar ω naught whole cube and then I have integral of d ϵ ϵ square divided by z inverse e to the power β ϵ minus 1 .

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$$\begin{aligned}
 N &= \frac{1}{h} \int_0^\infty \frac{\epsilon^2}{z^{-1} e^{\beta \epsilon} - 1} d\epsilon \\
 &= \frac{1}{2} \left(\frac{k_B T}{h \omega_0} \right)^3 \int_0^\infty d\epsilon \frac{\epsilon^2}{z^{-1} e^{\beta \epsilon} - 1} \quad (x = \beta \epsilon) \\
 &= \frac{1}{2} \left(\frac{k_B T}{h \omega_0} \right)^3 \int_0^\infty \frac{d(\beta \epsilon)}{\beta} \frac{(\beta \epsilon)^2}{z^{-1} e^{\beta \epsilon} - 1} = \frac{1}{2} \left(\frac{k_B T}{h \omega_0} \right)^3 \int_0^\infty dx \frac{x^2}{z^{-1} e^x - 1} \\
 &= \left(\frac{k_B T}{h \omega_0} \right)^3 \frac{1}{2} \int_0^\infty dx \frac{x^2}{z^{-1} e^x - 1} = \left(\frac{k_B T}{h \omega_0} \right)^3 \frac{1}{2} \int_0^\infty dx \frac{x^2}{e^x - z} \rightarrow S(z) \\
 &\quad \int_0^\infty \frac{x^2}{e^x - z} dx = \sum_{k=1}^{\infty} \frac{z^k}{k^3} \\
 &\quad z \rightarrow 1 \quad \int_0^\infty \frac{x^2}{e^x - 1} dx = \sum_{k=1}^{\infty} \frac{1}{k^3} = \zeta(3)
 \end{aligned}$$



This integral, now I can substitute x is equal to $\beta \epsilon$ and if x is equal to $\beta \epsilon$ you see, this means that, I have 1 over h naught h bar ω naught whole cube integration d of $\beta \epsilon$ ϵ square. I have divided by β and I have $\beta \epsilon$ square over z inverse e to the power $\beta \epsilon$ minus 1 divided by β square,

So that the expression takes a nice form ω naught whole cube integral 0 to infinity d x x square sorry, x square z inverse e to the power x minus 1 . And this is $k_B T$ over h naught

omega whole cube half of 0 to infinity d x x square z inverse e to the power x minus 1, but this form of the integral is very very familiar to me.

So, I know that this is going to be $k_B T \hbar \omega$ whole cube f of 3 plus z right. Now, clearly as you decrease the temperature your z also changes. So, you hit upon the limit where this function will have a limiting value of if you recall that f_m plus of z is sum over k equal to 1 to infinity, I have z to the power k divided by k to the power m and when I hit z to 1, I have f_m plus 1 going to be sum over k equal to 1 to infinity, 1 over k to the power m which is zeta m the Riemann zeta function.

So, this value of this function, now goes and hits the upper bound which is zeta of 3.

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$$N = \left(\frac{k_B T}{\hbar \omega_0} \right)^3 \zeta(3)$$
 Critical Temperature at which the Condensate starts to appear.

$$\zeta^m(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^m}$$

$$\zeta^m(1) = \sum_{k=1}^{\infty} \frac{1}{k^m} = \zeta^m$$

$$\zeta^3(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^3}$$

$$\frac{N_e}{N} = 1 \quad \text{For } T > T_c$$

$$\frac{N_e}{N} = \left(\frac{k_B T}{\hbar \omega_0} \right)^3 \zeta^3(x) \quad \text{For } T < T_c$$

$$\frac{N_e}{N} = \left(\frac{k_B T}{\hbar \omega_0} \right)^3 \zeta^3(1) = \left(\frac{k_B T}{\hbar \omega_0} \right)^3 \zeta^3(3)$$

$$\zeta^3(3) = \frac{1}{(k_B T_c)^3}$$

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So, your temporal the condition that the condensate starts to appear is given by N is going to be $k_B T_c \frac{h \bar{\omega}}{2\pi}^3 \zeta(3)$ and we put a subscript over here that denotes that this equation essentially gives me the critical temperature, at which the condensate starts to appear.

So, essentially it is at this temperature, you have the particles starting to populate the k equal to 0 momentum state. The ground sorry, but the k equal to 0, but the ground state of the system because it is no longer a free particle system one has to keep that in mind. Therefore, using our analysis that we did for the free particle gas, we know that in the excited states if I just look at this fraction N_ϵ divided by N the total number of particle this is going to be 1 for T greater than T_c .

So, once again then when you have high temperatures you will have $k_B T_c$ sorry, $k_B T$ over $h \bar{\omega}^3 \zeta(3)$, in this case you will have this equation that is valid and you have to determine the fugacity from this relation and that effectively tells you that z is to the lowest order, I know that $f^3 + z$ is going to be z to the lowest order. So, that z is going to be N times $h \bar{\omega}^3 k_B T^3$, this is going to be to the to the lowest order.

For T less than T_c , I have $f^3 + z$ being substituted by $\zeta(3)$. So, that you have n_ϵ for T less than T_c , one can do the very simple calculation, we will do it on the side and plug it in there N_ϵ over N is going to be I have $k_B T$ over $h \bar{\omega}^3 \zeta(3)$ divided by N . And if you see that this quantity is going to be using this relation I have $\zeta(3)$ if I use this relation over here, I write down essentially $\zeta(3)$ divided by N $1/h \bar{\omega}^3$ is going to be $1/k_B T_c^3$.

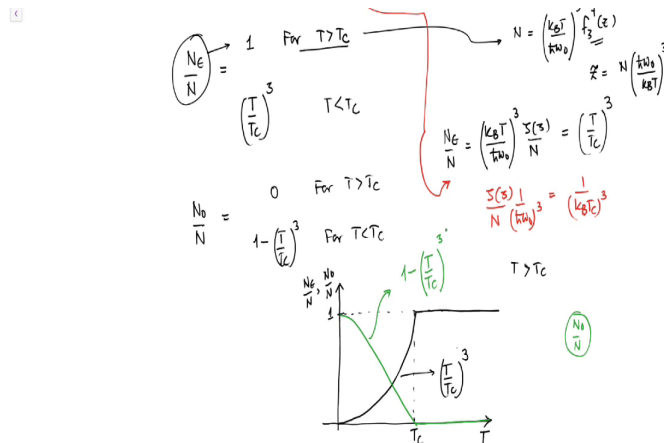
So, that this expression becomes T/T_c^3 . Remarkably, you see this factor has now changed, for an ideal Bose gas this factor was T/T_c raised to the power 3/2, but this is now T/T_c raised to the power 3 and this factor solely depends on the density of states. When we basically intuitively said that how why does a specific heat of an ideal Bose

gas near 0 temperature scales as T to the power $3/2$, we said that look I can excite particles for finite temperatures,

I can excite them and they are at most going to get energy levels go to energy levels with the momentum values which is k determined by $\hbar^2 k^2 / 2m$ is equal to $k_B T$. However, it should all and then we said that the total energy was volume times $k_B T$ raised to the power $d/2$ sorry $k_B T$ raised to the power d times $k_B T$, because each of these particles carry an thermal energy $k_B T$, but this $k_B T$ raised to the power d follows from the density of states.

So, even though you can still be in 3 dimension, but as you are seeing in this example my value of d the exponent that comes in is clearly different it is no longer $3/2$, but it is 3 and that is solely the property of density of states that you should keep in mind.

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For temperature for the ground state N_0/N is going to be 0 for T greater than T_c and it follows from this expression is going to be $1 - (T/T_c)^3$ for T less than T_c .

So, one can of course, plot this now. So, as we did for the free particle case we can plot this fraction of N_{exc}/N and N_0/N as a function of temperature. So, this is my T_c and this is my T . So, I know that for T greater than T_c my ratio of N_{exc}/N is unity. So, this remains like this and as I cross the critical temperature this expression follows T/T_c , let us write it here $(T/T_c)^3$.

In contrast, the fraction N_0/N the number of particles populating the ground state is 0 for all temperatures below T_c , because you can accommodate these particles in the excited states, and as you keep on reducing the temperature closer to below T_c , then essentially you start populating the ground state more and more, so that at T equal to 0 this ratio is 1 and therefore, you have a nice plot that goes.

So, this is let us do it a little bit more carefully; that goes like this and this is $1 - (T/T_c)^3$.