

Statistical Mechanics
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Lecture - 61
General Treatment of a Bose gas - Part 01

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$$\frac{C}{Nk_B} = 12 \frac{S(4)}{S(2)} - 9 \frac{S(3)}{S(2)}$$

At $T=T_c$, Specific Heat at $T=T_c$ when approaching from T_c^+

$$\frac{C}{Nk_B} = 12 \frac{S(4)}{S(2)}$$

Specific Heat at $T=T_c$ approach from T_c^-

$$\Rightarrow \leftarrow$$

$$T_c$$

$$\frac{\Delta C}{Nk_B} = 12 \frac{S(4)}{S(2)} - 9 \frac{S(3)}{S(2)} - 12 \frac{S(4)}{S(2)} = -9 \frac{S(3)}{S(2)}$$

Discontinuity in specific heat at $T=T_c$.



Welcome back. So, we were looking at the discontinuity in the specific heat for a harmonically trapped Bose gas. We will come back to this issue little later, but we want to consider now.

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$g(\epsilon) = C_d \epsilon^{d-1}$
 $C_{3/2} = \frac{2\pi gV}{h^3} (2m)^{3/2} \rightarrow$ free non-relativistic gas in 3D
 $C_3 = \frac{1}{2} \left(\frac{MgT}{\hbar \omega_0} \right)^3$
 $N = \int g(\epsilon) d\epsilon \frac{1}{z^{-1} e^{\beta\epsilon} - 1} = C_d \int d\epsilon \frac{\epsilon^{d-1}}{z^{-1} e^{\beta\epsilon} - 1} \quad x = \beta\epsilon$
 $= C_d \int_0^\infty \frac{d(\beta\epsilon)}{\beta^{d-1}} \frac{(\beta\epsilon)^{d-1}}{z^{-1} e^{\beta\epsilon} - 1}$
 $= \frac{C_d}{\beta^d}$



We now want to look at when the density of state goes as $C \epsilon^\alpha$ to the power minus 1. This is a slight change in notation because recall in earlier lecture I had Z said that the density of state goes as $\epsilon^{\alpha-1}$, but it is better that to be consistent with the degrees of freedom one writes $g(\epsilon)$ as $C \epsilon^{\alpha-1}$ and we know of two particular cases when $C_{3/2}$ is going to be $2\pi gV$ over h^3 twice $m^{3/2}$.

And this is the case for a free non relativistic gas in 3 dimension and we also know for C_3 which is the case we are looking at harmonically trapped gas and in this case this was $k_B T$

over $h \bar{\omega}$ naught whole cube half of this. So, idea is to take this general structure of the density of states where it depends on some exponent α right to work our way through.

So, then the particle number is integral $g(\epsilon) d\epsilon Z^{-1} e^{-\beta \epsilon}$ to the power α minus 1 and this gives me $C_\alpha \int d\epsilon \epsilon^{\alpha-1} Z^{-1} e^{-\beta \epsilon}$ to the power α minus 1. In this case again we use the transformation of variables which means we substitute x is equal to $\beta \epsilon$ to give me $d\epsilon = \beta^{-1} dx$ and then I have $\beta^{-1} dx$ raised to the power α minus 1 I have $Z^{-1} e^{-x}$ to the power α minus 1 and I have β^{-1} to the power α minus 1 and $1/\beta$.

So, that the expression takes the form $\beta^{-\alpha}$, one β cancels with the minus 1 β to the power minus 1 that you see over here, this β cancels with this and you are left out with C_α divided by $\beta^{\alpha-1}$ to the power α .

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$$\begin{aligned}
 &= C_\alpha \int_0^\infty d\epsilon \frac{(\beta \epsilon)^{\alpha-1}}{\beta^{\alpha-1} \epsilon^{\alpha-1} e^{\beta \epsilon} - 1} \\
 &= \frac{C_\alpha}{\beta^{\alpha-1}} \int_0^\infty dx \frac{x^{\alpha-1}}{e^x - 1} \quad \int_0^\infty \frac{x^{\alpha-1}}{e^x - 1} dx = \Gamma(\alpha) \zeta(\alpha) \\
 &= \frac{C_\alpha \Gamma(\alpha)}{\beta^{\alpha-1}} \zeta(\alpha) \\
 N &= \frac{C_\alpha \Gamma(\alpha)}{\beta^{\alpha-1}} \zeta(\alpha)
 \end{aligned}$$



And your integral is dx , x to the power $\alpha - 1$ Z inverse e to the power $x - 1$. Now, see this integral is related to my integrals that we had defined f_m plus of Z which is 1 over $m - 1$ factorial 0 to infinity dx x to the power $m - 1$ Z inverse e to the power $x - 1$.

Here if you compare these two integrals then you see that at factor of 1 by $m - 1$ is missing, but that is easily remedied. I know that $\Gamma(\alpha)$ is $\alpha - 1$ factorial. So, I am going to bring in a $\Gamma(\alpha)$ in the numerator and a $\Gamma(\alpha)$ in the denominator which makes it like this and this is now f_α plus of Z . So, that particle number is given by $C \Gamma(\alpha) \beta^\alpha f_\alpha$ plus of Z .

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$$N = \frac{C_\alpha \Gamma(\alpha)}{\beta^\alpha} \int_0^\infty \frac{e^{-x} x^{\alpha-1}}{Z} dx \quad \alpha > 1$$
 Ideal Bose Gas in 1D.

For $T < T_c$ $Z \rightarrow 1$ $\int_0^\infty e^{-x} x^{\alpha-1} dx \rightarrow \Gamma(\alpha)$

$$N = \frac{C_\alpha \Gamma(\alpha)}{\beta^\alpha} \Gamma(\alpha) \Rightarrow \beta_c^\alpha = \frac{C_\alpha \Gamma(\alpha) \Gamma(\alpha)}{N}$$
 Critical temperature at which the BE condensate appears. Condensation is in momentum space.



Now, of course, it is a standard it is just two steps now. So, if I now say that α is greater than 1 then it follows that for $T < T_c$ means, fugacity hits the value 1, in which case your $f_\alpha + Z$ goes to ζ_α .

So, that I can use this to determine the critical temperature at which the condensate is going to appear and that is given by βC_α raised to the power $\alpha \zeta_\alpha$, which implies we will use this later on βC_α is going to be $C_\alpha \gamma_\alpha \zeta_\alpha$ divided by N .

So, this defines the critical temperature at which the condensate the BE condensate appears and again this condensation is in momentum space not in the real space. Now, before we go further it is very interesting now that for a ideal Bose gas in 1D. So, let us just discuss this very briefly.

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appear. — 1 is in numerator space.

Ideal Bose gas in 1D

$$g(\epsilon) \sim \epsilon^{-1/2} \Rightarrow d = 1/2$$

$$N \sim \int_{1/2}^{\infty} z^{-\alpha} \epsilon^{-1/2} d\epsilon \quad Z \rightarrow 1 \quad \int_{1/2}^{\infty} z^{-\alpha} \epsilon^{-1/2} d\epsilon \rightarrow \infty \quad d < 1$$

$$N = \frac{C \Gamma(\alpha)}{\beta^\alpha} \int_{1/2}^{\infty} z^{-\alpha} \epsilon^{-1/2} d\epsilon$$

$$E = \int g(\epsilon) d\epsilon \frac{\epsilon}{z^{-\alpha} e^{\beta\epsilon} - 1}$$



For an ideal Bose gas in 1D my $g(\epsilon)$ goes as $\epsilon^{-1/2}$ which means and this implies that α is going to be half in our description that we have written down over here. Therefore, this means that N is proportional to $\int_{1/2}^{\infty} z^{-\alpha} \epsilon^{-1/2} d\epsilon$, but the curious thing is that as Z tends to 1, $\int_{1/2}^{\infty} z^{-\alpha} \epsilon^{-1/2} d\epsilon$ tends to infinity the series does not converge because α is less than 1.

And therefore, for a 1D ideal Bose gas you cannot have a Bose Einstein condensation. Now, let us quickly continue with this. So, this is my N , N is $C \Gamma(\alpha) / \beta^\alpha \int_{1/2}^{\infty} z^{-\alpha} \epsilon^{-1/2} d\epsilon$. The energy is $\int g(\epsilon) d\epsilon \frac{\epsilon}{z^{-\alpha} e^{\beta\epsilon} - 1}$.

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$$\begin{aligned}
 E &= \int g(\epsilon) d\epsilon \frac{\epsilon}{z^{-1} e^{\beta \epsilon} - 1} \\
 &= C_{\alpha} \int d\epsilon \frac{\epsilon^{\alpha-1} \cdot \epsilon}{z^{-1} e^{\beta \epsilon} - 1} \\
 &= \frac{C_{\alpha} \Gamma(\alpha+1)}{\beta^{\alpha+1} \Gamma(\alpha+1)} \int_0^{\infty} dx \frac{x^{\alpha}}{z^{-1} e^x - 1} \\
 E &= \frac{C_{\alpha} \Gamma(\alpha+1)}{\beta^{\alpha+1}} \zeta_{\alpha+1}^+(z)
 \end{aligned}$$

$x = \beta \epsilon$
 $\Gamma(\alpha+1) = \alpha!$

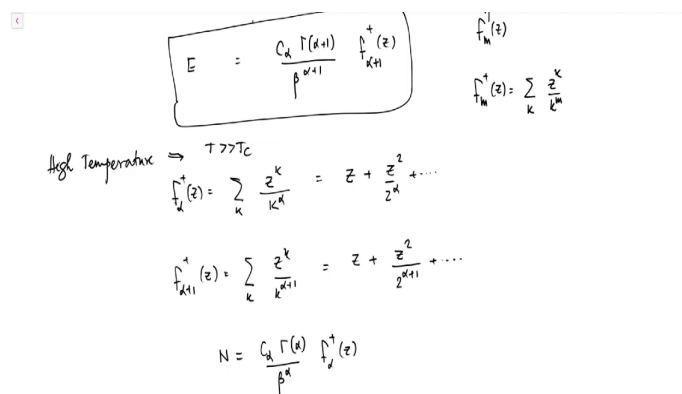


Which we will write down again as C alpha integral d epsilon epsilon to the power alpha minus 1 times an epsilon that comes epsilon to the power alpha minus 1 comes from the g epsilon and the epsilon is already there because it is an average of the energy and I have this. If I now substitute x equal to beta epsilon then I see that this answer is going to be C alpha is going to be beta raised to the power alpha plus 1 0 to infinity dx x to the power alpha divided by Z inverse e to the power x minus 1.

So, again comparing with the integrals that we had f plus integrals the Boson Bose integrals that we had defined I am missing a factor of 1 by alpha factor alpha factorial. So, gamma of alpha plus 1 is going to be alpha factorial. I bringing a gamma of alpha plus 1 and I bringing a gamma of alpha plus 1.

And that gives me that the energy is going to be $C \alpha \Gamma(\alpha + 1)$ divided by β raised to the power $\alpha + 1$ of $\alpha + Z$ right. So, I have two relations. One is the one this and sorry this has to be $\alpha + 1$, terribly sorry and I have this. The high temperature limit is the one which you are going interested in.

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$$E = \frac{C_\alpha \Gamma(\alpha+1) f_\alpha^+(z)}{\beta^{\alpha+1}}$$

$$f_\alpha^+(z) = \sum_k \frac{z^k}{k^\alpha}$$

High Temperature $\Rightarrow T \gg T_c$

$$f_1^+(z) = \sum_k \frac{z^k}{k^1} = z + \frac{z^2}{2} + \dots$$

$$f_{\alpha+1}^+(z) = \sum_k \frac{z^k}{k^{\alpha+1}} = z + \frac{z^2}{2^{\alpha+1}} + \dots$$

$$N = \frac{C_\alpha \Gamma(\alpha)}{\beta^\alpha} f_\alpha^+(z)$$



And for that I am going to use the high temperature expansion of the functions f_α of Z , f_α of Z and in this particular case this becomes sum over k Z to the power k , k to the power α , so that $f_{\alpha+1}$ of Z high temperatures which of course, always means that T is much much larger than T_c .

You are far away from the critical temperature and you have the expansion as sum over k Z to the power k α to the power k , sorry k to the power α which is Z plus Z square over 2 to the power $\alpha + 1$ plus higher order terms. And $f_{\alpha+1}$ of Z is going to be sum

over $k Z$ to the power k , k to the power $\alpha + 1$ which is going to be $Z + Z^2$ over 2 to the power $\alpha + 1$ plus higher order terms.

So, starting again from the expression for the particle number which I had $C \alpha \gamma$ α raised to the power β to the power $\alpha + 1$ of Z and the standard trick is that the fugacity must be determined from this relation.

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$$N = \frac{C \alpha \Gamma(\alpha)}{\beta^\alpha} \int_0^1 z^\alpha dz$$

$$\frac{\beta^\alpha N}{C \alpha \Gamma(\alpha)} = z + \frac{z^2}{2} + \dots$$

$$z = \frac{\beta^\alpha N}{C \alpha \Gamma(\alpha)} - \frac{z^2}{2} + \dots$$

$$z_1 = \frac{\beta^\alpha N}{C \alpha \Gamma(\alpha)}$$

$$z_2 = \frac{\beta^\alpha N}{C \alpha \Gamma(\alpha)} \left[1 - \frac{\beta^\alpha N}{C \alpha \Gamma(\alpha)} \frac{1}{2} + \dots \right]$$

$$N = \frac{C \alpha \Gamma(\alpha)}{\beta_c^\alpha} z^\alpha$$

$$\frac{N}{C \alpha \Gamma(\alpha)} = \frac{z^\alpha}{\beta_c^\alpha}$$



So, in order to determine the fugacity since I am at high temperatures, temperature is far away from my critical temperature I write this as $\beta \alpha C \alpha \gamma \alpha Z + Z^2$ raised to the power 2 to the power $\alpha + 1$ plus higher order term. Now, a perturbative expansion of the fugacity can be done. So, that to the lowest order I have $Z = 1$ as β to the power α and $C \alpha \gamma \alpha$.

So, let us write down the equation that I am going to use. That means, I can write down Z as β to the power $\alpha N C \alpha \gamma \alpha$ minus Z^2 over 2 to the power α plus higher order terms. And you can immediately see if I use again if I use the perturbative expansion then to the lowest order I ignore all higher orders of Z , I have β to the power α times $N C \alpha \gamma \alpha$.

And Z^2 is β to the power α times $N C \alpha \gamma \alpha$ $1 - \beta \alpha N C \alpha \gamma \alpha$ times 2 to the power α plus higher order terms. Now, you see $C \alpha$, $\gamma \alpha$ are all these quantities which are essentially a little bit tricky to measure. I mean I do not know I can only have an indirect idea or I can start from a model and I can try to figure out, but in principle here I can make my life easy and I can replace this over here.

So, $C \alpha \gamma \alpha$ divided by N , the condition for the condensation to happen at the temperature was given by $C \alpha \gamma \alpha \beta C \alpha$ times $\zeta \alpha$. So, this means, N by $C \alpha \gamma \alpha$ is going to be $\zeta \alpha$ divided by $\beta C \alpha$.

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$$\begin{aligned}
 Z &= \frac{\beta^\alpha N}{C^\alpha \Gamma(\alpha)} \left[1 - \frac{\zeta(\alpha)}{2^\alpha} \left(\frac{\beta}{Tc}\right)^\alpha + \dots \right] \\
 Z &= \frac{\beta^\alpha N}{C^\alpha \Gamma(\alpha)} \left[1 - \frac{\zeta(\alpha)}{2^\alpha} \left(\frac{Tc}{T}\right)^\alpha + \dots \right] \\
 E &= \frac{C^\alpha \Gamma(\alpha+1)}{\beta^{\alpha+1}} f_{\alpha+1}^+(Z) \\
 &= \frac{C^\alpha \Gamma(\alpha+1)}{\beta^{\alpha+1}} \left[Z + \frac{Z^2}{2^{\alpha+1}} + \dots \right]
 \end{aligned}$$



So, I will just write down this. $C^\alpha \Gamma(\alpha) \times [1 - \zeta(\alpha) \beta^\alpha / (2^\alpha T c)^\alpha + \dots]$ divided by $\beta^\alpha N$ gives me $\beta^\alpha N / [C^\alpha \Gamma(\alpha) (1 - \zeta(\alpha) \beta^\alpha / (2^\alpha T c)^\alpha + \dots)]$.

So, please note that you have T in the denominator and again you might have the desire to put T to 0 here and say claim that this goes to infinity, but we are in the high temperature limit. So, therefore, T actually you cannot take the limit of T to 0, but rather you should take the limit of T to infinity in which case of course, we recover the first result.

What about the energy? Energy was $C^\alpha \Gamma(\alpha+1) \beta^{\alpha+1} f_{\alpha+1}^+(Z)$ and I had $f_{\alpha+1}^+(Z)$ from the particle number equation and that Z I want to substitute over here. $C^\alpha \Gamma(\alpha+1) \beta^{\alpha+1} [Z + \frac{Z^2}{2^{\alpha+1}} + \dots]$

alpha gamma alpha plus 1 beta of alpha plus 1 and then if I expand this I have Z plus Z square divided by 2 to the power alpha plus 1 plus higher order terms.

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$$\begin{aligned}
 E &= \frac{C_\alpha \Gamma(\alpha+1)}{\beta^{\alpha+1}} f_{\alpha+1}(z) \\
 &= \frac{C_\alpha \Gamma(\alpha+1)}{\beta^{\alpha+1}} \left[z + \frac{z^2}{2^{\alpha+1}} + \dots \right] \\
 &= \frac{C_\alpha \Gamma(\alpha+1)}{\beta^{\alpha+1}} z \left[1 + \frac{z}{2^{\alpha+1}} + \dots \right] \\
 &= \frac{C_\alpha \Gamma(\alpha+1)}{\beta^{\alpha+1}} \frac{\beta^\alpha N}{C_\alpha \Gamma(\alpha)} \left[1 - \frac{\zeta(\alpha)}{2^\alpha} \left(\frac{T_c}{T} \right)^\alpha \right] \left[1 + \frac{\beta^\alpha N}{C_\alpha \Gamma(\alpha)} \frac{1}{2^{\alpha+1}} + \dots \right] \\
 &= \frac{N}{\beta} \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} \left[1 - \frac{\zeta(\alpha)}{2^\alpha} \left(\frac{T_c}{T} \right)^\alpha \right] \left[1 + \frac{\beta^\alpha N}{C_\alpha \Gamma(\alpha)} \frac{1}{2^{\alpha+1}} + \dots \right]
 \end{aligned}$$



So, this is C alpha gamma alpha plus 1 raised to the power beta alpha plus 1 times Z 1 plus Z raised to the power 2 to the power alpha plus 1 and all the higher orders. Z now I use from this relation. See then Z is given by C alpha gamma alpha plus 1 divided by beta raised to the power alpha and beta raised to the power alpha sorry, the denominator has to be alpha plus 1. The numerator is beta raised to the power alpha then I have a N then I have a C alpha and they have I have a gamma alpha.

The next is zeta alpha over 2 to the power alpha T c over T raised to the power alpha. I hope I had a gap times 1 plus beta alpha N divided by C alpha gamma alpha 1 over 2 to the power alpha plus 1 and of course, you will have multiplying this plus higher order term.

So, this this expression is going to again enter over here because that is a value of this, but we will ignore because after all it is a product of this term and this term. So, we will write this as C alpha, lot of things cancel out. So, first let us look at the cancellations here. C alpha, C alpha cancels out.

A beta alpha cancels with beta alpha and then I am left out with N over beta times gamma alpha plus 1 divided by gamma alpha 1 minus zeta alpha raise to the power 2 to the power alpha T c over T raised to the power alpha 1 plus beta alpha beta to the power alpha N C alpha gamma alpha 1 over 2 to the power alpha plus 1 and higher order terms.

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$$\begin{aligned}
 &= \frac{N}{\beta} \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} \left[1 - \frac{S(\omega)}{2^\alpha} \left(\frac{T_c}{T}\right)^\alpha \right] \left[1 + \frac{\beta^N}{C_\alpha \Gamma(\alpha)} \frac{1}{2^{\alpha+1}} + \dots \right] \\
 &= \frac{N}{\beta} \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} \left[1 - \frac{S(\omega)}{2^\alpha} \left(\frac{T_c}{T}\right)^\alpha + \dots \right] \left[1 + \frac{S(\omega)}{2^{\alpha+1}} \left(\frac{\beta}{\beta_c}\right)^\alpha + \dots \right] \beta^{\frac{1}{T}} \\
 &= N k_B T \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} \left[1 - \frac{S(\omega)}{2^\alpha} \left(\frac{T_c}{T}\right)^\alpha + \frac{S(\omega)}{2^{\alpha+1}} \left(\frac{T_c}{T}\right)^\alpha + \dots \right] \\
 &= N k_B T \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} \left[1 - \frac{S(\omega)}{2^\alpha} \left(\frac{T_c}{T}\right)^\alpha \left(1 - \frac{1}{2}\right) + \dots \right]
 \end{aligned}$$



N over beta alpha plus 1 divided by gamma alpha 1 minus zeta alpha 2 to the power alpha T c over T raised to the power alpha plus higher order terms which we always have and should not forget. And then again you see that N is going to be C alpha gamma alpha beta C alpha

zeta alpha. So, that N over C alpha gamma alpha is going to be 1 plus zeta alpha 2 to the power alpha plus 1 beta over beta C raised to the power alpha plus higher order terms.

Now, N by beta is N k B T gamma alpha plus 1 over gamma alpha. Let us do this. 1 minus zeta alpha 2 to the power alpha T c over T c over T raised to the power alpha and then you have plus 1 zeta alpha over 2 to the power alpha plus 1 T c over T raised to the power alpha plus higher order term because beta over beta C is essentially T c over T since beta goes as 1 over T.

Therefore, I have N k B T gamma alpha plus 1 over gamma alpha is going to be 1 minus zeta alpha 2 to the power alpha T c over T raised to the power alpha 1 minus half of because of this additional factor.

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$$= N k_B T \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} \left[1 - \frac{5(\alpha)}{2^\alpha} \left(\frac{T_c}{T}\right)^\alpha \left(1 - \frac{1}{2}\right)^{\frac{1}{2}} + \dots \right]$$

$$E = N k_B T \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} \left[1 - \frac{5(\alpha)}{2^{\alpha+1}} \left(\frac{T_c}{T}\right)^\alpha + \dots \right] \quad \begin{matrix} \Gamma(\alpha+1) = \alpha! \\ \Gamma(\alpha) = (\alpha-1)! \end{matrix}$$

$$E = \alpha N k_B T \left[1 - \frac{5(\alpha)}{2^{\alpha+1}} \left(\frac{T_c}{T}\right)^\alpha + \dots \right] \quad \left[\frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} = \frac{\alpha!}{(\alpha-1)!} = \alpha \right]$$

$$E = \alpha N k_B T \quad \begin{matrix} \alpha = 3 & g(\epsilon) \sim \epsilon^2 \\ E = 3 N k_B T \\ \alpha = 3/2 & g(\epsilon) \sim \epsilon^{1/2} \end{matrix}$$



And this gives me the energy as $N k_B T \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha + 1 - \zeta)}$ $\frac{\alpha}{2}$ to the power $\alpha + 1$ $\frac{T_c}{T}$ raised to the power α . Since this is half, I get a factor $\alpha + 1$ plus higher order terms. Now, $\Gamma(\alpha + 1)$ is $\alpha!$, $\Gamma(\alpha)$ is $(\alpha - 1)!$. So, $\alpha!$, so, this ratio of $\Gamma(\alpha + 1)$ divided by $\Gamma(\alpha)$ is $\alpha!$ divided by $(\alpha - 1)!$ which is just plain α .

So, that E over; so, first we write down this as E is going to be $\alpha N k_B T$ times $1 - \zeta$ of $\frac{\alpha}{2}$ to the power $\alpha + 1$ $\frac{T_c}{T}$ raised to the power α plus has higher order terms. So, at really high temperatures you recover the classical result of E is $\alpha N k_B T$. And this term, the term that you see over here is the first order correction as you come down in temperature. This is the first correction that you will notice right

So, for example, if α is equal to 3 g ϵ_{psa} will go as ϵ_{psa}^2 which is our case for a harmonically trapped Bose gas and in which case we saw that the energy was $3 N k_B T$.

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$$E = N k_B \frac{1}{\Gamma(\alpha)} \left[1 - \frac{1}{2^{\alpha+1}} \left(\frac{T_c}{T} \right)^\alpha \right]$$

$$E = \alpha N k_B T \left[1 - \frac{\zeta(\alpha) \left(\frac{T_c}{T} \right)^\alpha}{2^{\alpha+1}} \right]$$

$$\frac{\Gamma(\alpha+1)}{\Gamma(\alpha)} = \frac{\alpha!}{(\alpha-1)!} = \alpha$$

$E = \alpha N k_B T$

$\alpha = 3 \quad g(\epsilon) \sim \epsilon^2$
 $E = 3 N k_B T$

$\alpha = 3/2 \quad g(\epsilon) \sim \epsilon^{1/2}$
 $E = \frac{3}{2} N k_B T$



For alpha is equal to 3 half g epsa goes as epsa to the power half and E becomes 3 half N k B T.