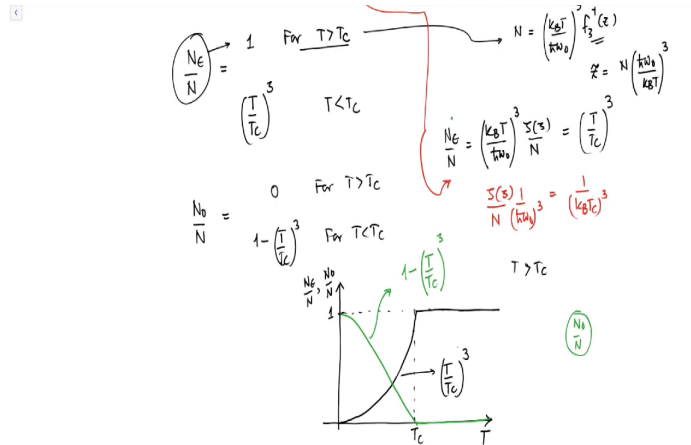


Statistical Mechanics
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Lecture - 60
Specific Heat of a Harmonically Trapped Bose Gas

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So, we have seen how the fraction behave N_ϵ over n and N_0 over N behaves. We now want to look at the energy.

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$$\begin{aligned}
 U &= \sum \epsilon_n \langle n \rangle \rightarrow \int g(\epsilon) d\epsilon \frac{\epsilon}{z^{-1} e^{\beta \epsilon} - 1} \\
 U &= \frac{1}{2} \frac{1}{(\hbar \omega_0)^3} \int_0^\infty d\epsilon \frac{\epsilon^3}{z^{-1} e^{\beta \epsilon} - 1} \quad x = \beta \epsilon \\
 &= \frac{1}{2} \frac{1}{(\hbar \omega_0)^3} \int_0^\infty \frac{1}{\beta} d(\beta \epsilon) \frac{(\beta \epsilon)^3}{z^{-1} e^{\beta \epsilon} - 1} \\
 &= \frac{1}{2} \frac{1}{(\hbar \omega_0)^3} \frac{1}{\beta^4} \int_0^\infty dx \frac{x^3}{z^{-1} e^x - 1} = 3 \left(\frac{k_B T}{\hbar \omega_0} \right)^3 k_B T \frac{1}{2 \cdot 15} \int_0^\infty \frac{x^3}{z^{-1} e^x - 1}
 \end{aligned}$$



And the energy is as usual the energy is sum over epsilon n average of n which is the occupation number and this becomes a continuous using the continuous density of state this goes to g epsilon d epsilon times epsilon divided by Z inverse e to the power beta epsilon minus 1. So, that we write down this as g epsilon is half 1 over h bar omega naught whole cube integral 0 to infinity d epsilon epsilon cube epsilon square times epsilon divided by Z inverse e to the power beta epsilon minus 1.

Now, as usual we will say will use the transformation of variable x equal to beta epsilon. So, that I have 0 to infinity 1 over beta d of beta epsilon and then I have an epsilon cube over here. So, that makes it beta epsilon whole cube and I have 1 over beta cube Z inverse e to the power beta epsilon minus 1, sorry there is a cube outside and over h bar omega naught.

So, this becomes half the beta cube and beta gives you beta to the power 4. So, I have h bar omega naught whole cube 1 over beta to the power 4, 0 to infinity dx x cube Z inverse e to the power x minus 1 which we rewrite as k B T over h bar omega naught whole cube times another factor of k B T and then I am left out with half 0 to infinity dx x cube Z inverse e to the power x minus 1.

Clearly, this integral is related to my function f m plus of Z which was 1 over m minus 1 factorial 0 to infinity dx x to the power m minus 1 Z inverse e to the power x minus 1. Now, you see that whatever I have within the integrant tells me that this is f 4 plus of z, but the factorial does not match. This is the 3 factorial for f 4 I have a half that is easily remedied by bringing a 3 factor in the denominator as well as in the numerator.

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$$= \frac{1}{2} \frac{1}{(\hbar\omega_0)^3} \frac{1}{\beta^4} \int_0^\infty dx \frac{x^3}{z e^x - 1} = \frac{1}{2} \left(\frac{k_B T}{\hbar\omega_0} \right)^3 \int_0^\infty \frac{x^3}{z e^x - 1} dx$$

$$U = 3 k_B T \left(\frac{k_B T}{\hbar\omega_0} \right)^3 \int_0^\infty \frac{x^3}{z e^x - 1} dx$$

$\int_0^\infty \frac{x^3}{z e^x - 1} dx \xrightarrow{z \rightarrow 1} \zeta(4)$

$$T < T_C \quad z \rightarrow 1$$

$$U = 3 k_B T \zeta(4) \left(\frac{k_B T}{\hbar\omega_0} \right)^3$$

$$U = 3 \zeta(4) k_B T \left(\frac{k_B T}{\hbar\omega_0} \right)^3 \sim T^4$$



So, I have $3 k_B T$ over $h \bar{\omega}$ naught whole cube and I have f_4 plus of Z and this is my energy I am looking at. Now, the idea is for T less than T_c , I know Z goes to 1. Therefore, my f_4 plus of Z since m is greater than 1 as Z tends to 1, this function value goes to zeta of 4.

So, I will replace this by zeta of 4 where I write down this as $3 k_B T$ zeta 4 and then I have $k_B T$ over $h \bar{\omega}$ naught whole cube. So, that U is equal to let us say $3 \zeta_4 k_B T$ and $k_B T$ over $h \bar{\omega}$ naught whole cube which implies the energy the internal energy scales with T to the power 4.

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$$\begin{aligned}
 T < T_c \quad Z \rightarrow 1 \\
 U &= 3 k_B T \zeta(4) \left(\frac{k_B T}{h \bar{\omega}_0} \right)^3 \\
 U &= 3 \zeta(4) k_B T \left(\frac{k_B T}{h \bar{\omega}_0} \right)^3 \sim T^4 \\
 C &= 3 \zeta(4) k_B \left(\frac{k_B}{h \bar{\omega}_0} \right)^3 \frac{dT}{dT} = 12 \zeta(4) k_B \left(\frac{k_B T}{h \bar{\omega}_0} \right)^3 \\
 C &= 12 k_B \zeta(4) \frac{N}{\zeta(3)} \frac{1}{T_c^3} T^3 = 12 N k_B \frac{\zeta(4)}{\zeta(3)} \left(\frac{T}{T_c} \right)^3
 \end{aligned}$$



The specific heat at constant volume is given by $3 \zeta_4$ is $\frac{dU}{dT}$. So, that I have k_B , let us keep k_B over here and then I have k_B over $h \bar{\omega}$ naught whole cube dT of T to the power 4 and that is $12 \zeta_4 k_B k_B T$ over $h \bar{\omega}$ naught whole cube. So, this

derivative brings in a factor 4 times T cube and this T cube I reobserve in the bracket to recast my equation for specific heat in this way.

Now, if you recall your N particle number was $k_B T$ over $h \bar{\omega}$ naught whole cube f_3 plus Z . For T greater than T_c from this is the equation from which you have to determine the fugacity, but for T less than T_c my life is little bit simpler because this function now becomes zeta of 3.

So, that N is equal to $k_B T$ over $h \bar{\omega}$ at T_c we will substitute for at T_c whole cube zeta of 3. Therefore, I can immediately see the expression and I can see that k_B over $h \bar{\omega}$ naught whole cube is nothing, but N over zeta 3 and 1 over T_c cube. So, my specific heat becomes $12 k_B zeta 4$ and then I have N over zeta 3 1 over T_c whole cube times T cube which takes a very simple form, which gives me $12 N k_B zeta 4$ over zeta 3 times T over T_c whole cube.

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$$\frac{C}{Nk_B} = 12 \frac{\zeta(4)}{\zeta(3)} \left(\frac{T}{T_c}\right)^3 \quad C \sim T^3 \text{ for } T < T_c$$

Exactly at $T = T_c$ $\frac{C}{Nk_B} = 12 \frac{\zeta(4)}{\zeta(3)}$

$$T > T_c \quad U = 3 k_B T \left(\frac{k_B T}{\hbar \omega_0}\right)^3 f_4^+(z) \quad \left(\frac{k_B T}{\hbar \omega_0}\right)^3 = \frac{N}{f_3^+(z)}$$

$$N = \left(\frac{k_B T}{\hbar \omega_0}\right)^3 f_3^+(z)$$



So, that C over $N k_B$ is going to be $12 \zeta(4)$ over $\zeta(3)$ times T over T_c whole cube. And exactly at T is equal to T_c , the specific heat is given by $12 \zeta(4)$ over $\zeta(3)$. The specific heat for T less than T_c would scale as T^3 for T less than T_c . What about the high temperature case? Well, for that we know that U was given by $3 k_B T$ $k_B T$ over $\hbar \omega_0$ whole cube f_4^+ of Z .

And N this is the case where we are looking at T greater than T_c and N is given by $k_B T$ over $\hbar \omega_0$ whole cube f_3^+ plus Z . So, I can now eliminate this $k_B T$ $\hbar \omega_0$ which is over here. So, I can write down $k_B T$ over $\hbar \omega_0$ whole cube as N over f_3^+ of Z .

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$$U = 3 k_B T \cdot \frac{N}{f_3^{\uparrow}(z)} f_4^{\uparrow}(z)$$

$$\frac{U}{N k_B} = 3 T \frac{f_4^{\uparrow}(z)}{f_3^{\uparrow}(z)}$$

$$\frac{C}{N k_B} = \frac{\partial}{\partial T} \left(\frac{U}{N k_B} \right)$$



And I have the expression U is equal to 3 k B T times N over f plus 3 of Z times f 4 plus of Z. So, therefore, U over N k B is going to be 3 T times f 4 plus of Z and f 3 plus of Z. So, we want to do the again repeat the elaborate calculation and its instructive to do it. The specific heat C over N k B is going to be del del T of U over N k B.

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$$\begin{aligned} \frac{C}{Nk_B} &= \frac{\partial}{\partial T} \left(\frac{U}{Nk_B} \right) \\ &= \frac{\partial}{\partial T} \left[3T \frac{f_4^+(z)}{f_3^+(z)} \right] = 3 \frac{f_4^+(z)}{f_3^+(z)} + 3T \left[\frac{f_3^+(z) \frac{df_4^+}{dT} - f_4^+(z) \frac{df_3^+}{dT}}{[f_3^+(z)]^2} \right] \\ \frac{C}{Nk_B} &= 3 \frac{f_4^+(z)}{f_3^+(z)} + 3T \frac{f_3^+(z) \frac{df_4^+}{dT} - f_4^+(z) \frac{df_3^+}{dT}}{[f_3^+(z)]^2} \quad \zeta \\ \frac{df_m^+}{dT} &= \frac{1}{z} f_{m-1}^+(z) \end{aligned}$$



This means this is going to be $\frac{\partial}{\partial T}$ of $3T$ times $\frac{f_4^+(z)}{f_3^+(z)}$ plus of Z $f_3^+(z)$ plus of Z , which simplifies to 3 times $\frac{f_4^+(z)}{f_3^+(z)}$ plus of Z divided by $f_3^+(z)$ plus of Z . First the derivative with respect to temperature and then you have plus $3T$ divided by $f_3^+(z)$ plus of Z whole square times $f_3^+(z)$ plus of Z $\frac{df_4^+}{dT}$ minus $f_4^+(z)$ $\frac{df_3^+}{dT}$ plus dT .

Let us be careful with this to see whether everything is consistent now. So, that $\frac{C}{Nk_B}$ is going to be $3 \frac{f_4^+(z)}{f_3^+(z)}$ plus of Z $f_3^+(z)$ plus of Z plus 3 times T $f_3^+(z)$ plus of Z $\frac{df_4^+}{dT}$ minus $f_4^+(z)$ $\frac{df_3^+}{dT}$ divided by $f_3^+(z)$ plus of Z square. Now, I know that $\frac{df_m^+}{dT}$ plus is $\frac{1}{z} f_{m-1}^+(z)$. This we did in the previous lectures times.

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$$\frac{C}{Nk_B} = 3 \frac{f_4^+(z)}{f_3^+(z)} + 3T \frac{f_3^+(z) \frac{d f_4^+(z)}{dz} - f_4^+(z) \frac{d f_3^+(z)}{dz}}{[f_3^+(z)]^2}$$

$\frac{1}{z} \frac{dz}{dT} = -\frac{3}{2T} \frac{f_3^+}{f_3^+ + 1/2}$

$$\frac{d f_m^+}{dT} = \frac{d f_m^+}{dz} \frac{dz}{dT}$$

$$= \left(\frac{1}{z} \frac{dz}{dT} \right) f_{m-1}^+(z)$$

$$\frac{d f_4^+}{dT} = \frac{1}{z} \frac{dz}{dT} f_3^+(z)$$

$$\frac{d f_3^+}{dT} = \frac{1}{z} \frac{dz}{dT} f_2^+(z)$$

$$N = \left(\frac{k_B T}{\hbar^3 \omega_0} \right)^3 f_3^+(z)$$



So, now, I know that $\frac{d}{dT}$ of f_m^+ is $\frac{d}{dz}$ of f_{m-1}^+ and then $\frac{dz}{dT}$. And $\frac{d f_m^+}{dT}$ is going to be $\frac{1}{z} \frac{dz}{dT} f_{m-1}^+$ as $\frac{dz}{dT}$. So, that this becomes $\frac{1}{z} \frac{dz}{dT}$ times f_{m-1}^+ of z . And this implies that $\frac{d}{dT}$ of f_4^+ is $\frac{1}{z} \frac{dz}{dT} f_3^+$. So, I have a derivative of $\frac{d}{dT}$ of f_4^+ which is $\frac{1}{z} \frac{dz}{dT} f_3^+$ and $\frac{d}{dT}$ of f_3^+ is going to be $\frac{1}{z} \frac{dz}{dT} f_2^+$.

So, we are left to determine these derivatives. Now, in the classical in the ideal Bose gas we have seen that this derivative $\frac{dz}{dT}$ is $-\frac{3}{2T} \frac{f_3^+}{f_3^+ + 1/2}$. So, word of caution is do not use this here because you have a different density of states. Please be careful in blindly using results. Instead we start from the same starting from point from where using which we derived such a relation that is to look at the particle number.

Particle number is given by for a harmonically trapped Bose gas is given by $k_B T$ over $\hbar \omega$ whole cube times f_3 of Z .

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$$N = \left(\frac{k_B T}{\hbar \omega_0} \right)^3 f_3^+(z)$$

$$\frac{d}{dT} \left(N \left(\frac{\hbar \omega_0}{k_B T} \right)^3 \right) = \frac{d}{dT} \left(f_3^+(z) \right)$$

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

$$= -3 N \frac{(\hbar \omega_0)^3}{T^4}$$

$\frac{d}{dT} f_3^+(z) = \frac{1}{z} \frac{dz}{dT} f_2^+(z)$



So, that I have N times $\hbar \omega$ over $k_B T$ whole cube is going to be f_3 of Z . Now, let us take a derivative with respect to temperature both in the left hand side as well as in the right hand side and let us look at the left hand side.

The left hand side is $\frac{d}{dT}$ of $N \left(\frac{\hbar \omega_0}{k_B T} \right)^3$ which is going to be $N \left(\frac{\hbar \omega_0}{k_B} \right)^3 \frac{d}{dT} \left(\frac{1}{T^3} \right)$ and that is a straightforward derivative. You are going to have minus 3 $N \left(\frac{\hbar \omega_0}{k_B} \right)^3 \frac{1}{T^4}$ and I have missed a k_B over here.

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$$N = \left(\frac{k_B T}{h \omega_0} \right)^3 f_3^+(z)$$

$$\frac{d}{dT} \left(N \left(\frac{h \omega_0}{k_B T} \right)^3 \right) = \frac{d}{dT} (f_3^+(z))$$

$$\frac{d}{dT} f_3^+(z) = \frac{d f_3^+(z)}{dz} \frac{dz}{dT}$$

$$= \frac{1}{z} f_2^+(z) \frac{dz}{dT}$$


$$= \frac{1}{z} \frac{dz}{dT} \cdot f_2^+(z)$$

$$\left(\frac{k_B T}{h \omega_0} \right)^3 = \frac{N}{f_3^+(z)}$$

$$\frac{d}{dT} N \left(\frac{h \omega_0}{k_B T} \right)^3 = N \left(\frac{h \omega_0}{k_B} \right)^3 \frac{d}{dT} \left(\frac{1}{T^3} \right)$$

$$= -3 N \left(\frac{h \omega_0}{k_B} \right)^3 \frac{1}{T^4}$$

$$= -\frac{3}{T} N \left(\frac{h \omega_0}{k_B T} \right)^3$$

$$= -\frac{3}{T} N \frac{f_3^+(z)}{N} = -\frac{3}{T} f_3^+(z)$$




So, that this $k_B T$ to the power 4. So, that I have minus 3 over T times N h bar omega naught divided by $k_B T$ whole cube. But, if you look at this expression then $k_B T$ h bar omega naught whole cube is going to be N divided by $f_3^+(z)$. And therefore, you have the answer minus 3 over T times N and I am going to use this expression over here noting that what I have here is just 1 over this value the left hand side.

So, that this gives me $f_3^+(z)$ divided by N and this answer is minus 3 over T $f_3^+(z)$. The right hand side is d/dT of $f_3^+(z)$ and that is going to be dz/dT of $f_3^+(z)$ times dz/dT and this derivative is $1/z^2$ plus z times dz/dT . So, that the left hand side is $1/z^2$ plus z times dz/dT times $f_2^+(z)$.

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$$\frac{1}{z} \frac{dz}{dT} = -\frac{3}{T} \frac{f_3^+(z)}{f_2^+(z)}$$

$$\frac{C}{Nk_B} = 3 \frac{f_4^+(z)}{f_3^+(z)} + 3T \frac{f_3^+(z) \frac{df_4^+(z)}{dT} - f_4^+(z) \frac{df_3^+(z)}{dT}}{[f_3^+(z)]^2}$$

$$= 3T \frac{f_3^+(z) \frac{df_4^+(z)}{dz} \frac{dz}{dT} - f_4^+(z) \frac{df_3^+(z)}{dz} \frac{dz}{dT}}{[f_3^+(z)]^2}$$



I can take this take this combine this to give me $\frac{1}{Z} \frac{dZ}{dT}$ is equal to $-\frac{3}{T} \frac{f_3^+(z)}{f_2^+(z)}$ plus of Z divided by $f_2^+(z)$. So, once I have this I take the expression of the specific heat which is going to be $3 \frac{f_4^+(z)}{f_3^+(z)}$ plus divided by $f_3^+(z)$ plus both functions of Z plus $3T$. Let us just write it down once again. It is a little bit laborious, but it is ok. So, I have $f_3^+(z)$ plus of $Z \frac{df_4^+(z)}{dT}$ minus $f_4^+(z) \frac{df_3^+(z)}{dT}$ divided by $[f_3^+(z)]^2$.

Let us take this expression and carry forward the calculation I know that I have the left hand I have this part we will add it at the right time. So, this is $3T$ times $f_3^+(z)$ plus of Z and this is dZ of $f_4^+(z)$ plus times dZ dT minus $f_4^+(z)$ plus of Z dZ of $f_3^+(z)$ plus times dZ dT divided by $f_3^+(z)$ plus of Z whole square.

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$$\begin{aligned}
 & 3T \frac{1}{z} \frac{dz}{dT} \left[\frac{f_3^+(z)}{f_3^+(z)} \right]^2 \\
 & 3T \left(\frac{1}{z} \frac{dz}{dT} \right) \left[\frac{f_3^+(z)^2 - f_4^+(z) f_2^+(z)}{f_3^+(z)} \right] \\
 & 3T \cdot \left(-\frac{3}{T} \right) \cdot \left[\frac{f_3^+(z)}{f_2^+(z)} \right] \cdot \left[1 - \frac{f_4^+(z) f_2^+(z)}{f_3^+(z)} \right] \\
 & 3 \frac{f_4^+(z)}{f_3^+(z)} - 9 \frac{f_3^+(z)}{f_2^+(z)} + 9 \frac{f_4^+(z)}{f_3^+(z)}
 \end{aligned}$$



So, that this is 3. This I already know this derivatives. This derivative is 1 by Z f 3 plus of Z and this derivative is 1 by Z f 2 plus Z. Therefore, I have 1 over Z dZ dT that comes outside as a common factor and then I have f 3 multiplying f 3 giving me f 3 plus Z whole square minus f 4 plus of Z f 2 plus of Z divided by f 3 plus of Z whole square.

This also I know I just calculated one by Z dZ dT and the answer is this. So, I take this and substitute over here to give me 3 times T minus 3 by T f 3 plus of Z divided by I have f 2 plus of Z and this is 1 minus f 4 plus of Z f 2 plus of Z divided by f 3 plus of Z whole square.

So, that this expression T T gets cancelled out and the first term you see is minus 9 f 3 plus of Z divided by f 2 plus of Z. The second expression is plus 9 f 4 plus of Z and if you see that

this factor of f_3 plus now cancels one factor of f_3 plus from the denominator and the f_2 plus completely cancels the f_2 plus over here.

So, that you have f_3 plus of Z . Now, look at it carefully and see let us add the first term. The first term is $3 f_4$ plus of Z divided by f_3 plus of Z . So, that this and this are the same terms, well same forms

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$$\frac{C}{Nk_B} = 12 \frac{f_4^+(z)}{f_3^+(z)} - 9 \frac{f_3^+(z)}{f_2^+(z)}$$

High temperature limit
 $f_n^+(z) \approx z$

$\frac{C}{Nk_B} \rightarrow 12 - 9 = 3 \rightarrow$ Classical limit. $C = 3Nk_B$

At $T = T_c$, $\frac{C}{Nk_B} = 12 \frac{5(4)}{5(3)} - 9 \frac{5(3)}{5(2)}$

$\frac{C}{Nk_B} = \frac{12}{4} \frac{5(4)}{5(3)}$
 Specific heat at T_c approach from T_c^-



Therefore, the specific heat now becomes 9 plus 3 is $12 f_4$ plus of Z divided by f_3 plus of Z minus $9 f_3$ plus of Z divided by f_2 plus of Z . Question is this looks very nice. Now, we go to check whether we have arrived at the right and expression. So, for that the first thing to look is the high temperature expansion sorry the high temperature limit.

And in the high temperature limit Z is very small and I know that all of this $f m$ plus Z is approximately Z . So, that the specific heat C over $N k_B$ which is 12 minus 9 which is equal to 3 and this is the classical result which is C is going to be $3 N k_B$. Now, the interesting thing is what happens at T equal to T_c ? At T equal to T_c one has C over $N k_B$ as 12 times $\zeta(4)$ divided by $\zeta(3)$ minus 9 times $\zeta(3)$ divided by $\zeta(2)$ the Riemann zeta function.

And here it is interesting because I clearly see that there is a difference right. There is a difference and this does not match the specific heat which we obtained at T equal to T_c which was C over $N k_B$ was 12 by 4 $\zeta(4)$ over $\zeta(3)$. This is the result of the specific heat at T_c approaching from T_c minus. So, you are approaching that critical temperature from below the critical temperature and once you do that this is the result that you get.

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$$\frac{C}{Nk_B} = 12 \frac{\zeta(4)}{\zeta(3)} - 9 \frac{\zeta(3)}{\zeta(2)}$$
 At $T=T_c$,

$$\frac{C}{Nk_B} = 12 \frac{\zeta(4)}{\zeta(3)}$$
 Specific heat at T_c when approaching from T_c^+

$$\frac{C}{Nk_B} = 12 \frac{\zeta(4)}{\zeta(3)}$$
 Specific heat at T_c approach from T_c^-

$$\frac{\Delta C}{Nk_B} = 12 \frac{\zeta(4)}{\zeta(3)} - 9 \frac{\zeta(3)}{\zeta(2)} - 12 \frac{\zeta(4)}{\zeta(3)} = -9 \frac{\zeta(3)}{\zeta(2)}$$
 Discontinuity in specific heat at $T=T_c$:



In contrast specific heat at T is equal to T_c when approaching from T_c plus. So, this is your T_c . T_c plus is approaching from this, T_c minus is this and when you approach from T_c plus you get this expression. So, there is a difference. And that difference ΔC over $N k_B$ is $12 \zeta(4)$ divided by $\zeta(3)$ minus 9 of $\zeta(3)$ divided by $\zeta(2)$ minus 12 ; sorry this is just 12 , not my mistake minus $12 \zeta(4)$ over $\zeta(3)$ which is minus $9 \zeta(3)$ over $\zeta(2)$.

So, there is a discontinuity in the specific heat in specific heat at the critical temperature T equal to T_c .