

# PHYS 522: Statistical Mechanics

## Homework #4

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1. Derive the virial expansion of the ideal Bose gas by inverting the relation  $n\lambda^3 = g_{3/2}(z)$  series to express  $z$  in terms of  $n\lambda^3$  and substitute it in the  $P/KT$  equation. Using this expression derive the expansion for  $C_v/Nk$  valid at high temperature limit.

**Solution:**

For high temperature  $N_0 \ll N$  the relation can be written as

$$n\lambda^3 = g_{3/2}(z) = z + \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \dots$$

To invert the series with usual technique we write the  $z$  as a power series in  $n\lambda^3$  as

$$z = c_1(n\lambda^3) + c_2(n\lambda^3)^2 + c_3(n\lambda^3)^3 + \dots$$

substituting the value of  $z$  into the first series we get

$$n\lambda^3 = [c_1(n\lambda^3) + \dots] + \left[ \frac{(c_1(n\lambda^3) + c_2(n\lambda^3)^2)^2}{2^{3/2}} \right] + \dots$$

Comparing the coefficients of like powers of  $\lambda^3$  in both sides we get

$$c_1 = 1; \quad c_2 + \frac{c_1^2}{2^{-3/2}} = 0 \quad c_3 + \frac{2c_1c_2}{2^{-3/2}} + \frac{c_1^3}{3^{-3/2}} = 0$$

Writing similarly we get

$$c_1 = 1; c_2 = \frac{-1}{2^{-3/2}} \quad c_3 = \frac{1}{4} - \frac{1}{3^{-3/2}}$$

Now the expression  $\ln Q$  becomes

$$\frac{PV}{NkT} = \frac{1}{n\lambda^3} \left( z + \frac{z^2}{2^{-5/2}} + \frac{z^3}{3^{-5/2}} + \dots \right)$$

Substituting the value of  $z$  from the series in  $n\lambda^3$  with the various coefficients  $c_1, c_2 \dots$  we get

$$\frac{PV}{NkT} = \sum_{l=1}^{\infty} a_l \left( \frac{\lambda^3}{v} \right)^{l-1}$$

This is the required virial expansion of the expression. Now for the specific heat at constant volume we have to find out  $\frac{\partial U}{\partial T}$ , this can be simplified as

$$\frac{C_v}{Nk} = \frac{1}{Nk} \left( \frac{\partial U}{\partial T} \right)_{N,V} = \frac{3}{2} \left[ \frac{\partial}{\partial T} \left( \frac{PV}{Nk} \right) \right]_v$$

In similar fashion for the expansion of  $g_{5/2}(z)$  we get

$$\frac{C_v}{Nk} = \sum_{l=1}^{\infty} \frac{3 \cdot 5 - 3l}{2} a_l \left( \frac{\lambda^3}{v} \right)^{l-1}$$

Substituting all the coefficient we get

$$\frac{C_v}{Nk} = \frac{3}{2} \left[ 1 + c_1 \left( \frac{\lambda^3}{v} \right) + c_2 \left( \frac{\lambda^3}{v} \right)^2 + \dots \right]$$

where the coefficients are  $c_1 = 0.088, c_2 = 0.0065, \dots$ . This is the expression of specific heat of Bose gas correct at high temperature.  $\square$

2. (**Pathria & Beale, 7.3**) Combining equation 7.1.24 and 7.1.26, and making use of the first two terms of formula (D.9) in Appendix D, show that, as  $T$  approaches  $T_c$  from above the parameter  $\alpha (= \ln z)$  of the ideal Bose gas assumes the form

$$\alpha = \frac{1}{\pi} \left( \frac{3\zeta(3/2)}{4} \right)^2 \left( \frac{T - T_c}{T} \right)^2$$

**Solution:**

We have from previous problem  $n\lambda^3 = g_{3/2}(z)$ . But at  $\lambda = \lambda_c$  we have  $z = 1$ . But for  $z = 1$

$$g_{3/2}(1) = 1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}} + \dots = \zeta(3/2)$$

Substituting this in the expression for the critical temperature and taking the ratio

$$\frac{T}{T_c} \equiv \left( \frac{\lambda}{\lambda_c} \right)^2 = \left( \frac{g_{3/2}(z)}{\zeta(3/2)} \right)^{-\frac{2}{3}}$$

The expression for  $g_{3/2}(z)$  can be expanded in terms of series the series expansion from appendix D.9 can be used to obtain

$$\frac{T}{T_c} = \left( \frac{\zeta(3/2) - 2\sqrt{\pi\alpha} + \dots}{\zeta(3/2)} \right)^{-\frac{2}{3}}$$

Since we have  $\alpha \ll 1$  we can make use of binomial expansion of the series

$$(1 + x)^n \approx 1 + nx; \quad x \ll 1$$

Using just the first two terms we get

$$\frac{T}{T_c} \approx 1 + 4 \frac{\sqrt{\pi\alpha}}{3\zeta(3/2)}$$

Now, this expression can be simplified further to get

$$4\sqrt{\pi\alpha} = 3\zeta(3/2) \left( \frac{T - T_c}{T_c} \right)$$

Squaring both sides leads to

$$\alpha = \frac{1}{\pi} \left( \frac{3\zeta(3/2)(T - T_c)}{4T} \right)^2$$

This is the required expression. □

3. Derive in detailed steps the following expression for an ideal Bose gas.

$$\frac{C_v}{Nk} = \frac{15g_{5/2}(z)}{4g_{3/2}(z)} - \frac{9g_{3/2}(z)}{4g_{3/2}(z)}$$

**Solution:**

For ideal Bose gas from 7.1.7 and 7.1.8 we get

$$\frac{P}{kT} = \frac{1}{\lambda^3} g_{5/2}(z)$$

$$\frac{N - N_0}{V} = \frac{1}{\lambda^3} g_{3/2}(z)$$

At high temperature we can assume that  $z \ll 1$  is very small and we can safely ignore  $N_0$ . We can take the ratio of these two quantities to get

$$\frac{PV}{NkT} = \frac{g_{5/2}(z)}{g_{3/2}(z)}$$

Also the internal energy can be calculated as

$$U \equiv - \left( \frac{\partial}{\partial \beta} \ln \mathcal{Q} \right)_{z,V} = kT^2 \left( \frac{\partial}{\partial T} \left( \frac{PV}{kT} \right) \right)_{z,v} = \frac{3}{2} kT \frac{V}{\lambda^3} g_{5/2}(z)$$

Now the expression for the specific heat is

$$C_v = \frac{\partial U}{\partial T} = \left[ \frac{\partial}{\partial T} \left( \frac{3}{2} T \frac{g_{5/2}(z)}{g_{3/2}(z)} \right) \right]_v$$

Now we can use the recurrence relation for the function  $g(z)$  as

$$z \frac{\partial}{\partial z} g_\nu(z) = g_{\nu-1}(z)$$

Also since the function  $g_{3/2}(z)$  is proportional to cube root of the square of the temperature we get

$$\left[ \frac{\partial}{\partial T} g_{3/2}(z) \right]_v = -\frac{3}{2T} g_{3/2}(z)$$

Combining these two expressions we get

$$\frac{1}{z} \left( \frac{\partial z}{\partial T} \right)_v = -\frac{3}{2T} \frac{g_{3/2}(z)}{g_{1/2}(z)}$$

Now carrying out the differentiation of the expression  $C_v$  we get

$$C_v = Nk \frac{3}{2} \frac{g_{5/2}(z)}{g_{3/2}(z)} + Nk \frac{\partial}{\partial T} \left( \frac{g_{5/2}(z)}{g_{3/2}(z)} \right) \frac{\partial z}{\partial T}$$

Using the previous expression for  $\frac{\partial z}{\partial T}$  and using the product rule in the differentiation we get

$$\frac{C_v}{Nk} = \frac{3}{2} \left[ \frac{5}{2} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{3}{2} \frac{g_{3/2}(z)}{g_{1/2}(z)} \right]$$

Simplifying the expression gives

$$\frac{C_v}{Nk} = \frac{15}{4} \frac{g_{5/2}(z)}{g_{3/2}(z)} - \frac{9}{4} \frac{g_{3/2}(z)}{g_{1/2}(z)}$$

This is the required expression for the specific heat of bosons in high temperature limit. □

#### 4. Prove the following for and atomic Bose gas with spin $S$

(a) Its density of state is given by:

$$g(E) = 2\pi V (2S+1) \left( \frac{2m}{h^2} \right)^{3/2} E^{1/2}$$

#### Solution:

If we consider atomic non-interating atomic gas with spin  $S$ , then for each momentum state, there are  $2S+1$  spin states. Then the grand partition function becomes

$$\mathcal{Q} = \prod_i \mathcal{Q}_i^{2S+1}$$

The grand potential becomes

$$\Phi = -kT \ln \mathcal{Q} = kT(2S+1) \sum_i \ln \left( 1 \pm e^{-\beta(\epsilon-\mu)} \right)$$

Approximating the sum with the integration we get

$$\Phi = kT(2S+1) \int_0^\infty \ln \left( 1 + e^{-\beta(\epsilon-mu)} \right) g(E) dE$$

Here  $g(E)$  is the density of states which can be simplified for uniformly distributed particles as

$$g(k)dk = \frac{4\pi k^2(2S+1)dk}{(2\pi/L)^3} = \frac{(2S+1)VK^2dk}{2\pi^2}$$

With volume  $V = L^3$  and  $E = \frac{\hbar^2 k^2}{2m}$  we get

$$g(E)dE = \frac{(2S+1)V\sqrt{E}dE}{(2\pi)^2} \left(\frac{2m}{\hbar^2}\right)^{3/2}$$

Using  $\hbar = \frac{h}{2\pi}$  and writing the density of states we get

$$g(E) = 2\pi V(2S+1)\sqrt{E} \left(\frac{2m}{h}\right)^{3/2}$$

Which is the required density of states. □

(b) Then show that its Bose-Einstein temperature is given by

$$T_c = \frac{h^2}{2\pi mk} \left[ \frac{n}{2.612(2S+1)} \right]^{2/3}$$

**Solution:**

Now the total number of particles  $N$  can be obtained as

$$N = \int_0^\infty \frac{g(E)dE}{e^{\beta(\epsilon-\mu)} + 1}$$

Substituting the density function we get

$$N = \left[ 2\pi V \left(\frac{2m}{h^2}\right)^{3/2} \right] \int_0^\infty \frac{\sqrt{E}dE}{z^{-1}e^{\beta E} - 1}$$

The integrand can be recognized as the Einstein function  $g_{3/2}(z)$ . so we get

$$N = \frac{(2S+1)V}{\lambda^3} g_{3/2}(z)$$

For  $T = T_C$  we can consider  $z$  comparable to unity, thus, we have  $z = 1$ , substituting this we get  $g_{3/2}(1) = \zeta(3/2) = 2.612$

$$\frac{n\lambda^3}{2S+1} = \zeta(3/2) = 2.612$$

Making this substitution and recognizing  $\lambda = \left[\frac{h^2}{2\pi mkT}\right]^{1/2}$  Rearranging we get

$$T_c = \frac{h^2}{\pi mk} \left[ \frac{n}{2.612(2S+1)} \right]$$

where we have made use of  $n = \frac{N}{V}$ . This gives the expression for the critical temperature of Bose gas. □