Ex3240: Bose gas in a uniform gravitational field

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The problem¹:

Consider an ideal Bose gas of particles of mass m in a uniform gravitational field of acceleration g.

(1) Show that the phenomenon of Bose-Einstein condensation in this gas sets in at a temperature T_c given by

$$T_c \approx T_c^0 \left[1 + \frac{8}{9} \frac{1}{\zeta(3/2)} \sqrt{\frac{\pi m g L}{k T_c^0}} \right],$$

where L is the height of the tank and $mgL \ll kT_c^0$ $(T_c^0 = T_c^0(g = 0))$.

(2) Show that the condensation is accompanied by a discontinuity in the specific heat of the gas:

$$(\Delta C_V)_{T=T_c} \approx -\frac{9}{8\pi} \zeta(3/2) N k \sqrt{\frac{\pi m g L}{k T_c^0}}$$

Hint: You might find use in the following expansion of the polylogarithmic functions at $\alpha = 0$:

$$Li_{\nu}(e^{-\alpha}) = \frac{\Gamma(1-\nu)}{\alpha^{1-\nu}} + \sum_{i=0}^{\infty} \frac{(-1)^{i}}{i} \zeta(\nu-i)\alpha^{i}.$$

The solution:

(1) The single-particle Hamiltonian is given by

$$H = \frac{\vec{p}^2}{2m} + mgh \equiv \varepsilon + mgh. \tag{1}$$

The average occupation of the gas (ideal Bose gas) is

$$\langle n_e \rangle = \frac{1}{z^{-1} \mathrm{e}^{\beta m g h} \mathrm{e}^{\beta \varepsilon} - 1},\tag{2}$$

where e denotes eigenvalues of H, $\beta = 1/kT$ and z is the fugacity of the gas which is related to the chemical potential μ through the formula $z \equiv e^{\mu/kT}$. The total number of particles is therefore

$$N \equiv \sum_{e} \langle n_e \rangle = \sum_{e} \frac{1}{z^{-1} \mathrm{e}^{\beta m g h} \mathrm{e}^{\beta \varepsilon} - 1}.$$
(3)

Dividing the container into boxes of surface A and height dh, we replace the summation on the r.h.s of eq. (3) by integration. In doing so, we make use of the known expression for the density of states of free particles in 3D;

$$g(\varepsilon, h)d\varepsilon dh = (2\pi A/\hbar^3)(2m)^{3/2}\varepsilon^{1/2}d\varepsilon dh \equiv cA\varepsilon^{1/2}d\varepsilon dh.$$
(4)

We, however, note that by substituting this expression into our integrals we are inadvertently giving a weight zero to the energy level $\varepsilon + mgh = 0$. It is therefore advisable to take this particular state out of the sum in question before carrying out the integration. We thus obtain:

$$N = cA \int_0^\infty \int_0^L \frac{\varepsilon^{1/2} d\varepsilon dh}{z^{-1} e^{\beta \varepsilon} e^{\beta mgh} - 1} + N_0 = cA(kT)^{3/2} \Gamma(3/2) \int_0^L Li_{3/2}(z e^{-\beta mgh}) dh + N_0, \quad (5)$$

¹In its original version; R.K. Pathria and P.D. Beale, "Statistical Mechanics", Elsevier Ltd., Chapter 7; problem 7.10. (2011)

where N_0 is the number of particles in the ground state and $Li_{\nu}(x)$ are Bose-Einstein functions, which obey

$$x\frac{\partial Li_{\nu}(x)}{\partial x} = Li_{\nu-1}(x).$$
(6)

On substituting $ze^{-\beta mgh} = x$ in eq. (5) we get:

$$N_{exited} = cA(kT)^{3/2}\Gamma(3/2) \int_0^L x \frac{\partial Li_{5/2}(x)}{\partial x} \frac{\partial x}{\partial h} dh = cA(kT)^{3/2}\Gamma(3/2) \int_z^{ze^{-\beta mgL}} \left(-\frac{kT}{mg}\right) \frac{\partial Li_{5/2}(x)}{\partial x} dx = cA \frac{(kT)^{5/2}}{mg} \Gamma(3/2) [Li_{5/2}(z) - Li_{5/2}(ze^{-\beta mgL})].$$

$$(7)$$

We recall that condensation appears at that temperature in which the chemical potential equals the ground energy. For our particular case this last assertion entails: $\epsilon_{min} = 0 \Rightarrow ze^0 = 1 \Rightarrow z = 1$. Therefore for $T \to T_c$ from below, z of course equals 1 and we can legitimately use the expansion of $Li_{5/2}(e^{-\beta mgL})$ for T which obeys $mgL/k \ll T_c^0 \leq T < T_c$. Doing so we obtain:

$$N_e \approx cA \frac{(kT)^{5/2}}{mg} \Gamma(3/2) \left(\zeta(5/2) - \zeta(5/2) - \Gamma(-3/2) \left(\frac{mgL}{kT} \right)^{3/2} + \zeta(3/2) \frac{mgL}{kT} \right) = cAL(kT)^{3/2} \Gamma(3/2) \left(\zeta(3/2) - \frac{4}{3} \sqrt{\pi} \sqrt{\frac{mgL}{kT}} \right).$$
(8)

We know² that in the absence of gravitational field (g = 0) for $T = T_c^0$:

$$N'_e(T = T_c^0) = N = cAL(kT_c^0)^{3/2} \Gamma(3/2)\zeta(3/2).$$
(9)

On the other hand, for $T = T_c$, eq. (8) becomes

$$N_e(T = T_c) = N \approx cA(kT_c)^{3/2} \Gamma(3/2) \left(\zeta(3/2) - \frac{4}{3}\sqrt{\frac{\pi mgL}{kT_c}}\right).$$
 (10)

The total number of particles when g = 0 (eq. 9) equals the total number of particles when $g \neq 0$ (eq. 10). Therefore, combining the above results³, we obtain the desired expression:

$$cA(kT_c^0)^{3/2}\Gamma(3/2) \approx cA(kT_c)^{3/2}\Gamma(3/2) \left(1 - \frac{4}{3}\frac{1}{\zeta(3/2)}\sqrt{\frac{\pi mgL}{kT_c}}\right)$$

$$\Rightarrow T_c \approx T_c^0 \left(1 - \frac{4}{3}\frac{1}{\zeta(3/2)}\sqrt{\frac{\pi mgL}{kT_c}}\right)^{-2/3}$$

..
so that finally, recalling $mgL \ll kT_c^0 (< kT_c)$, we get

$$T_c \approx T_c^0 \left[1 + \frac{8}{9} \frac{1}{\zeta(3/2)} \sqrt{\frac{\pi m g L}{k T_c^0}} \right].$$
 (11)

²See lecture notes.

$$N_0(T = T_c^0) = N - N'(T = T_c^0) \approx cAL\Gamma(3/2)\zeta(3/2)[(kT_c)^{3/2} - (kT_c^0)^{3/2}].$$

³We could, alternatively, calculate eq. (8) at $T = T_c^0 < T_c$; following the same reasoning concerning the equal number of particles in both systems, we know that

(2) We consider the behavior of the total energy E as a function of T and μ , with the constraint of fixed number of particles N; we know that

$$\left(\frac{dE}{dT}\right)_{N,V} = \left(\frac{\partial E}{\partial T}\right)_{\mu} + \left(\frac{\partial E}{\partial \mu}\right)_{T} \left(\frac{\partial \mu}{\partial T}\right).$$
(12)

The first term of the r.h.s of eq. (12) is continuous at $T = T_c$, therefore the only singular behavior possible is of $\partial_T \mu$. In fact, the discontinuity is given by:

$$(\Delta C_V)_{T=T_c} = C(T_{c+}) - C(T_{c-}) = \left(\frac{dE}{dT}\right)_{T=T_c} = \left(\frac{\partial E}{\partial \mu}\right)_{T=T_c} \left(\frac{\partial \mu}{\partial T}\right)_{T=T_c^+}.$$
(13)

Using equations (2) and (4), we get an expression for the total energy:

$$E = cA \int_0^L \int_0^\infty \frac{(\varepsilon + mgh)\varepsilon^{1/2}d\varepsilon dh}{z^{-1}\mathrm{e}^{\beta\varepsilon}\mathrm{e}^{\beta mgh} - 1}.$$
(14)

On substituting $\beta \varepsilon = a$, we obtain:

$$E = cA(kT)^{5/2} \int_0^L \int_0^\infty \frac{a^{3/2} dadh}{z^{-1} e^a e^{\beta mgh} - 1} + cA(kT)^{3/2} mg \int_0^L \int_0^\infty \frac{ha^{1/2} dadh}{z^{-1} e^a e^{\beta mgh} - 1} = cA(kT)^{5/2} \Gamma(5/2) \int_0^L Li_{5/2}(ze^{-\beta mgh}) dh + cA(kT)^{3/2} mg \Gamma(3/2) \int_0^L hLi_{3/2}(ze^{-\beta mgh}) dh.$$
(15)

Using eq. (6), on substituting $ze^{-\beta mgh} = x$, and integrating by parts we obtain:

$$cA(kT)^{5/2}\Gamma(5/2) \int_{0}^{L} x \frac{\partial Li_{7/2}(x)}{\partial x} \frac{\partial x}{\partial h} dh = cA(kT)^{5/2}\Gamma(5/2) \int \left(-\frac{kT}{mg}\right) \frac{\partial Li_{7/2}(x)}{\partial x} dx =$$

$$= \frac{ckT}{mg} A(kT)^{5/2}\Gamma(5/2) [Li_{7/2}(z) - Li_{7/2}(ze^{-\beta mgL})],$$
(16)

$$cA(kT)^{3/2}mg\Gamma(3/2)\int_{0}^{L}hLi_{3/2}(x)dh = \dots =$$

= $cA(kT)^{3/2}mg\Gamma(3/2)\pi \left[-\frac{kT}{mg}Li_{5/2}(ze^{-\beta mgL})L - \left(\frac{kT}{mg}\right)^{2} [Li_{7/2}(ze^{-\beta mgL}) - Li_{7/2}(z)] \right].$ (17)

Combining the results⁴ and using equation (6) again we obtain the derivative $\partial_z E$:

$$\frac{\partial E}{\partial z} = cA(kT)^{5/2} \frac{1}{z} \left[\frac{5}{4} \sqrt{\pi} \frac{kT}{mgL} [Li_{5/2}(z) - Li_{5/2}(ze^{-\beta mgL})] - \frac{1}{2} \sqrt{\pi} Li_{3/2}(ze^{-\beta mgL})L \right].$$
(18)

Now, we know that the total number of particles is constant, meaning that its differential with respect to the temperature equals zero. Going back to eq. (5) we differentiate the number of particles in order to find $\partial_T z$. After a fair amount of algebra we obtain:

$$\left(\frac{\partial z}{\partial T}\right)_{T>T_c} = -\frac{3}{2T} z \frac{Li_{5/2}(z) - Li_{5/2}(ze^{-\beta mgL})}{Li_{3/2}(z) - Li_{3/2}(ze^{-\beta mgL})}.$$
(19)

⁴NOTE:

$$\Gamma(5/2) = \frac{3}{4}\sqrt{\pi}$$
; $\Gamma(3/2) = \frac{1}{2}\sqrt{\pi}$; $\Gamma(-1/2) = -2\sqrt{\pi}$.

The specific heat discontinuity is therefore:

$$(\Delta C_V)_{T=T_c} = \left(\frac{\partial E}{\partial \mu}\right) \left(\frac{\partial \mu}{\partial T}\right) = \left(\frac{\partial E}{\partial z}\frac{\partial z}{\partial \mu}\right) \left(\frac{\partial \mu}{\partial z}\frac{\partial z}{\partial T}\right) = = \frac{3}{2}kcA\frac{(kT_c)^{5/2}}{mg}\Gamma(3/2)\frac{Li_{5/2}(z) - Li_{5/2}(ze^{-\beta_c mgL})}{Li_{3/2}(z) - Li_{3/2}(ze^{-\beta_c mgL})} \times \left[\frac{mgL}{kT_c}Li_{3/2}(ze^{-\beta_c mgL}) - \frac{5}{2}[Li_{5/2}(z) - Li_{5/2}(ze^{-\beta_c mgL})]\right]$$

$$(20)$$

As $T \to T_c$ from above, $z \to 1$. Additionally by recognizing the number of excited particles (eq. (7)), which equals the total number of particles at $T = T_c$, we obtain

$$(\triangle C_V)_{T=T_c} = \frac{3}{2}Nk \frac{\left[\frac{mgL}{kT_c}Li_{3/2}(e^{-\beta_c mgL}) - \frac{5}{2}[Li_{5/2}(1) - Li_{5/2}(e^{-\beta_c mgL})]\right]}{Li_{3/2}(1) - Li_{3/2}(e^{-\beta_c mgL})}.$$
(21)

Using the expansion of the relevant polylogarithmic functions at $\frac{mgL}{kT_c} \approx \frac{mgL}{kT_c^0} = 0$ to the lowest order⁴ (under the framework of the given limit $mgL \ll kT_c^0$) we obtain the required result:

$$(\Delta C_V)_{T=T_c} \approx \frac{3}{2} Nk \frac{\left[\frac{mgL}{kT_c^0} \zeta(3/2) - \frac{5}{2} \zeta(3/2) \frac{mgL}{kT_c^0}\right]}{2\sqrt{\pi} \sqrt{\frac{mgL}{kT_c^0}}} = -\frac{9}{8\pi} \zeta(3/2) Nk \sqrt{\frac{\pi mgL}{kT_c^0}}.$$
 (22)