Bose Einstein Condensate in 3D

Problem statement

Start with the following expression,

$$pV = k_B T \ln\left(\prod_k \left(\frac{1}{1 - e^{-\beta(\epsilon_k - \mu)}}\right)\right) = -k_B T \sum_k \ln\left(1 - ze^{-\beta\epsilon_k}\right)$$

and derive,

$$p = \frac{k_B T}{\lambda^3} \sum_{l=0}^{\infty} \frac{z^l}{l^{5/2}}$$

Solution

Given equation is,

$$pV = k_B T \ln\left(\prod_k \left(\frac{1}{1 - e^{-\beta(\epsilon_k - \mu)}}\right)\right) = -k_B T \sum_k \ln\left(1 - ze^{-\beta\epsilon_k}\right) \tag{25}$$

where I am using $z = e^{\beta\mu}$ as the fugacity.

Comment on BEC - Might need later

We recall that when we derive the Bose-Einstein distribution, we make the following approximation,

$$\sum_{\vec{k}} \approx \int g(E)\, dE \tag{26}$$

where

$$g(E) = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \tag{27}$$

Because of the $\sqrt{E}$ in the integrand, $E = 0$ states are not taken into consideration when we do the sum over k. Those states become crucial when we drop the temperatures lower and lower (which is the basis of the BEC as we can recall learning in class). Using the Bose-Einstein distribution, we found that the correction needed (for the missing $E = 0$ states can be written as,

$$n_0 = \frac{1}{z^{-1} - 1} \tag{28}$$

For most of the values in $z \in (0, 1)$ the number of particles in n_0 is very low and the approximation for the sum to integral holds really well (as we are usually dealing with a set of particles as large as $\mathcal{O}(10^{23})$. But as $z \to 1$ the number of particles starts to get macroscopic.
For our current computations we are trying to mimic the derivation for Eq. 4.92 in the script. We carefully identify that, while deriving 4.92, $z \ll 1$ is an assumption made, and proceed for this part with the same assumption i.e. we assume eq.(26) is valid.

Handwritten solution continued on next page!

$$pV = -k_BT \sum_k \ln(1 - ze^{-\beta E_k}) = -k_BT \int g(E) \ln(1 - ze^{-\beta E_k})\, dE$$

Where, $g(E) = \varkappa E^{1/2}$, $\varkappa = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$

$$= -\varkappa k_BT \underbrace{\int E^{1/2} \ln(1 - ze^{-\beta E})\, dE}_{I}$$

$$\boxed{\begin{aligned} &u = \ln(1 - ze^{-\beta E}), \quad \frac{du}{dE} = \frac{1}{1 - ze^{-\beta E}}(-ze^{-\beta E})(-\beta) \\ &\qquad\qquad\qquad\qquad du = \frac{\beta z e^{-\beta E}}{1 - ze^{-\beta E}}\, dE \\ &dv = E^{1/2} dE, \quad v = \int dv = \int E^{1/2} dE = \frac{2}{3}E^{3/2} \end{aligned}}$$

$$= -\varkappa k_BT \left[\underbrace{\frac{2}{3}\ln(1 - ze^{-\beta E}) E^{3/2} \Big|_0^\infty}_{} - \int \frac{2}{3} E^{3/2} \frac{\beta z e^{-\beta E}}{(1 - ze^{-\beta E})}\, dE \right]$$

This term goes to zero (Mathematica attached)

$$= \frac{2}{3}\varkappa \frac{\cancel{k_BT}}{\cancel{k_BT}} \int E^{3/2} \frac{1}{(z^{-1}e^{\beta E} - 1)}\, dE$$

$$= \frac{2}{3} \int \varkappa E^{1/2} \frac{E}{(z^{-1}e^{\beta E} - 1)}\, dE$$

$$= \frac{2}{3} \int \frac{g(E)\, E}{(z^{-1}e^{\beta E} - 1)}\, dE = \frac{2}{3} E$$

$$pV = \frac{2}{3}\int dE \, \frac{E\, g(E)}{z^{-1}e^{\beta E}-1}$$

$g(E) = \chi E^{1/2}$

$\chi = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}$

Let $\beta E = x$; $\frac{dx}{dE} = \beta \Rightarrow dE = \frac{dx}{\beta}$

$E = \frac{x}{\beta}$

Integrat^n Bounds remain same.

$$= \frac{2}{3}\chi \int \frac{dx}{\beta} \frac{E^{3/2}}{z^{-1}e^{x}-1}$$

$$= \frac{2}{3}\chi \int \frac{dx}{\beta} \frac{1}{\beta^{3/2}} \frac{x^{3/2}}{z^{-1}e^{x}-1}$$

$$= \frac{2}{3}\frac{\chi}{\beta^{5/2}} \boxed{\int dx \frac{x^{3/2}}{z^{-1}e^{x}-1}} \rightarrow g_{5/2}(z)\,.\,\Gamma\left(\tfrac{5}{2}\right)$$

$$\frac{\chi}{\beta^{5/2}} = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(k_BT)^{3/2}(k_BT) = \frac{V}{4\pi^2}\left(\frac{2mk_BT}{\hbar^2}\right)^{3/2} k_BT$$

Recall that $\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$

$$= \frac{V}{4\pi^2}\left(\frac{2(2\pi)mk_BT}{(2\pi)\hbar^2}\right)^{3/2} k_BT$$

$$= \frac{V}{4\pi^2}(4\pi)^{3/2}\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} k_BT$$

$$= V\frac{2}{\sqrt{\pi}}\frac{k_BT}{\lambda^3}$$

$$\therefore \; pV = \frac{2}{3}V\frac{2}{\sqrt{\pi}}\frac{k_BT}{\lambda^3} g_{5/2}(z)\,\Gamma\left(\tfrac{5}{2}\right) = \frac{4}{3}\frac{V}{\sqrt{\pi}}\frac{k_BT}{\lambda^3} g_{5/2}(z)\,\Gamma(5/2)$$

We know $\Gamma\left(\frac{5}{2}\right) = \frac{3\sqrt{\pi}}{4}$ which cancels out the prefactor of $\frac{4}{3\sqrt{\pi}}$

$$\Rightarrow p\cancel{V} = \cancel{V}\frac{k_BT}{\lambda^3} g_{5/2}(z) \Rightarrow \quad p = \frac{k_BT}{\lambda^3}\sum_{l=0}^{\infty}\frac{z^l}{l^{5/2}}$$

□

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In[66]:= Limit[x^(3/2) Log[1 - z Exp[-x β]], x → 0, Assumptions → {β > 0, 0 < z < 1}]

Out[66]= 0

In[67]:= Limit[x^(3/2) Log[1 - z Exp[-x β]], x → ∞, Assumptions → {β > 0, 0 < z < 1}]

Out[67]= 0
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$$g_n(z) = \frac{1}{\Gamma(n)} \int_0^\infty dx \frac{x^{n-1}}{z^{-1}e^x - 1} \tag{29}$$

Sometimes $g_n(z)$ is also represented by $\mathrm{Li}_n(z)$ these functions are called Polylogarithms. With some manipulation we can show that these Polylogarithms can be represented by a sum,

$$\begin{aligned} g_n(z) &= \frac{1}{\Gamma(n)} \int dx \frac{zx^{n-1}e^{-x}}{1 - ze^{-x}} \\ &= \frac{1}{\Gamma(n)} z \int dx x^{n-1} e^{-x} \sum_{m=0}^{\infty} z^m e^{-mx} \\ &= \frac{1}{\Gamma(n)} \sum_{m=1}^{\infty} z^m \int dx x^{n-1} e^{-mx} \\ &= \frac{1}{\Gamma(n)} \sum_{m=1}^{\infty} \frac{z^m}{m^n} \int du u^{n-1} e^{-u} \end{aligned} \tag{30}$$

The integral that appears in the last line above is nothing but the definition of the gamma function (n). This means that we can write,

$$g_n(z) = \sum_{m=1}^{\infty} \frac{z^m}{m^n} \tag{31}$$

Solution 9.(b)

We know that BEC does not occur in 2D. Hence, we can safely use the $\sum_k \approx \int g(E)\, dE$ approximation.

$$E = \int \frac{g_{2D}(E) E z e^{-\beta E}\, dE}{1 - ze^{-\beta E}} \tag{32}$$

$$= \frac{Vm}{2\pi\hbar^2} \sum_{i=1}^{\infty} z^{i+1} \int_0^\infty E e^{-\beta E(i+1)} \tag{33}$$

$$\tag{34}$$

$$
\begin{aligned}
E &= \int \frac{g_{2\text{D}}(E)\, dE}{z^{-1}e^{\beta E} - 1} && (35)\\
&= \frac{Vm}{2\pi\hbar^2} \int \frac{dE}{z^{-1}e^{\beta E} - 1} && (36)\\
&= \frac{Vm}{2\pi\hbar^2\beta^2} && (37)\\
&= \frac{Vm}{2\pi\hbar^2\beta^2} \sum_{j=1}^{\infty} \frac{z^j}{j^2} && (38)
\end{aligned}
$$

Now its relation to PV is given by,

$$
\begin{aligned}
\frac{PV}{k_B T} &= -\sum_k \log\left(1 - ze^{-\beta E_k}\right) && (39)\\
&= -\frac{Vm}{2\pi\hbar^2} \int_0^{\infty} \log\left(1 - ze^{-\beta E}\right) dE && (40)\\
&= -\frac{Vm}{2\pi\hbar^2} \int dE \int d\beta \frac{Eze^{-\beta E}}{1 - ze^{-\beta E}} && (41)\\
&= -\frac{Vm}{2\pi\hbar^2} \int d\beta \frac{1}{\beta^2} \sum_{l=1}^{\infty} \frac{z^l}{l^2} && (42)
\end{aligned}
$$

Giving us,

$$PV = E \tag{43}$$

Solution.(c) (1 page) + Solution.(d) (1 Page)

We have :
$$\frac{P}{k_B T} = \rho + B_2(T)\rho^2 + B_3(T)\rho^3 + \dots$$
$$B_2(T) = -\left(\frac{1}{2^{3/2}} - \frac{1}{2^{5/2}}\right)\lambda^3$$

On the other side, we also know
$$\frac{P}{k_B T} = \frac{1}{\lambda^3}\left(z + \frac{z^2}{2^{3/2}} + \frac{z^3}{2^{5/2}} + \dots\right)$$

where , $z = a_0 + a_1\rho + a_2\rho^2 + a_3\rho^3 + \dots$

From all this we have a relation between $\underline{z}$ & $\underline{\rho}$.
$$\rho = \frac{1}{\lambda^3}\left[z + \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \dots\right]$$

- In order to get B_3, we first need a_3,
  ↳ We get this by collecting all ρ^3 in → $\rho = \frac{1}{\lambda^3}\left(z + \frac{z^2}{2^{3/2}} + \frac{z^3}{2^{5/2}} + \dots\right)$
  ↳ $a_3 = \frac{\lambda^9}{4} - \frac{\lambda^9}{3\sqrt{3}}$

Last min Comment : Printing before class forgot to add code here, Sorry! Mathematica

Next → for B_3, we group ρ^3 term in :
$$\frac{PV}{k_B T} = \frac{1}{\lambda^3}\left(z + \frac{z^2}{2^{5/2}} + \dots\right)$$

$$\frac{a_3}{\lambda^3} - \frac{\lambda^6}{8} + \frac{\lambda^6}{9\sqrt{3}} = B_3 \xrightarrow{\text{Plug in } a_3}$$

$$\underline{B_3(T) = \left(\frac{9\sqrt{3} - 2}{72\sqrt{3}}\right)\lambda^6}$$

ROUGH PART
(i) $\Delta S = \int_{T_1}^{T_2} \frac{C(T)}{T} dT$
(ii) $C_V = T \frac{\partial S}{\partial T}\Big\|_V$
(iii) $\lambda = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$

- We know from part (a) of this problem:

$$p = \frac{2}{3}\frac{E}{V} = \frac{k_BT}{\lambda^3} g_{5/2}(z)$$

$$= k_BT\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} g_{5/2}(z)$$

$$= k_B\left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2} T^{5/2}\, g_{5/2}(z)$$

$$\therefore E = \frac{3}{2}\left[k_B\left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2}\right] T^{5/2}\, g_{5/2}(z)\; V$$

We can plug this into

$$\frac{C_V}{V} = \frac{1}{V}\frac{dE}{dT} = \frac{3}{2}\left[k_B\left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2}\right]\frac{d}{dT}\left(T^{5/2} g_{5/2}(z)\right) \quad \frac{\cancel{V}}{\cancel{V}}$$

$$= \frac{3}{2}\left[k_B\left(\frac{mk_B}{2\pi\hbar^2}\right)^{3/2}\right]\left(\frac{5}{2}T^{3/2} g_{5/2}(z) + T^{5/2}\frac{d g_{5/2}(z)}{dT}\right)$$

$$= \frac{15}{4}k_B\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} g_{5/2}(z) + \frac{3}{2}k_BT\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2}\frac{d g_{5/2}(z)}{dz}\frac{dz}{dT}\Bigg)$$

$$= \frac{15}{4}\frac{k_B}{\lambda^3} g_{5/2}(z) + \frac{3}{2}\frac{k_BT}{\lambda^3}\frac{dg_{5/2}}{dz}\frac{dz}{dT}$$

$$\boxed{\text{As we have, } g_n(z) = \sum_{m=1}^{\infty}\frac{z^m}{m^n} \Rightarrow \frac{d}{dz}g_n(z) = \frac{1}{z}g_{n-1}(z)}$$

$$= \underbrace{\frac{15}{4}\frac{k_B}{\lambda^3}}_{C_1} g_{5/2}(z) + \underbrace{\frac{3}{2}\frac{k_BT}{\lambda^3}\frac{1}{z}\frac{dz}{dT}}_{C_2} g_{3/2}(z)$$

- From eqn.(ii) in the rough part (right top) of the page, we can see that for $\frac{S}{V}$ we will have the same relation with $C_1 \to \tilde{C}_1$ & $C_2 \to \tilde{C}_2$ (New prefactors)