2. A closed container of volume V with a classical gas $\left(E_p = \frac{p^2}{2m}, PV = Nk_BT\right)$ of $N \gg 1$ indistinguishable particles. The inner surfaces of the container's walls have $N_s \gg 1$ similar traps (potential wells of small size). Each trap can hold only one particle, in one of g_s degenerate states; energy $\Delta > 0$ is required to free the particle from the trap.

(a) Assuming that the chemical potential μ of the system is known, calculate the number N_g of particles in the gas phase (i.e. in the volume of the container). What condition should be imposed on N_g for the gas to behave classically?

the Grand Canonical ensemble lets us write the partition function of the N_s independent traps as (with Z_{gas} on next page),

$$Z_{traps} = \prod_i^{N_s} \sum_n e^{-\beta(E_n - N_n\mu)} = \prod_i^{N_s} \sum_n^{g_s} e^{-\beta n(\Delta - \mu)}$$

why here?? (But OK)

??

where we used $E = n\Delta$ for a trap with $n \leq g_s$ particles in it and $\beta = 1/k_BT$.

(I cannot understand this

for $e^{-\beta(\Delta-\mu)} < 1$ we can use the geometric series

$$\sum_i^N x^i = \frac{1 - x^{N+1}}{1 - x} \quad \text{for } x < 1$$

$$\therefore Z_{traps} = \prod_i^{N_s} \frac{1 - e^{-\beta(g_s+1)(\Delta-\mu)}}{1 - e^{-\beta(\Delta-\mu)}} = \left[\frac{1 - e^{-\beta(g_s+1)(\Delta-\mu)}}{1 - e^{-\beta(\Delta-\mu)}}\right]^{N_s}$$ X

see model solution

While the Grand Canonical ensemble also lets us →

write the partition function of the gas phase independently (μ is parametrizing their interface, and $Z_{tot} = Z_{gas} \cdot Z_{trapped}$) ✓ OK

So $$Z_{gas} = \sum_i e^{-\beta(E_i - N_i\mu)} = \prod_p^{\infty} \sum_n^{N} e^{-\beta n\left(\frac{p^2}{2m} - \mu\right)}$$

assume $N \to \infty$ for simplicity.

$\therefore$ in $N \to \infty$ limit

$$Z_{gas} = \prod_p^{\infty} \frac{1}{1 - e^{-\beta\left(\frac{p^2}{2m} - \mu\right)}}$$

Now, $$N_{gas} = \frac{1}{Z_{gas}} \sum_i N_i e^{-\beta(E_i - N_i\mu)} = \frac{1}{\beta}\frac{d}{d\mu} \ln(Z_{gas})$$

$$N_{gas} = \frac{1}{\beta}\frac{d}{d\mu}\left[-\sum_p^{\infty} \ln\left(1 - e^{-\beta\left(\frac{p^2}{2m} - \mu\right)}\right)\right]$$

Where $\sum_p^{\infty}$ can be turned into a $p=0$ piece and a $\int d^3\vec{p}$ piece by taking

$$\sum_{\text{states}} \simeq \int d^3_{\text{state vector}} = \frac{1}{(2\pi)^3}\frac{1}{\hbar^3}\int d^3\vec{p}\, d^3\vec{q} = \frac{V}{(2\pi\hbar)^3}\cdot 4\pi \int dp\, p^2$$

and $E_n \to E = \frac{p^2}{2m}$ & $dE = \frac{p}{m}dp$

$$\therefore dp\, p^2 = dE \cdot m \cdot \frac{p^2}{p} = dE\, m \cdot \sqrt{2mE}$$

then $\sum = \int g(E)dE \quad \therefore \quad g(E) = \frac{V}{-}\left(\frac{2m}{-}\right)^{3/2} E^{1/2}$

$$\frac{\partial}{\partial\mu} \ln\left(1 - e^{-\beta\left(\frac{p^2}{2m}-\mu\right)}\right) = \frac{-(\beta)\cdot e^{-\beta\left(\frac{p^2}{2m}-\mu\right)}}{1-e^{-\beta\left(\frac{p^2}{2m}-\mu\right)}}$$

$$\therefore N_{gas} = -\frac{1}{\beta}\frac{V}{4\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}\int_0^\infty dE\cdot E^{1/2}\cdot -\beta\frac{1}{e^{\beta(E-\mu)}-1} + \underset{\uparrow}{Z(p=0)} \quad \overset{\frac{z}{1-z}}{''}$$

separating out the condensate part

$$= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}\int_0^\infty \frac{dx\, x^{1/2}\cdot\frac{1}{\beta^{3/2}}}{z^{-1}e^{x}-1} + \left(\frac{V}{4\pi^2}\left(\frac{2m}{\hbar}\right)^{3/2}\left(\frac{z}{1-z}\right)\right)$$

fugacity $z = e^{\beta\mu}$

↑ bound states, non-classical gas states,

$$\boxed{N_{gas\,\text{classical}} = \frac{V}{4\pi^2}\left(\frac{2m}{\hbar\beta^3}\right)^{3/2} g_{3/2}(z)\,\Gamma(3/2)}$$

which is a well known function of z (and $g_{3/2}(1) = \zeta(3/2)$)

So, in order for N_{gas} to behave classically we need to have the chemical potential above zero, otherwise the number of particles stuck in the bound states becomes appreciable.

wrong coeff, and functional dep. on $\hbar$.

wrong!!

From the very beginning, it was given that the gas is classical (i.e. $\mu < 0$ and $-\mu \gg T$), so that you could get the result very simply - see the model solution.

b) From the Z_{trap} on page 1 we have

P(a trap to have a particle ~~particle~~ in it)

$$P(1) = \frac{1}{Z_{1trap}} \cdot e^{-\beta(\Delta-\mu)} = e^{-\beta(\Delta-\mu)} \cdot \left[\frac{1-e^{-\beta(\Delta-\mu)}}{1-e^{-\beta(g_s+1)(\Delta-\mu)}}\right]^{N_s}$$

And $N_{trapped} = \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln(Z_{1trap}) = \frac{\frac{1}{\beta}\cdot N_s}{Z_{1trap}}\left[\frac{\beta(g_s+1)\cdot -e^{-\beta(g_s+1)(\Delta-\mu)}}{1-e^{-\beta(\Delta-\mu)}} + \left(1-e^{-\beta(g_s+1)(\Delta-\mu)}\right)\cdot -\frac{\left(-e^{-\beta(\Delta-\mu)}\cdot\beta\right)}{\left(1-e^{-\beta(\Delta-\mu)}\right)^2}\right]$

$$\boxed{N_{trapped} = N_s \cdot \left[\frac{(g_s+1)\cdot -e^{-\beta(g_s+1)(\Delta-\mu)}}{1-e^{-\beta(g_s+1)(\Delta-\mu)}} + \frac{e^{-\beta(\Delta-\mu)}}{(1-e^{-\beta(\Delta-\mu)})}\right]}$$

× see model solution

c) What is $\mu(N_{trap}, N_{gas})$

We know we have N total particles, which must sum to $N_{gas} + N_{trap}$.

$\therefore N = N_{trap} + N_{gas}$ ✓, and even better is that from our separating out the $p=0$ condensed states from our N_{gas} integration we know that

$$N - N_{gas} = \underbrace{\frac{V}{4\pi^2} \cdot \left(\frac{2m}{\hbar}\right)^{3/2} \frac{e^{\beta\mu}}{1-e^{\beta\mu}}}_{\text{how does this relate to your result on the previous page?}} = N_{trap}$$

So the equation which defines the chemical potential of our system is

$$\underbrace{\frac{1}{e^{-\beta\mu}-1}}_{N_{trapped}??} = \left(\frac{\hbar}{2m}\right)^{3/2} \frac{4\pi^2}{V} \cdot N_s \cdot \underbrace{\left[\frac{e^{-\beta(\Delta-\mu)}}{1-e^{-\beta(\Delta-\mu)}} - (g_s+1)\frac{e^{-\beta(g_s+1)(\Delta-\mu)}}{1-e^{-\beta(g_s+1)(\Delta-\mu)}}\right]}_{N_{trapped}??}$$

Where is N_{gas}?

E) for $\frac{N_{gas}}{N_s} \ll 1$ what happens $\rightarrow$ calculate pressure.

↳ this means there are very many spots available for particles to fall into traps, and $\therefore$ we may treat $\mu \rightarrow$ small

$$\frac{1}{e^{-\beta\mu}-1} \rightarrow \frac{1}{1-\beta\mu-1} \sim \frac{k_BT}{\mu} = \left(\frac{\hbar^2}{2m}\right)^{3/2} \frac{4\pi^2}{V} N_s \left[\frac{1}{e^{\beta\Delta}(1-\mu)-1} - \frac{(g_s+1)}{e^{\beta(g_s+1)\Delta}(1-(g_s+1)\mu)-1}\right]$$

let μ be small even here.

$$\therefore \boxed{\mu = \frac{k_BT \cdot V}{N_s\, 4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[\frac{1}{e^{\beta\Delta}-1} - \frac{(g_s+1)}{e^{\beta(g_s+1)\Delta}-1}\right]^{-1}}$$

and then $P = -\frac{\Phi}{V} = +\frac{1}{V\beta} \ln\left(\mathcal{Z}(\mu \to \text{small})\right)$

$$= -\frac{k_B T}{V} \int_0^\infty \underbrace{g(E)}_{\text{given before in part a)}} dE \ln\left(1 - e^{-\beta(E - \underbrace{\mu}_{\mu \text{ given as above}})}\right)$$

and this integral is highly non-trivial, though for μ really small we can use

$\ln(1-x) \simeq -x$ to proceed

$$= +\frac{k_B T}{V} \cdot \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty E^{1/2} dE \cdot e^{-\beta(E-\mu)}$$

$\left(x = E^{1/2},\ dx = \frac{1}{2} E^{-1/2} dE \right.$

$dE = 2 E^{1/2} dx$

$$\underbrace{2 \cdot \int_0^\infty dx\, e^{-\beta x^2}}\, e^{\beta\mu}$$

$$2 \cdot \sqrt{\frac{\pi}{\beta}}\, \underbrace{e^{\beta\mu}}_{(1+\beta\mu)}$$

so $P = \frac{k_B T}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot 2\sqrt{\pi} \cdot \sqrt{k_B T} \left[1 + \frac{V}{N_s 4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \left(\frac{1}{e^{\beta\mu} - 1} - \frac{(\gamma_s+1)}{e^{\beta(\gamma_s+1)} - 1}\right)\right]^{-1}$

which looks kind of wrong honestly.

D) Now do $N/N_s \gg 1$ → as in there are very few sites & μ large

for $\mu \gg 0$ we get $z = e^{\beta\mu} \gg 1$ and we get

$$\frac{1}{e^{-\beta\mu}-1} \simeq -(1+e^{-\beta\mu}) \simeq +\beta\mu = \left(\frac{\hbar}{2m}\right)^{3/2}\frac{4\pi^2}{V}\cdot N_s\cdot\left[-\cancel{1}-\left(-(g_s+\cancel{1})\right)\right]$$

$$\therefore \boxed{\mu = k_B T\left(\frac{\hbar}{2m}\right)^{3/2}\frac{4\pi^2}{V} N_s g_s}$$

1/4

and $P = -\frac{\Phi}{V} = \frac{1}{V\beta}\ln\left(\mathcal{Z}(\mu \to \text{large})\right)$

$$= \frac{k_B T}{V}\int_0^\infty g(E)\,dE\,\ln\left(1-e^{-\beta(E-\mu)}\right)$$

large ∴ dominates

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

I don't know how to perform this integral.

F) In summary, the gas pressure is significantly affected by the particle condensation into traps when the temperature reaches the low critical temperature of T_c defined at $z=1$ in the N_{gas} formula from part A). We then see that for $T < T_c$ the $N_{trapped}$ goes like $1-\left(\frac{T}{T_c}\right)^{2/3}$ (arguing from the generalized $g(E) = C E^{\alpha-1}$ formulation of BEC problems) ⟶

Similarly we expect for gas to condense more readily when the number of available traps to fall into begin to compete with the number of available microstates in the gas phase. This happens for $N_s \gg N_{gas}$.