1 Classical ideal gas in 2D

(a) μ can be found by first finding the total average number of particles in the system $N \equiv \langle N \rangle$, which will be a function of $N = N(\underline{\underline{\mu}}, T, V)$ and then solving it for μ as a function of N, i.e. $\mu = \mu(\underline{\underline{N}}, T, V)$.

So, need to find $N \equiv \langle N \rangle$ first.
From the definition:

$$\underbrace{N \equiv \langle N \rangle}_{\substack{\text{total} \\ \text{average} \\ \text{number} \\ \text{of particles} \\ \text{known to} \\ \text{be present}}} = \underbrace{\sum_{\underline{n}}}_{\substack{\text{over} \\ \text{all} \\ \text{orbitals}}} \underbrace{\langle N(E_{\underline{n}}) \rangle}_{\substack{\text{average} \\ \text{occupancy} \\ \text{of an} \\ \text{orbital} \\ \text{at energy } E_{\underline{n}}}}$$

(ignore spin and spin multiplicity)

In the classical regime, the average occupancies are given by the classical Boltzmann distribution function

$$\langle N(E_{\underline{n}}) \rangle \equiv f_c(E_{\underline{n}}) = e^{-(E_{\underline{n}} - \mu)/k_B T}$$

Next, the sum $\sum_{\underline{n}} \equiv \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty}$ — in 2D

Thus

$$N \equiv \langle N \rangle = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} e^{-(E_{\underline{n}} - \mu)/k_B T}$$

where $E_{\underline{n}} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n^2$ (as in problem No. 1)

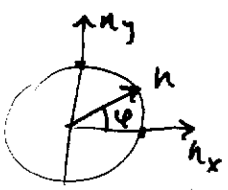
Convert the Σ's into continuos integrals

$$\rightarrow \simeq \int_1^{\infty} dn_x \int_1^{\infty} dn_y \, e^{-(E_{\underline{n}} - \mu)/k_B T}$$

approx.

$$\simeq \int_0^{\infty} dn_x \int_0^{\infty} dn_y \, e^{-(E_{\underline{n}} - \mu)/k_B T}$$

$n = \sqrt{n_x^2 + n_y^2}$



in polar coordinates $\int_0^{\infty} n\,dn \int_0^{2\pi} d\varphi (..) = 2\pi \int_0^{\infty} n\,dn (..)$,

taking only the positive quadrant acounts for $\frac{1}{4}$ of the full range

$$= \frac{1}{4} \cdot 2\pi \int_0^{\infty} dn \cdot n \cdot e^{-(E_n - \mu)/k_B T}$$

$$= e^{\mu/k_B T} \, \frac{\pi}{2} \int_0^{\infty} dn \; n \; e^{-E_n/k_B T}$$

$E_{\underline{n}}$ is given above

$$= e^{\mu/k_B T} \, \frac{\pi}{2} \int_0^{\infty} \underbrace{dn \; n}_{n\,dn = \frac{1}{2} d(n^2)} \, e^{-\frac{\hbar^2 \pi^2}{2mL^2 k_B T} n^2}$$

$$= e^{\mu/k_BT} \; \frac{\pi}{2} \; \frac{1}{2} \int_0^\infty d(n^2) \; e^{-\frac{\hbar^2\pi^2}{2mL^2k_BT} n^2}$$

define $\dfrac{\hbar^2\pi^2}{2mL^2k_BT} n^2 = x$

$$= e^{\mu/k_BT} \frac{\pi}{4} \cdot \frac{2mL^2k_BT}{\hbar^2\pi^2} \underbrace{\int_0^\infty dx \; e^{-x}}_{=1}$$

$$= \frac{mL^2k_BT}{2\pi\hbar^2} e^{\mu/k_BT} \qquad (L^2 \equiv A)$$

Thus $$\boxed{N = \frac{m A k_BT}{2\pi\hbar^2} e^{\mu/k_BT}}$$

$\hookrightarrow N = N(T,\mu,A)$

Solve for μ:

$$\mu = k_BT \ln\left(\frac{2\pi\hbar^2 N}{m A k_BT}\right) \equiv \mu(T,N,A)$$

(b) $U = \sum_{\underline{n}} E_{\underline{n}} \underbrace{\langle N(E_{\underline{n}}) \rangle}_{e^{-(E_{\underline{n}} - \mu)/k_B T}}$

in the classical regime (Boltzmann distribution)

$$\rightarrow \simeq \frac{1}{4} \cdot 2\pi \int_0^\infty n\, dn\, E_n\, e^{-(E_n - \mu)/k_B T}$$

$$= e^{\mu/k_B T} \frac{\pi}{2} \int_0^\infty dn \cdot n \left(\frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n^2 \right) e^{-\frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 \frac{1}{k_B T} n^2}$$

$$= e^{\mu/k_B T} \frac{\pi}{2} \cdot \frac{\hbar^2 \pi^2}{2mL^2} \int_0^\infty dn\, n^3\, e^{-\frac{\hbar^2 \pi^2}{2mL^2 k_B T} n^2}$$

define $\boxed{\frac{\hbar^2 \pi^2}{2m L^2 k_B T} n^2 \equiv x^2}$

$$= e^{\mu/k_B T} \frac{\pi}{2} \frac{\hbar^2 \pi^2}{2mL^2} \cdot \left(\frac{2mL^2 k_B T}{\hbar^2 \pi^2} \right)^{2} \underbrace{\int_0^\infty dx\, x^3\, e^{-x^2}}_{=\frac{1}{2}}$$

(Table integral)

$$= e^{\mu/k_B T} \frac{1}{2} \frac{\pi}{2} \frac{\hbar^2 \pi^2}{2mL^2} \frac{(2mL^2)^2 (k_B T)^2}{(\hbar^2 \pi^2)^2}$$

$$= e^{\mu/k_BT} \frac{\cancel{\pi}}{2\cancel{4}} \frac{\cancel{2}m L^2 (k_B T)^2}{\hbar^2 \pi^{\cancel{2}}}$$

$$= e^{\mu/k_BT} \frac{m A (k_B T)^2}{2\pi \hbar^2}$$

Thus $$\boxed{U = \frac{m A (k_BT)^2}{2\pi\hbar^2} e^{\mu/k_BT}}$$

Also

$$U = k_BT \underbrace{\frac{m A k_B T}{2\pi\hbar^2} e^{\mu/k_BT}}_{= \langle N \rangle \equiv N \text{ (from (a))}}$$

$$\therefore \boxed{U = N k_B T}$$

$$\frac{U}{N} = k_B T$$ → this is expected in the <u>classical regime</u>, in 2D by the equipartition theorem: $\frac{1}{2} k_B T$ contribution from each degree of freedom

(classical regime = high temperature)

(c) To find S we first find

$$F = U - TS \quad \left(\text{then} \quad S = \frac{U-F}{T} \right)$$

F – ? can be found using the definition of $\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V}$

$$\Rightarrow \quad F = \int_0^N \underbrace{\mu}_{\text{from (a) } \mu = \mu(T, \underline{\underline{N}}, A)} dN'$$

$$= \int_0^N dN' \cdot k_B T \ln\left(\frac{2\pi\hbar^2 N'}{m A k_B T}\right) =$$

$$= k_B T \int_0^N dN' \left[\ln N' + \ln\left(\frac{2\pi\hbar^2}{m A k_B T}\right)\right] =$$

$$= k_B T \underbrace{\int_0^N dN' \ln N'}_{N \ln N - N} + k_B T \ln\left(\frac{2\pi\hbar^2}{m A k_B T}\right) \underbrace{\int_0^N dN'}_{N}$$

(use $\int \ln x \, dx = x \ln x - x$)

$$= k_B T \left[N \ln N - N + N \ln \frac{2\pi\hbar^2}{A m k_B T} \right]$$

$$\therefore \quad S = \frac{U-F}{T} = \underbrace{\frac{U}{T}}_{\substack{k_B N \\ \text{(from (b))}}} - \frac{F}{T}$$

$$= k_B N - k_B \left[\underbrace{N \ln N} - N + N \underbrace{\ln \frac{2\pi\hbar^2}{m A k_B T}} \right]$$

$$= k_B N \left[-\ln \frac{2\pi\hbar^2}{m A k_B T} - \ln N + 2 \right]$$

$$= k_B N \left[\ln \frac{m A k_B T}{2\pi\hbar^2 N} + 2 \right]$$

Thus (in 2D)

$$\boxed{S' = k_B N \left[\ln\left(\frac{A}{N} \cdot \frac{m k_B T}{2\pi\hbar^2} \right) + 2 \right]}$$

this is the 2D version of the Sackur-Tetrode equation

with $\frac{N}{A}$ taking the role of 2D "concentration"

and $\frac{m k_B T}{2\pi\hbar^2} \equiv n_Q^{(2D)}$ taking the role of the 2D <u>quantum concentration</u>

2 Quantum density of an ideal gas on the extreme relativistic regime.

$$E_{\underline{n}} = \frac{\pi \hbar c}{L} n \quad , \quad \text{where} \quad n = |\underline{n}| = \sqrt{n_x^2 + n_y^2 + n_y^2},$$

and (n_x, n_y, n_z) can take positive integers

$n_x = 1, 2, 3 \ldots$, $n_y = 1, 2, 3 \ldots$, $n_z = 1, 2, 3, \ldots$

Density of states : $D(E) = \dfrac{d\mathcal{N}(E)}{dE}$

where $\mathcal{N}(E)$ is the number of single-particle states in the energy range from 0 to E.

From $E_n = \dfrac{\pi \hbar c}{L} n$, the ~~largest~~ value of n corresponding to E is

$$n(E) = \frac{L}{\pi \hbar c} E$$

The derivations are similar to those in Lecture 12, except the energies are different [in Lecture 12, $E_{\underline{n}} = \dfrac{\hbar^2 \pi^2}{2mL^2} n^2$)

in 3D : $\mathcal{N}(E) = (2S+1)\,\frac{1}{8}\,\frac{4\pi}{3}\,n(E)^3$

$$= (2S+1)\,\frac{1}{8}\,\frac{4\pi}{3}\,\frac{L^3}{(\pi\hbar c)^3}\,E^3$$

$$\therefore\ D_3(E) = \frac{d\mathcal{N}(E)}{dE} = (2S+1)\,\frac{V\,E^2}{2\pi^2\hbar^3 c^3} \qquad (V = L^3)$$

in 2D : $\mathcal{N}(E) = (2S+1)\,\frac{1}{4}\pi n^2(E) = (2S+1)\,\frac{1}{4}\pi\,\frac{L^2}{(\pi\hbar c)^2}\,E^2$

$$\therefore\ D_2(E) = \frac{d\mathcal{N}(E)}{dE} = (2S+1)\,\frac{A}{2\pi\hbar^2 c^2}\,E \qquad (A = L^2)$$

in 1D : $\mathcal{N}(E) = (2S+1)\,n(E) = (2S+1)\,\frac{L}{\pi\hbar c}\,E$

$$\therefore\ D_1(E) = \frac{d\mathcal{N}(E)}{dE} = (2S+1)\,\frac{L}{\pi\hbar c} \quad \text{—— const.}$$

3 (a) Total average number of particles

$$N = \underbrace{\sum_{n} \sum_{S_z=-S}^{+S}}_{\substack{\text{sum}\\ \text{over}\\ \text{all}\\ \text{orbitals}}} \underbrace{f(E_n)}_{\substack{\text{average}\\ \text{occupancy}\\ \text{of an orbital}}} = (2S+1) \sum_{n} f(E_n)$$

[Fermi-Dirac or Bose-Einstein distribution functions, or their classical limit – the Boltzmann distribution function]

$$\xrightarrow{\text{in 3D}} (2S+1)\,\frac{1}{8}\,4\pi \int_0^\infty dn\, n^2 f(\underbrace{E_n}_{\hookrightarrow\, E_n = \frac{\pi\hbar c}{L} n})$$

$\left(\text{or} = \int_0^\infty dE\, D(E)\, f(E) \right.$, where $D(E)$ – from Problem 3 $\left. \right)$

For fermionic/bosonic atoms, the required integral would be:

$$N = (2S+1)\,\frac{1}{8}\,4\pi \int_0^\infty dn \frac{n^2}{\exp\left(\frac{\frac{\pi\hbar c}{L} n - \mu}{k_B T}\right) \pm 1}$$

"+" – fermions

"−" – bosons

If evaluated numerically, this integral determines N as a function of μ and T (and V), $N = N(\mu, T, V)$. This can be solved (numerically) to give

$\mu = \mu(N, T, V)$

Alternatively, using $N = \int_0^\infty dE\, D(E) f_{F/B}(E)$

For fermions: $$N = \frac{(2S+1)V}{2\pi^2 \hbar^3 c^3} \int_0^\infty dE \frac{E^2}{e^{\frac{E-\mu}{k_B T}} + 1}$$

For bosons: $$N = \frac{(2S+1)V}{2\pi^2 \hbar^3 c^3} \int_0^\infty dE \frac{E^2}{e^{\frac{E-\mu}{kT}} - 1}$$

where we took $D(E)$ (in 3D) from problem 3.

(b) Fo the classical Boltzmann distribution:

$$f_c(E_n) = \frac{1}{e^{(E_n-\mu)/k_B T}} = e^{-\frac{E_n-\mu}{k_B T}}$$

we get:

$$N = (2S+1)\,\frac{1}{8}\,4\pi \int_0^\infty dn\; n^2\; e^{-\frac{E_n-\mu}{k_BT}}$$

$$\left(\text{or}\quad N = \int_0^\infty dE\; D(E)\; e^{-\frac{E-\mu}{k_BT}}\right)$$

$$= (2S+1)\,\frac{\pi}{2}\; e^{\mu/k_BT} \int_0^\infty dn\; n^2\; e^{-E_n/k_BT}$$

$$= (2S+1)\,\frac{\pi}{2}\, e^{\mu/k_BT} \int_0^\infty dn\; n^2\; e^{-\frac{\pi\hbar c}{Lk_BT}n}$$

$$\text{def}:\; x \equiv \frac{\pi\hbar c}{Lk_BT}\, n$$

$$= (2S+1)\,\frac{\pi}{2}\, e^{\mu/k_BT}\,\frac{1}{\left(\frac{\pi\hbar c}{Lk_BT}\right)^3}\,\underbrace{\int_0^\infty dx\; x^2 e^{-x}}_{=\,2\ \text{(from tables of integrals)}}$$

$$= (2S+1)\,\frac{(k_BT)^3}{\pi^2\hbar^3c^3}\, V\, e^{\mu/k_BT}\;,\ \text{where}\ V = L^3$$

Thus

$$\boxed{N = (2S+1)\,\frac{V}{\pi^2\hbar^3c^3}\,(k_BT)^3\, e^{\mu/k_BT}}$$

The same result follows from

$$N = \int_0^\infty dE\; D(E)\; e^{(E-\mu)/k_BT} = e^{\mu/k_BT}\int_0^\infty dE\, D(E)\, e^{E/k_BT}$$

$= \ldots$ (see page 16)

(c) From the result for N in part (b),

$$e^{-\mu/k_BT} = (2S+1)\,\frac{(k_BT)^3}{\pi^2\hbar^3c^3}\,\frac{V}{N}$$

$$= (2S+1)\,\frac{\overbrace{\left(\frac{k_B^3T^3}{\pi^2\hbar^3c^3}\right)}^{\xrightarrow{\text{def.}}\ n_Q}}{\underbrace{\left(\frac{N}{V}\right)}_{\to\ n\ \text{(concentration)}}}$$

Define

$$\boxed{n_Q = \frac{k_B^3\,T^3}{\pi^2\hbar^3c^3}}$$ — quantum concentration (for extreme relativistic particles)

In the classical regime $e^{-\mu/k_BT} \gg 1$

(so that $f_{F(B)} \ll 1$ for all energies including $E=0$)

Therefore

$$e^{-\mu/k_BT} \gg 1 \quad \left(\text{with } e^{-\mu/k_BT} = (2S+1)\,\frac{n_Q}{n}\right)$$

implies

$$(2S+1)\,\frac{n_Q}{n} \gg 1$$

or $\boxed{n \ll n_Q}$ (if S is not too large)

$\hookrightarrow$ classical regime

$\therefore$ $\boxed{n \gtrsim n_Q}$ — quantum regime

$$N = \int_0^\infty dE \; \underbrace{D(E)} \; e^{(E-\mu)/k_BT}$$

$$\hookrightarrow D(E) = \frac{(2S+1)\,V}{2\pi^2\hbar^3c^3}\,E^2 \quad \left(\text{from problem 3 in 3D}\right)$$

$$= \frac{(2S+1)}{2\pi^2\hbar^3c^3}\, e^{\mu/k_BT} \int_0^\infty dE\; E^2\, e^{-E/k_BT}$$

def.: $x \equiv \frac{E}{k_BT}$

$$= \frac{(2S+1)}{2\pi^2\hbar^3c^3}\, e^{\mu/k_BT}\,(k_BT)^3 \underbrace{\left(\int_0^\infty dx\, x^2 e^{-x}\right)}_{=2}$$

$$= (2S+1)\frac{V}{\pi^2\hbar^3c^3}(k_BT)^3\, e^{\mu/k_BT}$$

Quantum temperature:

Rewrite $e^{-\mu/k_BT} = (2S+1)\,\frac{k_B^3T^3}{\pi^2\hbar^3c^3}\,\frac{V}{N}$ as

$$e^{-\mu/k_BT} = (2S+1)\frac{T^3}{\left(\frac{\pi^2\hbar^3c^3}{k_B^3}\right)\underbrace{\left(\frac{N}{V}\right)}_{=n}}$$

define: $\boxed{T_Q = \frac{\pi^2\hbar^3c^3}{k_B^3\, n}}$ — quantum temperature

$\therefore\; e^{-\mu/k_BT} = (2S+1)\,\frac{T^3}{T_Q^3} \gg 1$ implies $\underline{\underline{T \gg T_Q}}$

— classical regime ; and $\underline{\underline{T \lesssim T_Q}}$ — quantum regime

4 To find $\frac{U}{N}$, need to find each, N and U first.

$$N \equiv \langle N \rangle = \sum_{\underline{n}} \langle N(E_{\underline{n}}) \rangle$$

(neglect spin, assume $S=0$ then $2S+1=1$)

where $\langle N(E_{\underline{n}}) \rangle$ is the thermal average occupancy of a single-orbital state of energy $E_{\underline{n}}$. In the classical regime $\langle N(E_{\underline{n}}) \rangle$ is given by the Boltzmann distribution function

$$\langle N(E_{\underline{n}}) \rangle \equiv f_c(E_{\underline{n}}) = e^{-(E_{\underline{n}} - \mu)/k_B T}$$

Therefore

$$N = \sum_{\underline{n}} \langle N(E_{\underline{n}}) \rangle = \sum_{\underline{n}} f_c(E_{\underline{n}})$$

$$\xrightarrow{\text{in 3D}} \frac{1}{8} 4\pi \int_0^\infty dn \, n^2 \, e^{-(E_{\underline{n}} - \mu)/k_B T}$$

$$= \frac{\pi}{2} e^{\mu/k_B T} \int_0^\infty dn \, n^2 \, e^{-\frac{\hbar \pi c}{L k_B T} n}$$

define $x \equiv \frac{\hbar \pi c}{L k_B T} n$

$$= \frac{\pi}{2} e^{\mu/k_B T} \left(\frac{L k_B T}{\hbar \pi c}\right)^3 \underbrace{\int_0^\infty dx\, x^2 e^{-x}}_{=2}$$

$$= e^{\mu/k_B T} \frac{L^3 (k_B T)^3}{\pi^2 \hbar^3 c^3} \qquad (L^3 = V)$$

Thus

$$\boxed{N = \frac{V (k_B T)^3}{\pi^2 \hbar^3 c^3} e^{\mu/k_B T}}$$

$$\boxed{\int_0^\infty dx\, x^n e^{-ax} = \frac{n!}{a^{n+1}} \quad (n = 1, 2, 3, \dots)}$$

Next U: (total energy)

$$U = \sum_{\underline{n}} E_{\underline{n}} \langle N(E_{\underline{n}}) \rangle = \sum_{\underline{n}} E_{\underline{n}} \underbrace{f_c(E_{\underline{n}})}$$

in the classical regime – Boltzmann distribution

$$f_c(E_n) = e^{-(E_n - \mu)/k_B T}$$

$$\longrightarrow \frac{1}{8} 4\pi \int_0^\infty dn\, n^2 E_{\underline{n}} f_c(E_{\underline{n}}) =$$

$$= \frac{\pi}{2} \int_0^\infty dn\, n^2 E_n\, e^{-(E_n - \mu)/k_B T}$$

$$= \frac{\pi}{2} e^{\mu/k_B T} \int_0^\infty dn\, n^2 \left(\frac{\pi \hbar c}{L} n\right) e^{-\frac{\pi \hbar c}{L k_B T} n}$$

def $\quad x \equiv \frac{\pi \hbar c}{L k_B T} n$

$$= e^{\mu/k_B T} \frac{\pi}{2} \left(\frac{\pi \hbar c}{L}\right) \left(\frac{L k_B T}{\pi \hbar c}\right)^4 \underbrace{\int_0^\infty dx\, x^3 e^{-x}}_{=3!=6}$$

Thus

$$U = e^{\mu/k_B T} \cdot 3\pi k_B T \cdot \left(\frac{L k_B T}{\pi \hbar c}\right)^3$$

$$\boxed{U = e^{\mu/k_B T} \frac{3V (k_B T)^4}{\pi^2 \hbar^3 c^3}}$$

$$\boxed{\int_0^\infty dx\, x^n e^{-x} = n!}$$

Combine the results for N and U to find $\frac{U}{N}$

$$\frac{U}{N} = \frac{e^{\mu/k_B T} 3V (k_B T)^4}{\pi^2 \hbar^3 c^3 \cdot e^{\mu/k_B T} \frac{V (k_B T)^3}{\pi^2 \hbar^3 c^3}} =$$

$$= 3 k_B T$$

Thus $\boxed{\frac{U}{N} = 3 k_B T}$

— $k_B T$ per degree of freedom for relativistic particles (instead of $\frac{1}{2} k_B T$ per degree of freedom for non-relativistic particles)