PHY 252 S: HW # 3

Q1: Definitions

(a) Scale height – a height at which the pressure of an ideal gas, for instance, decreases by the fraction $e^{-1} \simeq 0.37$ in an external gravity field. The characteristic height for an isothermal (hypotetical) atmosphere of the Earth is

$$h_s \simeq 8.5 \text{ km} \simeq 5 \text{ mi}.$$

(b) Absolute activity – that part of the Boltzmann factor in the grand partition function (Gibbs sum) which is associated with the chemical potential μ. $\Rightarrow$ $\lambda \equiv \exp(\mu/\tau)$

More precisely we can say that it is part of the Gibbs factor: $\exp(N\mu - \varepsilon)/\tau$

(c) Orbital – an energy state of the Schrödinger equation in the one-particle approximation. This is useful in the weakly interacting particle regime, whereby the orbital model allows us to approximate an exact quantum state of the Schrödinger equation of a system of N particles in terms of an approximate quantum state that is constructed by assigning the N particles to orbitals, which are solutions to a one-particle Schrödinger equation. Usually there is an infinity of states available for occupancy. The term "orbital" is used even when there is no analogy to a classical orbit or to a Bohr orbit. It simply denotes energy state! The orbital model is an exact solution to the N-particle problem only if there are no interactions between the particles.

(d) Pauli exclusion principle – a principle which states that each orbital can by occupied b 0 or 1 fermion of the same species. It forms the basis for Fermi-Dirac statistics. Examples: electrons in the shell model of the atom; electrons in the conduction band in solid-state physics; nucleons (protons & neutrons) in the shell model of the nucleus; etc.

(e) Bose-Einstein distribution function – distribution function obeyed by bosons (particles with integral value of the spin). The occupancy rule for bosons is that each orbital can ~~be~~ be occupied by any number of bosons, so that bosons have an essentially different quality than fermions. Systems of bosons can have rather different physical properties from those of fermions. Examples: photons and phonons whose number is not conserved; any excitation of an oscillator; atoms of ^{4}He; etc.

Note: The carriers of all 4 fundamental interactions (gravitational, electromagnetic, weak and strong) are bosons!

Q 2: (A) KK 5.8 Carbon monoxide poisoning.

(a) In the absence of CO we have a Gibbs sum for 2-level system

$$\mathcal{Z}_2 = 1 + \lambda(O_2)\exp(-\varepsilon_A/\tau)$$

Therefore the fraction f of Hb occupied by O_2 is

$$f_{O_2} = \frac{\lambda(O_2)\exp(-\varepsilon_A/\tau)}{1+\lambda(O_2)\exp(-\varepsilon_A/\tau)} =$$

$$= \frac{1}{\lambda^{-1}(O_2)\exp(\varepsilon_A/\tau)+1}$$

$$\therefore \quad \lambda^{-1}(O_2)\exp(\varepsilon_A/\tau)+1 = \frac{1}{f_{O_2}}$$

$$\exp(\varepsilon_A/\tau) = \lambda(O_2)\left(\frac{1}{f_{O_2}}-1\right)$$

$$\varepsilon_A = \tau\ln\left[\lambda(O_2)\left(\frac{1}{f_{O_2}}-1\right)\right]$$

$$\therefore \quad \underline{\underline{\varepsilon_A = k_B T\ln\left[\lambda(O_2)\left(\frac{1}{f_{O_2}}-1\right)\right]}} \; //$$

$$\varepsilon_A = (1.38066\times10^{-16}[\mathrm{erg\,K^{-1}}])\times(273.16\,\mathrm{K}+37^\circ\mathrm{C})\times$$

$$\times\ln\left[10^{-5}\times\left(\frac{10}{9}-1\right)\right] =$$

$$= 4.28\times10^{-14}[\mathrm{erg}]\times[-5\ln(10)-\ln(9)] =$$

$$= 4.28 \times 10^{-14} [\text{erg}] [-5 \times 2.3026 - 2.197] =$$

$$= -13.71 \times 4.28 \times 10^{-14} [\text{erg}] =$$

$$\varepsilon_A \cong -5.868 \times 10^{-13} [\text{erg}] = -\frac{5.868 \times 10^{-13}}{1.60219 \times 10^{-12}} [\text{eV}]$$

$$\therefore \boxed{\varepsilon_A \cong -3.6625 \times 10^{-1} = -0.366 [\text{eV}]}$$

(b) With CO we have a Gibbs sum for 3-level system

$$\mathcal{Z}_3 = 1 + \lambda(O_2) \exp(-\varepsilon_A/\tau) + \lambda(CO) \exp(-\varepsilon_B/\tau)$$

and the fraction f of Hb occupied by O_2 is

$$f_{O_2} = \frac{\lambda(O_2) \exp(-\varepsilon_A/\tau)}{1 + \lambda(O_2) \exp(-\varepsilon_A/\tau) + \lambda(CO) \exp(-\varepsilon_B/\tau)}$$

$$= \frac{1}{1 + \lambda^{-1}(O_2) \exp(\varepsilon_A/\tau) + \lambda(CO) \lambda^{-1}(O_2) \exp[(\varepsilon_A - \varepsilon_B)/\tau]}$$

or better

$$1 + \lambda(O_2) \exp(-\varepsilon_A/\tau) + \lambda(CO) \exp(-\varepsilon_B/\tau) =$$

$$= \lambda(O_2) \exp(-\varepsilon_A/\tau) \cdot \frac{1}{f_{O_2}}$$

$$\therefore \lambda(CO) \exp(-\varepsilon_B/\tau) = \lambda(O_2) \exp(-\varepsilon_A/\tau) \left[\frac{1}{f_{O_2}} - 1\right] - 1 \quad (**)$$

Take logarithm of both sides

$$\boxed{\ln[\lambda(CO)] - \frac{\varepsilon_B}{\tau} = \ln\left\{\lambda(O_2)\exp(-\varepsilon_A/\tau)\left[\frac{1}{f_{O_2}}-1\right]-1\right\}}$$

where

$$-\frac{\varepsilon_A}{\tau} = -\frac{(-0.366[eV])}{k_B T} = \frac{0.366\times 1.60219\times 10^{-12}[erg]}{4.28\times 10^{-14}[erg]} =$$

$$= +0.137\times 10^{2} = \underline{\underline{13.7}}$$

and $\lambda(O_2)\times e^{+13.7}\times(10-1)-1 = 10^{-5}\times e^{+13.7}\times 9-1 \simeq$

$$= 9\times 8.909 - 1 = \underline{79.181}$$

$$\therefore\quad \varepsilon_B = \left(\ln[\lambda(CO)] - \ln\left\{\lambda(O_2)\exp(-\varepsilon_A/\tau)\left[\frac{1}{f_{O_2}}-1\right]-1\right\}\right)\times\tau$$

or $\varepsilon_B = k_B T\left(\ln[\lambda(CO)] - \ln\left\{\lambda(O_2)\exp(-\varepsilon_A/\tau)\left[\frac{1}{f_{O_2}}-1\right]-1\right\}\right)$

$$\varepsilon_B = 4.28\times 10^{-14}[erg]\left(-7\ln(10) - \ln 79.181\right) =$$

$$= -4.28\times 10^{-14}[erg]\left(7\times 2.3026 + 4.372\right) =$$

$$= -4.28\times 10^{+14}[erg]\times(20.49) =$$

$$= -\frac{8.7697\times 10^{-13}}{1.60219\times 10^{-12}}[eV] = -5.4736\times 10^{-1}[eV]$$

$$\therefore\quad \boxed{\varepsilon_B \simeq -0.5473[eV]}$$

A very similar result we will obtain if we disregard -1 in $(**)$. Then

$$\ln[\lambda(CO)] - \frac{\varepsilon_B}{\tau} = \ln[\lambda(O_2)] - \frac{\varepsilon_A}{\tau} + \ln\left(\frac{1}{f_{O_2}} - 1\right)$$

$$\therefore \quad \frac{\varepsilon_B}{\tau} - \ln[\lambda(CO)] = \frac{\varepsilon_A}{\tau} - \ln[\lambda(O_2)] - \ln\left(\frac{1}{f_{O_2}} - 1\right)$$

$$\therefore \quad \boxed{\varepsilon_B = \varepsilon_A + \tau\left\{\ln[\lambda(CO)] - \ln[\lambda(O_2)] - \ln\left(\frac{1}{f_{O_2}} - 1\right)\right\}}$$

where

$$\ln[\lambda(CO)] = -7 \times \ln(10) = -16.118$$

$$\ln[\lambda(O_2)] = -5 \times \ln(10) = -11.513$$

$$\ln\left(\frac{1}{f_{O_2}} - 1\right) = \ln(10-1) = \ln(9) = +2.197$$

$$\therefore \quad \varepsilon_B = \varepsilon_A + k_B T\{-16.118 + 11.513 - 2.197\} =$$

$$= \varepsilon_A - 6.802 \times 4.28 \times 10^{-14}\,[\text{erg}] =$$

$$= \varepsilon_A - 2.911 \times 10^{-13}\,[\text{erg}] =$$

$$= \varepsilon_A - \frac{2.911 \times 10^{-13}}{1.60219 \times 10^{-12}}\,[\text{eV}] = \underline{\varepsilon_A - 0.1817\,[\text{eV}]}$$

$$\therefore \quad \boxed{\varepsilon_B = -0.548\,[\text{eV}]}$$

(B) Possible states

○——○ ← $\varepsilon_0 = 0.00$ [eV]

$$\left.\begin{array}{l} ●\!\!-\!\!-\!\!○ \leftarrow \varepsilon_1 = -0.55\,[eV] \\ ○\!\!-\!\!-\!\!● \leftarrow \varepsilon_2 = -0.55\,[eV] \end{array}\right\} = \varepsilon_A \longrightarrow \mathcal{Z}_1 = 1 + 2\lambda \exp(-\varepsilon_A/\tau) + \lambda \exp(-\varepsilon_B/\tau)$$

●——● ← $\varepsilon_4 = -1.30$ [eV] $\} = \varepsilon_B$

$$\tau = k_B T = 2.67 \times 10^{-2}\,[eV]$$

For the fraction of the singly occupied states we have

$$f_s = \frac{2\lambda \exp(-\varepsilon_A/\tau)}{1 + 2\lambda \exp(-\varepsilon_A/\tau) + \lambda \exp(-\varepsilon_B/\tau)} =$$

$$= \frac{1}{1 + \frac{1}{2}\lambda^{-1} \exp(\varepsilon_A/\tau) + \frac{1}{2}\exp[(\varepsilon_A - \varepsilon_B)/\tau]}$$

where $\lambda = n/n_Q = p/\tau n_Q$; $p_0 \equiv n_Q \tau \exp(\varepsilon_A/\tau)$

$$\therefore\ f_s = \frac{1}{1 + \frac{1}{2}\frac{p_0}{p} + \frac{1}{2}\exp[(\varepsilon_A - \varepsilon_B)/\tau]}$$

$$\therefore\ \boxed{f_s = \frac{2p}{p_0 + p\left(2 + \exp[(\varepsilon_A - \varepsilon_B)/\tau]\right)}}$$

For the fraction of the doubly occupied states we have, accordingly:

$$f_d = \frac{\lambda \exp(-\varepsilon_B/\tau)}{1 + 2\lambda \exp(-\varepsilon_A/\tau) + \lambda \exp(-\varepsilon_B/\tau)}$$

$$= \frac{1}{1 + 2\exp[(\varepsilon_B - \varepsilon_A)/\tau] + \lambda^{-1}\exp(\varepsilon_B/\tau)}$$

where $\lambda = n/n_Q = P/\tau n_Q$; $P_0 \equiv n_Q \tau \exp(\varepsilon_B/\tau)$

$$\therefore f_d = \frac{1}{1 + 2\exp[(\varepsilon_B - \varepsilon_A)/\tau] + \frac{P_0}{P}}$$

$$\therefore \boxed{f_d = \frac{P}{P_0 + P(1 + 2\exp[(\varepsilon_B - \varepsilon_A)/\tau])}}$$

Now,

$$\frac{\varepsilon_A - \varepsilon_B}{\tau} = \frac{-0.55 + 1.30\,[eV]}{2.67 \times 10^{-2}\,[eV]} \cong +28.1$$

$$\frac{\varepsilon_B - \varepsilon_A}{\tau} = \frac{-1.30 + 0.55\,[eV]}{2.67 \times 10^{-2}\,[eV]} \cong -28.1$$

Therefore

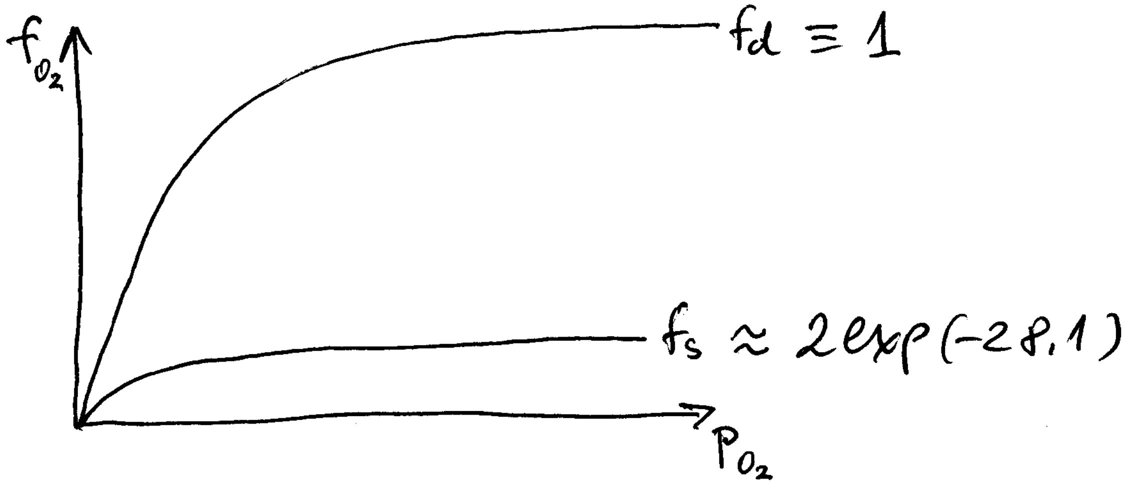
$$f_s = \frac{2P}{P_0 + P(2+\exp(+28.1))} \approx \frac{2P}{P_0 + P\exp(+28.1)} \approx$$

$$\approx 2\exp(-28.1)$$

and

$$f_d = \frac{P}{P_0 + P(1+2\exp(-28.1))} \approx$$

$$\approx \frac{P}{P_0 + P}$$ ← Langmuir adsorption isotherm



The fraction of the singly occupied sites are exponentially suppressed compared to doubly occupied sites.

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Q3: KK 5.12 Ascent of sap in trees.

Water vapor is considered in the Earth's atmosphere an ideal gas which obeys the barometric pressure equation (known in Meteorology as the hydrostatic equation):

$$p(h) = p(0)\exp(-Mgh/\tau) = p(0)\exp(-h/h_c)$$

In our case: $p(0) = n_0$; $p(h) = r n_0$

$$\tau \equiv k_B T = 1.38066\times 10^{-16}\,[\mathrm{erg/K}] \times (273.16\mathrm{K} + 25^\circ\mathrm{C}) =$$

$$= 4.1166\times 10^{-14}\,[\mathrm{erg}]$$

$$g = 980\,[\mathrm{cm/s^2}]$$

$$M_{H_2O} = (2H_1 + O_{16})\times 1[\mathrm{a.u.}] = 18\times 1.660566\times 10^{-24}\,[\mathrm{gm}]$$

$$= 29.89\times 10^{-24}\,[\mathrm{gm}] \approx 30\times 10^{-24}\,[\mathrm{gm}]$$

$$r = 0.9$$

and assuming isothermal atmosphere, we have

$$r\cancel{n_0} = \cancel{n_0}\exp(-M_{H_2O}\,gh/\tau)$$

$$\therefore\ h = -\frac{\tau}{M_{H_2O}\,g}\ln(r) =$$

$$= -\frac{4.1166\times 10^{-14}\,[\mathrm{erg}]}{(30\times 10^{-24}\,[\mathrm{gm}])\times 980\,[\mathrm{cm/s^2}]}\ln(0.9) =$$

$$= 0.10536 \times 1.4 \times 10^{-4} \times 10^{-14+24} [cm]$$

$$= 0.10536 \times 1.4 \times 10^{6} [cm] =$$

$$= 0.10536 \times 1.4 \times 10^{4} [m] =$$

$$= 0.10536 \times 14 [km] \simeq$$

$$\simeq \underline{\underline{1.475 [km]}} //$$

Note: we found the characteristic height to be

$$h_c \simeq 14 [km]$$

which is roughly the depth of the troposphere! We also found that the maximum height of the water rise is

$$h_{max}^{H_2O} \simeq 1.475 [km]$$

which is exactly the assumed height of the Planetary Boundary Layer (PBL)! The troposphere contains almost all of the moisture in the Earth's atmosphere, and nearly 90% of it is contained in the Planetary Boundary Layer (PBL). On these grounds we can conclude that our solution is of the right order!

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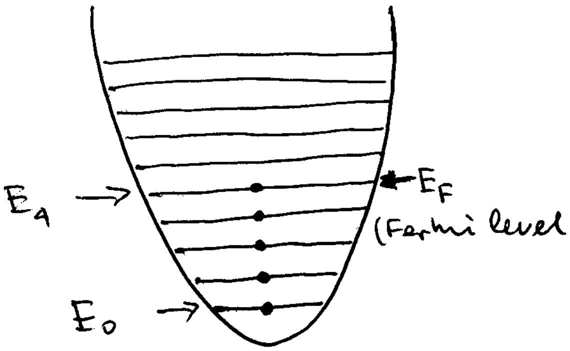
Q. 4: We assume 5 spinless particles distributed over nondegenerate, evenly spaced levels, and which can assume the form of identical fermions, identical bosons or distinguishable classical particles. The partition function in general is given by:

$$Z_C = Z_1 Z_2 Z_3 \times \cdots \times Z_N \leftarrow \text{for N classical particles}$$

$$Z_Q = \frac{1}{N!} Z_1 Z_2 Z_3 \times \cdots \times Z_N \leftarrow \text{for N quantum particles}$$

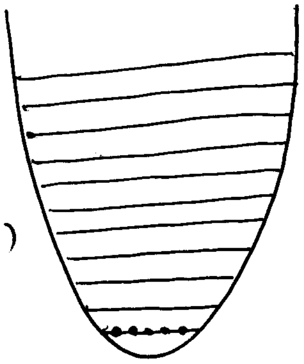
(a)

Fermions



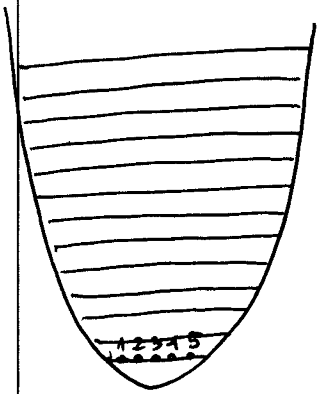
Pauli exclusion principle

Bosons



Bose-Einstein condensate

Classical



Distinguishable particles (unrealizable in Nature)

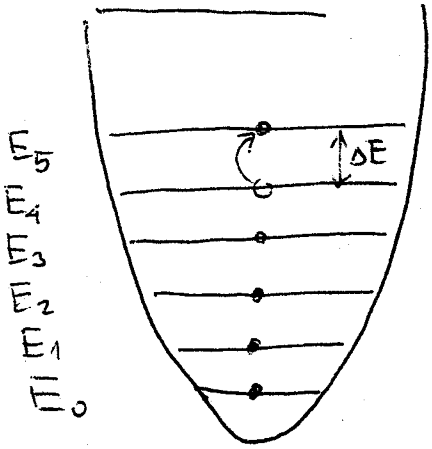
$$Z_F = \frac{1}{5!} e^{-(\sum_{i=0}^{4} E_i)/\tau} \qquad Z_B = \frac{1}{5!} e^{-(\sum_{i=0}^{4} E_0)/\tau} \qquad Z_c = e^{-5E_0/\tau}$$

Ground state assume to be at T = 0!

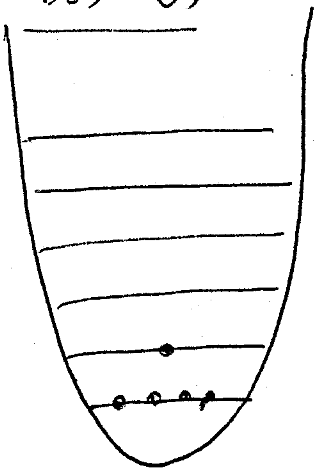
Ground state is also non-degenerate!

(b)

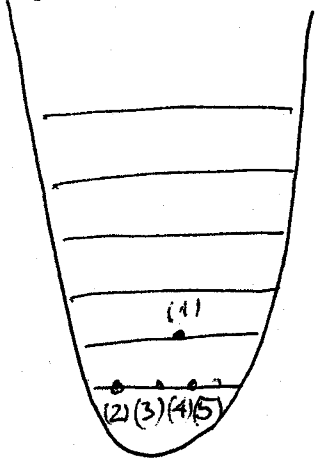
Fermions



Bosons



Classical



$E_0+E_1+E_2+E_3+E_5$

(1+2+3+4+6)

1- state

$4E_0 + E_1 \Rightarrow (4+2)$

(1+1+1+1+2)

1 - state

indistinguishable quantum particles

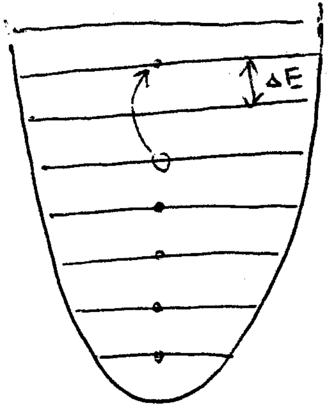
$4E_0 + E_1$

(1+1+1+1+2)

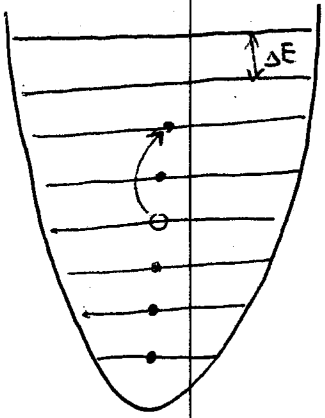
5 - states

distinguishable classical particles

(c) **Fermions:**



+2ΔE units of energy



(1+2+3+4+7)

(1+2+3+5+6)

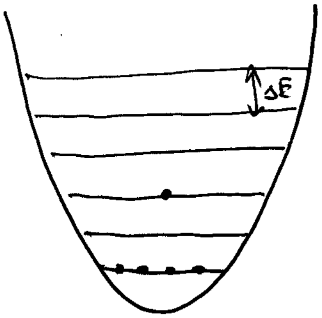
2 - states

For $+3\Delta E$ we have

$$\left\{\begin{array}{l} 1+2+3+4+(5+3) = 1+2+3+4+8 \\ 1+2+3+(4+3)+5 = 1+2+3+5+7 \\ 1+2+(3+3)+4+5 = 1+2+4+5+6 \end{array}\right\}$$

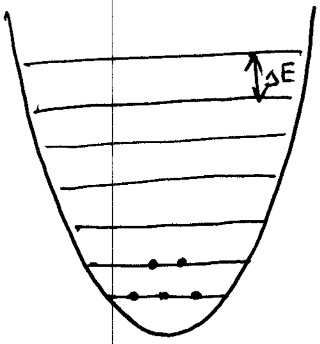
3 - system states

Bosoms:



(1+1+1+1+3)

$+2\Delta E$
units of
energy



(1+1+1+2+2)

2 - states

For $+3\Delta E$ we have

$$\left\{\begin{array}{l} 1+1+1+1+(1+3) = 8 \\ 1+1+1+(1+1)+(1+2) = 8 \\ 1+1+(1+1)+(1+1)+(1+1) = 8 \end{array}\right\}$$

3 - system states

<u>Classical:</u> The total energy of the system is exactly that of Bosons, but we have count different multiplicities for distinguishable particles.

+2ΔE units of energy

$(\underbrace{1+1+1+1}+\underbrace{3}) \Rightarrow g(4,1) = 5 \leftarrow \{\text{any one of } \underset{1-5}{} \text{ particles}\}$

$(\underbrace{1+1+1}+\underbrace{2+2}) \Rightarrow g(3,2) =$

$$= \begin{bmatrix} 1,2 \\ 1,3 \\ 1,4 \\ 1,5 \end{bmatrix} + \begin{bmatrix} 2,3 \\ 2,4 \\ 2,5 \end{bmatrix} + \begin{bmatrix} 3,4 \\ 3,5 \end{bmatrix} + \begin{bmatrix} 4,5 \end{bmatrix} =$$

$$= 4 + 3 + 2 + 1 = 10$$

$\therefore\ g(+2\Delta E) = g(4,1) + g(3,2) = 5 + 10 = \underline{\underline{15}}$ //

15 - system states

+3ΔE units of energy

$(\underbrace{1+1+1+1}+\underbrace{4}) \Rightarrow g(4,1) = 5 \leftarrow \{\text{any one of } \underset{1-5}{} \text{ particles}\}$

$(\underbrace{1+1+1}+\underbrace{2}+\underbrace{3}) \Rightarrow g(3,1,1) \equiv g(3,2) \equiv 10$

$(\underbrace{1+1}+\underbrace{2}+\underbrace{2}+\underbrace{2}) \Rightarrow g(2,3) =$

$$\begin{bmatrix} 1,2,3 \\ 1,2,4 \\ 1,2,5 \end{bmatrix} + \begin{bmatrix} 1,3,4 \\ 1,3,5 \end{bmatrix} + \begin{bmatrix} 1,4,5 \end{bmatrix} +$$

$$\begin{bmatrix}2,3,4\\2,3,5\end{bmatrix} + [2,4,5] + [3,4,5] =$$

$$= 3 + 2 + 1 + 2 + 1 + 1 = 10$$

$$\therefore\ g(+3\Delta E) = g(4,1) + g(3,2) + g(2,3) =$$

$$= 5 + 10 + 10 = \underline{\underline{25}}\ /\!/$$

<u>25 - system states</u>

(d) As we see, the main difference between the bosonic and classical system is the large multiplicity factor for the classical distinguishable particles. Therefore there are many more available states for the classical system than for the quantum one. This leads to the fact that the entropy of the classical system is much larger than the entropy of the quantum one. This tells you that with classical particles it would be much more difficult to obtain Bose - Einstein condensation!

Q5: (A) KK 6.1 Derivative of Fermi-Dirac function.

$$f(\varepsilon) = \frac{1}{\exp[(\varepsilon-\mu)/\tau]+1}$$

$$\therefore -\frac{\partial f(\varepsilon)}{\partial \varepsilon}\Big|_{\varepsilon=\mu} = +\frac{\exp[(\varepsilon-\mu)/\tau]\cdot\left(\frac{1}{\tau}\right)}{\{\exp[(\varepsilon-\mu)/\tau]+1\}^2}\Big|_{\varepsilon=\mu} = \frac{e^0}{\{\underbrace{e^0+1}_{2}\}^2}\,\frac{1}{\tau} = \underline{\underline{(4\tau)^{-1}}}$$

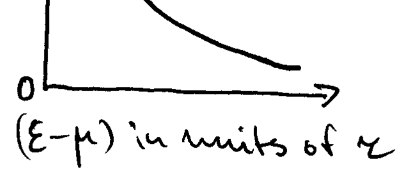
(B) Derivative of Bose-Einstein distribution function

$$f(\varepsilon) = \frac{1}{\exp[(\varepsilon-\mu)/\tau]-1}$$

$$\therefore \frac{\partial f(\varepsilon)}{\partial \varepsilon}\Big|_{\varepsilon=\mu} = -\frac{\exp[(\varepsilon-\mu)/\tau]\cdot(1/\tau)}{\{\exp[(\varepsilon-\mu)/\tau]-1\}^2}\Big|_{\varepsilon=\mu} =$$

$$= -\frac{e^0}{\{e^0-1\}^2}\cdot\left(\frac{1}{\tau}\right) = -\frac{1}{(1-1)^2}\cdot\left(\frac{1}{\tau}\right) = -\infty$$

$$\therefore -\frac{\partial f(\varepsilon)}{\partial \varepsilon}\Big|_{\varepsilon=\mu} = \underline{\underline{\infty}}$$ ← for fixed temperature!



For bosons the derivative of the distribution function at the chemical potential is independent of temperature, and is infinite.