KING FAHD UNIVERSITY of PETROLIUM and MINERALS Physics Department Statistical Mechanics I (Phys-530) Fall 2005 Help Session # 1

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1- A box is separated by a partition which divides its volume in the ratio 3:1. The larger portion of the box contains 1000 molecules of Ne gas; the smaller, 100 molecules of He gas. A small hole is punctured in the partition, and one waits until equilibrium is attained.

a. Find the mean number of molecules of each type on either side of the partition.

b. What is the probability of finding 1000 molecules of Ne gas in the larger portion and 100 molecules He gas in the smaller (i.e., the same distribution as in the initial system)?

- 2- A system of N molecules of type 1 and M molecules of type 2 confined within a box of volume V. The molecules are supposed to interact very weakly so that they constitute an ideal gas mixture.
- a) How does the total number of states in the range between E and $E+\Delta E$ depend on the volume of this system? Treat the problem in microcanonical system.
- b) Use this result to find the equation of state of this system, i.e. to find the its mean pressure P as a function of V and T.
- 3- Consider an ensemble of N = 18 distinguishable molecule systems of fixed energy $U = 6\varepsilon$ and a fixed volume such that the only individual molecule energy states are fixed as 0, ε , and 2ε . If N_i is the number of molecules in state *i* (=0, 1, 2), show by explicit calculation that the full ensemble average and the average in the most probable distribution for (N_i/N) are practically identical.
- 4- Consider an ensemble of N = 4 distinguishable molecule systems of fixed energy $U = 12 \varepsilon$ and a fixed volume such that the only individual molecule energy states are fixed as 1, 2ε , 3ε , and 4ε . If N_i is the number of molecules in state i (= 1, 2, 3, 4). Determine the number of possible macrostates and find the number of microstates associated with the macrostates.
- 5- Consider an ensemble of N = 4 distinguishable molecule systems of fixed energy $U = 10\varepsilon$ and a fixed volume such that the only individual molecule energy states are fixed as 1, 2 ε , 3 ε , and 4 ε . If N_i is the number of molecules in state i (= 1, 2, 3, 4). Determine the number of possible macrostates and find the number of microstates associated with the macrostates.
- 6- A box is separated by a partition which divides its volume in the ratio 3:1. The larger portion of the box contains 1000 molecules of Ne gas; the smaller, 100 molecules of He gas. A small hole is punctured in the partition, and one waits until equilibrium is attained. a) find the mean number of molecules of each type on either side of the

partition. b) What is the probability of finding 1000 molecules of Ne gas in the larger portion and 100 molecules He gas in the smaller (i.e., the same distribution as in the initial system)?

7- Some substance has the entropy function

$$S = aV^{\frac{1}{2}}(NE)^{\frac{1}{4}}$$

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where N is the number of moles, and a is a constant with the appropriate units. A cylinder is separated by a fixed partition into two halves, each of volume 1 m^3 . One mole of the substance with energy of 200 J is placed in the left half, while two moles of the substance with energy of 400 J is placed in the right half.

- a) Assuming that the partition conducts heat, what will be the distribution of energy between left and right at equilibrium?
- b) Assuming the partition moves freely and also conducts heat, what will be the volumes and energies of the samples in both sides at equilibrium?

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- A box is separated by a partition which divides its volume in the ratio 3:1. The larger portion of the box contains 1000 molecules of Ne gas; the smaller, 100 molecules of He gas. A small hole is punctured in the partition, and one waits until equilibrium is attained.
 - a. Find the mean number of molecules of each type on either side of the partition. In equilibrium, the densities on both sides of the box are the same. Thus, in the larger volume, the mean number will be

$$(\frac{3}{4})(1000 \text{ Ne}) + (\frac{3}{4})(100 \text{ He}) = 750 + 75 = 825$$

In the other side, it is

$$1100 - 825 = 275$$

b. What is the probability of finding 1000 molecules of Ne gas in the larger portion and 100 molecules He gas in the smaller (i.e., the same distribution as in the initial system)?

$$p = (\frac{3}{4})^{1000} (\frac{1}{4})^{100} \approx 10^{-185}$$

 A system of N molecules of type 1 and M molecules of type 2 confined within a box of volume V. The molecules are supposed to interact very weakly so that they constitute an ideal gas mixture. Since

$$\Omega(E) \propto V^N \Sigma(E)$$

then for two noninteracting species with total energy $E = E_1 + E_2$.

a. How does the total number of states in the range between E and $E + \Delta E$ depend on the volume of this system? treat the problem in microcanonical system.

$$Ω(E) = Ω_1(E_1)Ω_2(E_2) = CV^{N_1+N_2}Σ_1(E_1)Σ_2(E_2)$$

b. Use this result to find the equation of state of this system, i.e. to find the its mean pressure P as a function of V and T.

$$\begin{split} \ln(\Omega(E)) &= (N_1 + N_2) \ln V + \ln C + \ln(\Sigma_1 \Sigma_2) \\ \overline{P} &= \frac{1}{\beta} \left(\frac{\partial}{\partial V} \ln \Omega \right) = \frac{1}{\beta} \frac{(N_1 + N_2)}{V} \Longrightarrow \\ \overline{P}V &= (N_1 + N_2) kT \end{split}$$

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Example: Consider an ensemble of N = 18 distinguishable molecule systems of fixed energy $U = 6\varepsilon$ and a fixed volume such that the only individual molecule energy states are fixed as 0, ε , and 2ε . If N_i is the number of molecules in state i (=0, 1, 2), show by explicit calculation that the full ensemble average and the average in the most probable distribution for (N_i/N) are practically identical.

Solution: the following constrains:

 $N_o + N_1 + N_2 = 18,$ And $N_o(0) + N_1\varepsilon + N_2(2\varepsilon) = 6\varepsilon$

have the following distributions:

Energy	Macrostates			
	а	b	с	d
2ε	3	2	1	0
3	0	2	4	6
0	15	14	13	12
$w_i = \frac{N!}{\prod_{i=1}^r N_i!}$	816	18,360	42,840	18,564

With $\Omega = w_a + w_b + w_c + w_d = 80,580$

Distribution "c" is the most probable, and even in this few-molecule case, $ln(\Omega) = 11.3$ and $ln(w_c) = 10.7$ do not differ greatly and both are of order N = 18. The number of distribution (M = 4) is also of order N.

In the most probable distribution

$$\frac{N_o}{N} = \frac{13}{18} = 0.722, \quad \frac{N_1}{N} = \frac{4}{18} = 0.222, \quad \frac{N_2}{N} = \frac{1}{18} = 0.056.$$

The full ensemble average may be calculated as follows: The total number of molecules in all the replicas of the system is given by: 18 w = 1,450,440 of which the number in the zero state are:

(816)(15)(1) + (18,360)(14)(1) + (42,840)(13)(1) + (18,564)(12)(1) = 1,048,968.

____0

_____6

____12

3 _____ 0 ____

___2

ß

____2 ____1

_____14 _____13

____4

21

2ε _____ 3

ε____3

0 ____ 15

a

The inclusion of the factor (1) is due to the equal a priori probability. The weight factor w_i differ because of the great difference in the number of micromolecular ways in which these modes of occupation can be realized. Finally,

 $\frac{\overline{N_o}}{N} = \frac{1,048,968}{1,450,440} = 0.723$, similarly $\frac{\overline{N_1}}{N} = 0.220$, and $\frac{\overline{N_2}}{N} = 0.057$.

These ensemble results agree with the most probable results.