

الفرقة الثالثة (فيزياء)

مادة (إحصائية)

الزمن ساعتان

جامعة بنها

كلية التربية

دور يناير 2011

تاريخ الامتحان: 2011/1/15

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ورقة كاملة

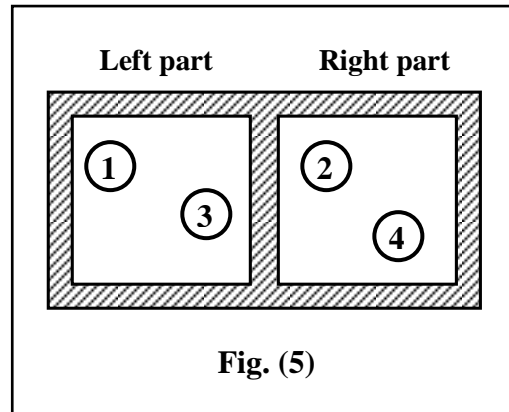
1. Write on the total ways in which four molecules of a gas can be distributed between two halves of a vessel. (comment on the results)

----- Solution -----

The second law of thermodynamics states that irreversible process proceed so that the entropy of the system of bodies participating in a process grows, tending to a maximum value. The maximum value of the entropy is reached when the system arrives at a state of equilibrium.

At the same time, we have seen that the irreversibility of heat process itself is connected with the fact that the transition to the equilibrium states more probable in comparison with all other transitions. This is why we only observe such changes of state in which a system passes from a less probable to a more probable state. The similarity in the behavior of the two quantities – entropy and probability – is striking: both of them grow upon a transition to equilibrium. It is therefore natural to relate the entropy of a system in a certain state to the probability of this state. This relationship was discovered by L. Boltzmann.

First of all we must define more precisely the concept of the probability of a state. This can be done in the simplest way if we use the example of distribution of gas molecules in the volume of a vessel.



Imagine a vessel divided into two parts as in Fig. (5), and let it contain, for example, four molecules each of which will be given a definite number to enable us to "distinguish" them from one another. It is easy to see by simple calculations that these four molecules can be arranged in the two halves of the vessel in 16 different ways. A definite state of the system corresponds to each of them. For instance, the state in which the left hand part of the vessel contains one molecule and the right hand part three differs from the state when these two parts contain two and two molecules. Let us see in how many ways of the total number of possible arrangements of the molecules each state of our system can be realized. It is not difficult to calculate that, for example, only one arrangement (combination) creates a state when the left hand part of the vessel does not contain a single molecule. The state "one in the left hand, three in the right hand part" can be accomplished in four ways. The greatest number of combinations results in a state when there will be two molecules in

each of the two parts, i.e. the molecules will be uniformly distributed between the two halves of the vessel.

We can show in general that if a vessel contains N molecules and they are numbered, then they can be distributed in 2^N ways between the two halves of the vessel. Among this total number of different combinations, the number (W) of combinations when one half of the vessel contains (n) molecules and the other half ($N - n$) molecules is determined by the equation

$$W = \frac{N!}{n!(N - n)!}$$

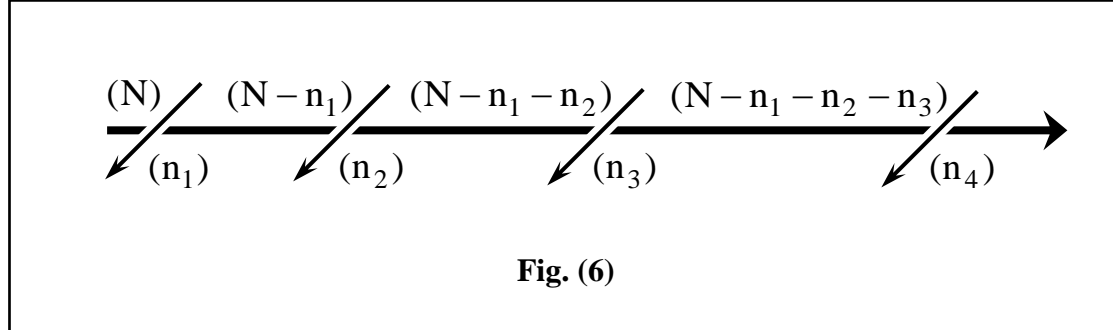
It is simple to convince ourselves that at any value of (N) the value of (W) will be the greatest when $n = N/2$, i.e. uniform distribution of the molecules throughout the volume of the vessel is accomplished in the greatest number of ways.

The following table shows all the possible ways of distributing four molecules between two parts of a vessel.

n_1 at left	n_2 at right	at left	at right	$W = \frac{N!}{n!(N-n)!}$
0	4	---	1, 2, 3, 4	1
1	3	1 2 3 4	2, 3, 4 1, 3, 4 1, 2, 4 1, 2, 3	4
2	2	1, 2 1, 3 1, 4 2, 3 2, 4 3, 4	3, 4 2, 4 2, 3 1, 4 1, 3 1, 2	6
3	1	1, 2, 3 1, 2, 4 1, 3, 4 2, 3, 4	4 3 2 1	4
4	0	1, 2, 3, 4	---	1
Total ways				$2^4 = 16$

When the number of molecules (N) is very great, the number of ways in which the molecules are distributed uniformly in the volume of the vessel becomes great in comparison with any other non-uniform distribution. We now calculate the number of ways of realizing this situation. In order to make these calculations, let us first calculate the number of ways of putting n_1 particles of N particles in one box, then n_2 out of $N - n_1$ in the second box, and so on until we have exhausted all of the particles.

With the help of the representation of Fig. (6), the number of ways of choosing n_1 particles out of N particles is given by



$$W_1 = \frac{N!}{(N - n_1)! n_1!}$$

and the number of ways of choosing n_2 out of $N - n_1$ is:

$$W_2 = \frac{(N - n_1)!}{(N - n_1 - n_2)! n_2!}$$

and so the number of ways of achieving this arrangement is

$$W = W_1 \times W_2 \times W_3 \times \dots$$

$$\begin{aligned} W &= \frac{N!}{(N - n_1)! n_1!} \times \frac{(N - n_1)!}{(N - n_1 - n_2)! n_2!} \times \frac{(N - n_1 - n_2)!}{(N - n_1 - n_2 - n_3)! n_3!} \times \dots \\ &= \frac{N!}{n_1! \times n_2! \times n_3! \times \dots} \\ &= N! \prod_i \frac{1}{n_i!} \end{aligned}$$

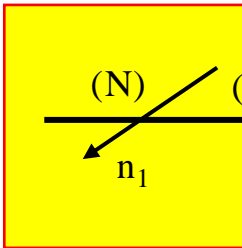
We seek the most probable distribution of n_i which we assume to be more probable than any other distribution

2. Prove the following relation for the occupation number n_i due

$$\text{to Boltzmann distribution } n_i = \sum_i \frac{N}{Z} e^{\varepsilon_i / kT}$$

----- Solution -----

Let the number of allowed states associated with the energy ε_i be g_i . Let us first calculate the number of ways of putting n_1 particles of N particles in one box, then n_2 out of $N - n_1$ in second, and so on until we have exhausted all of the particles. The number of ways of choosing n_1 particles out of N particles is given by



$$W_1 = \frac{N!}{(N - n_1)! n_1!} \quad (1)$$

and the number of choosing n_2 out of $N - n_1$ is:

$$W_2 = \frac{(N - n_1)!}{(N - n_1 - n_2)! n_2!} \quad (2)$$

and the number of ways of achieving this arrangement is

$$\begin{aligned} W &= W_1 \cdot W_2 \cdots \\ &= \frac{N!}{(N - n_1)! n_1!} \cdot \frac{(N - n_1)!}{(N - n_1 - n_2)! n_2!} \cdots \\ &= \frac{N!}{n_1! n_2! \cdots n_i!} \\ W &= N! \prod_i \frac{g_i^{n_i}}{n_i!} \quad (3) \end{aligned}$$

$$\begin{aligned}\ln W &= \ln N! + \sum_i (n \ln g_i - n \ln n_i!) \\ &= N \ln N + \sum_i (n \ln g_i - n \ln n_i)\end{aligned}$$

To obtain the most probable distribution, we maximize Eq. (3) with $dN = 0$:

$$\delta \ln W = \sum_i (\ln g_i - n \ln n_i - \frac{n_i}{n_i}) \delta n_i = 0$$

$$\delta \ln W = \sum_i (\ln g_i - n \ln n_i - 1) \delta n_i = 0$$

but

$$\delta N = \sum_i \delta n_i = 0 \quad (4)$$

$$\delta U = \sum_i \epsilon_i \delta n_i = 0 \quad (5)$$

multiply Eq. (4) by $\alpha + 1$ and Eq. (5) by $-\beta$ and add the resulting equations to each other:

$$\sum_i (\ln g_i - n \ln n_i + \alpha - \beta \epsilon_i) \delta n_i = 0 \quad (6)$$

Since n_i is vary independent,

$$\ln g_i - n \ln n_i + \alpha - \beta \epsilon_i = 0$$

or

$$\ln \frac{g_i}{n_i} + \alpha - \beta \epsilon_i = 0 \quad (7)$$

Solving Eq. (7) for n_i gives

$$n_i = \frac{N}{Z} g_i e^{-\beta \epsilon_i}$$

2 Find the relation between the partition function Z and U, S and F.

----- Solution -----

(a) Relation between Z and U

Since

$$Z = \sum_i g_i e^{\epsilon_i / KT}$$

differentiate Z with respect to T, holding V constant,

$$\begin{aligned} \left(\frac{\partial Z}{\partial T} \right)_V &= \sum_i g_i \left(\frac{\epsilon_i}{KT^2} \right) e^{\epsilon_i / KT} \\ &= \frac{1}{KT^2} \sum_i \epsilon_i g_i e^{\epsilon_i / KT} \\ &= \frac{1}{KT^2} \frac{\sum_i n_i \epsilon_i}{\sum_i n_i} g_i e^{\epsilon_i / KT} \\ &= \frac{ZU}{NKT^2} \end{aligned}$$

It follow that

$$U = NKT^2 \left(\frac{\partial \ln Z}{\partial T} \right)_V \quad (8)$$

and U may be calculated once lnZ is known as a function of T and V.

(b) Relation between Z and S

The entropy S is related to the order or distribution of the particles, through the relation:

$$S = K \ln W$$

but

$$\ln W = - \sum_i n_i \ln \frac{n_i}{g_i} + N \ln N$$

Hence

$$S = K \ln W = K \left[- \sum_i n_i \ln \frac{n_i}{g_i} + N \ln N \right]$$

By using the relation

$$n_i = \frac{N}{Z} g_i e^{-\varepsilon_i / KT}$$

we have

$$\frac{n_i}{g_i} = \frac{N}{Z} e^{-\varepsilon_i / KT}$$

then

$$\begin{aligned} S &= K \ln W = K \left[- N \ln N + N \ln Z + \frac{U}{KT} + N \ln N \right] \\ &= NKT \ln Z + \frac{U}{T} \end{aligned} \tag{9}$$

and S may be calculated once $\ln Z$ is known as a function of T and V.

(c) Relation between Z and F

The property of the system is defined by its Helmholtz function F which is given by:

$$F = U - TS$$

This equation can be evaluated in terms of the partition function Z. By using the entropy S, Eq. (8), we get

$$\begin{aligned} F &= U - T \left(NK \ln Z + \frac{U}{T} \right) \\ F &= -NKT \ln Z \end{aligned} \tag{10}$$

and F may be calculated once $\ln Z$ is known as a function of T and V.

(d) Relation between Z and P

Since

$$F = U - TS$$

then

$$dF = dU - TdS - SdT$$

From the first law of thermodynamics:

$$TdS - dU = PdV$$

By substituting

$$dF = -PdV - SdT$$

at constant temperature $SdT = 0$, then

$$P = -\left(\frac{\partial F}{\partial V}\right)_T$$

but

$$\frac{\partial F}{\partial V} = -NKT \frac{\partial \ln Z}{\partial V}$$

So

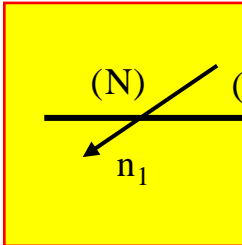
$$P = NKT \left(\frac{\partial \ln Z}{\partial V}\right)_T$$

and P may be calculated once $\ln Z$ is known as a function of T and V.

3. (b) Prove the following relation for the occupation number n_i due to Bose-Einstein Statistics $n_i = \frac{g_i}{e^{(\alpha+\epsilon_i)/KT} - 1}$.

----- **Solution** -----

Let the number of allowed states associated with the energy ϵ_i be g_i . Let us first calculate the number of ways of putting n_1 particles of N particles in one box, then n_2 out of $N - n_1$ in second, and so on until we have exhausted all of the particles. The number of ways of choosing n_1 particles out of N particles is given by



$$W_1 = \frac{N!}{(N - n_1)! n_1!} \quad (1)$$

and the number of choosing n_2 out of $N - n_1$ is:

$$W_2 = \frac{(N - n_1)!}{(N - n_1 - n_2)! n_2!} \quad (2)$$

and the number of ways of achieving this arrangement is

$$\begin{aligned} W &= W_1 \cdot W_2 \cdots \\ &= \frac{N!}{(N - n_1)! n_1!} \cdot \frac{(N - n_1)!}{(N - n_1 - n_2)! n_2!} \cdots \\ &= \frac{N!}{n_1! n_2! \cdots n_i!} \\ W &= N! \prod_i \frac{g_i^{n_i}}{n_i!} \quad (3) \end{aligned}$$

$$\begin{aligned}\ln W &= \ln N! + \sum_i (n \ln g_i - n \ln n_i!) \\ &= N \ln N + \sum_i (n \ln g_i - n \ln n_i)\end{aligned}$$

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but

$$\delta N = \sum_i \delta n_i = 0 \quad (4)$$

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multiply Eq. (4) by $\alpha + 1$ and Eq. (5) by $-\beta$ and add the resulting equations to each other:

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Since n_i is vary independent,

$$\ln g_i - n \ln n_i + \alpha - \beta \epsilon_i = 0$$

or

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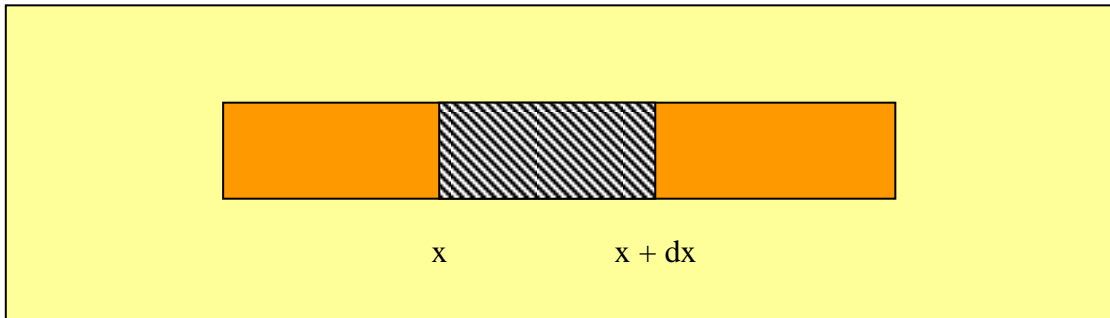
Solving Eq. (7) for n_i gives

$$n_i = \frac{N}{Z} g_i e^{-\beta \epsilon_i}$$

4. Write a short note about the vibrational spectrum of crystals.

----- **Solution** -----

Let us examine the propagation of an elastic wave in a long bar. The wave equation in one dimension is



$$\frac{\partial^2 \varphi}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} = 0 \quad (1)$$

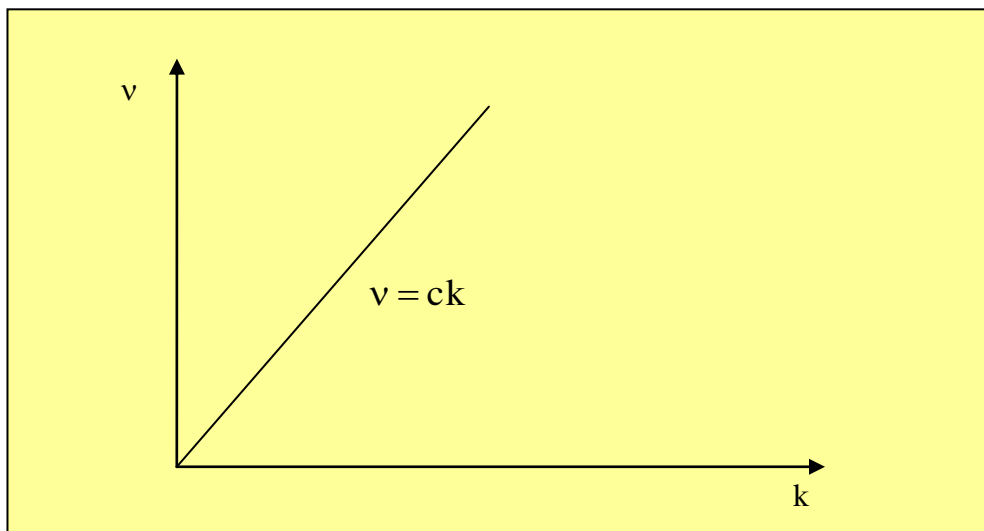
The solution of this equation is

$$\varphi = Ae^{i(kx - vt)} \quad (2)$$

Substituting Eq. (2) in (1) leads to

$$v = ck \quad (3)$$

The last equation is known as the dispersion relation which represents a straight line as in the figure

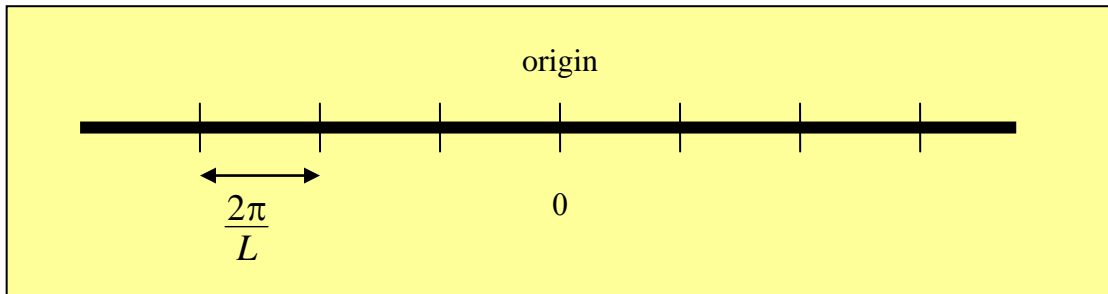


The boundary conditions require that

$$\varphi(0) = \varphi(L) \quad (4)$$

Substituting by Eq. (2) in (4) gives

$$k = n \frac{2\pi}{L}, \quad n = 0, \pm 1, \pm 2, \dots \quad (5)$$



The density of states is

$$g(\nu)d\nu = \frac{L}{2\pi} dk \quad (6)$$

In one dimension

$$g(\nu) = \frac{L}{2\pi} \frac{1}{c}$$

In three dimension

$$g(\nu) = \frac{3V}{2\pi^2} \frac{\nu^2}{c^3} \quad (7)$$

