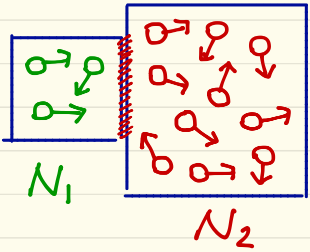
HH0056 Most Probable configurations

Consider two boxes of ideal gas in thermal contact:



BEFORE: system 1: U_{10} system 2: U_{20} and $\boxed{U_{10}+U_{20}=U}$

After thermal contact $\rightarrow$ equilibrium

Energy is conserved ($U=\text{const}$) Make a wild guess about U_1 & U_2?

$$\boxed{\frac{U_1}{N_1} \overset{?}{=} \frac{U_2}{N_2}} \quad \text{i.e. } U_1 = \frac{N_1}{N_1+N_2}U \quad U_2 = \frac{N_2}{N_1+N_2}U$$

Is this the right answer?

① Thermalization by 1d scattering

Consider two types of gas molecules: Let's compute the energy transfer due to collisions.

$$\boxed{\begin{aligned} v_1' &= \frac{m_1-m_2}{m_1+m_2}v_1 + \frac{2m_2}{m_1+m_2}v_2 \\ v_2' &= \frac{2m_1}{m_1+m_2}v_1 + \frac{m_2-m_1}{m_1+m_2}v_2 \end{aligned}}$$

$$\Delta K_1 = -\Delta K_2 = \frac{1}{2}m_1\left(v_1'^2 - v_1^2\right)$$

$$= \frac{m_1}{2}\left[\left(\frac{m_1-m_2}{m_1+m_2}\right)^2 v_1^2 - v_1^2 + \frac{4m_2^2}{(m_1+m_2)^2}v_2^2 + \frac{4(m_1-m_2)m_2}{(m_1+m_2)^2}v_1v_2\right]$$

After some algebra ...

$$\boxed{\Delta K_1 = \frac{4m_1m_2}{(m_1+m_2)^2}\left[\frac{1}{2}m_2v_2^2 - \frac{1}{2}m_1v_1^2 + \frac{1}{2}(m_1-m_2)v_1v_2\right]}$$

Although $\Delta K_1 \neq 0$ for each collision, in thermal equilibrium, the net energy flow should average to zero, i.e. $\langle \Delta K_1 \rangle = 0$!

$$\underbrace{\left\langle \frac{1}{2}m_2v_2^2 \right\rangle - \left\langle \frac{1}{2}m_1v_1^2 \right\rangle}_{\text{only these two terms survive!}} + \frac{1}{2}(m_1-m_2)\langle v_1v_2 \rangle = 0$$

only these two terms Survive!

$\rightarrow \langle v_1 \rangle \langle v_2 \rangle = 0$, velocity dist. are independent ☺

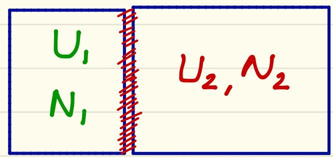
The equilibrium condition is $\left\langle \frac{1}{2} m_2 v_2^2 \right\rangle = \left\langle \frac{1}{2} m_1 v_1^2 \right\rangle$
That is to say, the energies in equilibrium are

$$\boxed{\frac{U_2}{N_2} = \frac{U_1}{N_1}}$$

as guessed. This simple example reveals the notion of "temperature".

In this case, it's natural to define $\boxed{\tau = \left\langle \frac{1}{2} m v^2 \right\rangle}$ 1d only

2 Thermal equilibrium:



Consider two systems in thermal contact. Because the total energy $E = E_1 + E_2$ is conserved, the multiplicity function can be written as ~

$$\boxed{g(N,E) = \sum_{E_1} g_1(N_1, E_1)\, g_2(N_2, E - E_1)}$$

Here I use E_i as variables and U_i as average energy.

The largest term in the sum corresponds to the most probable configuration, satisfying the condition:

$$d(g_1 g_2) = 0 \rightarrow \left(\frac{\partial g_1}{\partial E_1}\right)_{N_1} g_2\, dE_1 + \left(\frac{\partial g_2}{\partial E_2}\right)_{N_2} g_1\, dE_2 = 0, \quad dE_1 + dE_2 = 0$$

Thus, we obtain the necessary for the most probable configuration

$$\boxed{\frac{1}{g_1}\left(\frac{\partial g_1}{\partial E_1}\right)_{N_1} = \frac{1}{g_2}\left(\frac{\partial g_2}{\partial E_2}\right)_{N_2}}$$

E_1, E_2 satisfy the condition $\rightarrow U_1, U_2$

The remaing step is to show that U_1, U_2 for the most probabe conf. are the average energies in thermal equilibrium.

The fundamental assumption of statistical systems in thermal equilibrium is a closed system is equally likely to be in any of the quantum states accessible to it. That is to say, the probability to find the systen in state s is $P(s) = 1/g$!!

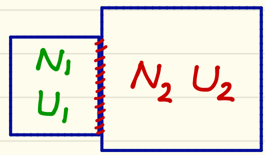
Furthermore, the multiplicity for the most probable conf. $g_1(U_1)g_2(U_2)$ is much larger than other terms in the sum. In consequence,

$$\boxed{g(N,E) = \sum_{E_1} g_1(E_1)\, g_2(E-E_1) \approx g_1(U_1)\, g_2(U_2)}$$

Well.... Some people write E as U. This is of course right.

Because the ensemble space is dominated by the most probable conf., the average energies of the subsystems are very close to U_1, U_2. In the following, we would like to demonstrate the dominance of the most probable configuration.

3 Two spin systems in thermal contact:



$$g(N,E) = \sum_{E_1} g_1(N_1,E_1)\, g_2(N_2,E_2)$$

where $N_1+N_2=N$ and $E_1+E_2=E$

The energy of the spin system is $E(S) = -2mBS$, $S=S_1+S_2$

$$g_1(N_1,E_1)\, g_2(N_2,E_2) = g_1(0)\, g_2(0) \exp\left(-\frac{2S_1^2}{N_1} - \frac{2S_2^2}{N_2}\right)$$

$$\rightarrow \boxed{g_1 g_2 = \exp\left\{-\frac{1}{2m^2B^2}\left[\frac{E_1^2}{N_1} + \frac{(E-E_1)^2}{N_2}\right]\right\}}$$

The most probable conf. $\rightarrow$ MAX $(g_1 g_2)$.

$$\frac{2E_1}{N_1} - \frac{2(E-E_1)}{N_2} = 0 \rightarrow \frac{U_1}{N_1} = \frac{U_2}{N_2} = \frac{U}{N}$$

equilibrium condition ☺

It means each spin has the same average energy.

Expand around the most probable conf.,

$$E_1 = U_1 + \Delta, \quad E_2 = U_2 - \Delta \rightarrow \begin{aligned} E_1^2 &= U_1^2 + 2U_1\Delta + \Delta^2 \\ E_2^2 &= U_2^2 - 2U_2\Delta + \Delta^2 \end{aligned}$$

$$g_1 g_2 = (g_1 g_2)_{max} \exp\left[-\frac{1}{2m^2B^2}\left(\cancel{\frac{2U_1\Delta}{N_1}} + \frac{\Delta^2}{N_1} - \cancel{\frac{2U_2\Delta}{N_2}} + \frac{\Delta^2}{N_2}\right)\right]$$

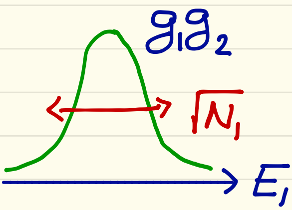
$$\boxed{g_1 g_2 = (g_1 g_2)_{max} \exp\left[-\frac{\Delta^2}{m^2B^2}\left(\frac{N_1+N_2}{2N_1N_2}\right)\right]}$$

If the deviation Δ satisfies the criterion on the left, its multiplicity $g_1 g_2 \ll (g_1 g_2)_{max}$. We thus show that the sum over all possible states is dominated by the most probable configuration. The criterion simplifies when $N_2 \gg N_1$ (One system is much larger)

$$\boxed{\frac{\Delta}{mB} \gg \sqrt{\frac{2N_1N_2}{N_1+N_2}}},$$

$$\boxed{\frac{\Delta}{mB} \gg \sqrt{N_1}}$$

This $\sqrt{N}$ criterion turns out to be quite general :)



The width of $\sqrt{N_1}$ doesn't seem small at all. What do we say $g_1 g_2$ is "Sharp"? Well, if one plots $g_1 g_2$ versus $\varepsilon \equiv E_1/N_1$, it becomes rather sharp with vanishingly small width of order $1/\sqrt{N_1} \rightarrow 0$ in thermodynamic limit.

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