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Energy distribution in ionization and dissociation

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We consider a (classical) gas of identical molecules (atoms), each with mass M at thermal equlibrium. As long as the thermal energy per molecule is smaller than the ionization (dissociation) energy of a molecule, the thermal energy is taken up in translation, rotation, vibration, etc motion. The coresponding thermal energy E per molecule for translation generates a molecular momentum $\mathbf{P}$, such that $E = P^2/2M$. If the thermal energy excedes the ionization (dissociation) energy E_i the momentum and energy conservation laws are

$$\begin{gathered}\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 \ \ , \\ E = p_1^2/2m_1 + p_2^2/2m_2 \ \ , \end{gathered} \tag{1}$$

where E is the excess energy which generates the momenta $\mathbf{p}_{1,2}$ of the two molecular fragments (*e.g.*, an ion and an electron) with masses $m_{1,2}$. Equations (1) lead to

$$p_1^2 - 2\frac{\mu}{m_2}P\cos\theta \cdot p_1 - \left(2\mu E - \mu P^2/m_2\right) = 0 \ \ , \tag{2}$$

where $\mu = m_1 m_2/M$ is the reduced mass ($M = m_1 + m_2$) and θ is the angle made by $\mathbf{P}$ with $\mathbf{p}_1$; the solutions of equation (2) are .

$$p_1 = \frac{\mu}{m_2}P\cos\theta \pm \sqrt{2\mu E - \frac{\mu}{m_2}P^2\left(1 - \frac{\mu}{m_2}\cos^2\theta\right)} \ \ . \tag{3}$$

Let us assume $m_2 \ll m_1$ and $E \gg P^2/2m_2$; then, we get from equation (3) $p_1 \simeq \sqrt{2m_2E}$ and the energies

$$E_1 = p_1^2/2m_1 \simeq \frac{m_2}{m_1}E \ \ , \ \ E_2 \simeq E \ \ ; \tag{4}$$

we can see that the high amount of excess energy is taken by the lighter fragments, in the proportion of the mass ratio, as expected ($E_1/E_2 \simeq m_2/m_1$); the magnitudes of the momenta are close to each other (since $\mathbf{P}$ is small). In the opposite limit, when $E \ll P^2/2m_2$, the ionization (dissociation) takes place in the forward direction ($\theta \simeq 0$) and the energy is kept, practically, by the heavier fragment. The same energy distribution is valid for ionization produced by high electric fields.

In elastic binary collisions the two fragments preserve their energy distribution and the scattering angles, only the relative momentum changes direction; this follows from the conservation laws

$$\begin{gathered}\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_1^{'} + \mathbf{p}_2^{'} \ \ , \\ p_1^2/2m_1 + p_2^2/2m_2 = p_1^{'2}/2m_1 + p_2^{'2}/2m_2 \ \ , \end{gathered} \tag{5}$$

where $\mathbf{p}'_{1,2}$ are momenta after collision; indeed, from the second equation (5) we get $E_2 = E'_2$ and $E_1 = E'_1$ and, from the first equation (5), we get $\varphi \simeq \varphi'$, where φ is the angle made by $\mathbf{p}_1$ with $\mathbf{p}_2$ and φ' is the angle made by $\mathbf{p}'_1$ with $\mathbf{p}'_2$.

The energy $P^2/2M + E$ is a measure of the mean energy; it is $(2N + N_0)T$, where N is the original number of atoms which are ionized and N_0 is the number of atoms which remain neutral. Since $E \gg P^2/2M$ we may write $(2N + N_0)T \simeq E$. On the other hand we have from the above calculations $E_1 \simeq \frac{m_2}{m_1}(2N + N_0)T = NT_1$ and $E_2 \simeq (2N + N_0)T = NT_2$, where the temperatures $T_{1,2}$ are given by $T_1 \simeq \frac{m_2}{m_1}(2 + N_0/N)T$ and $T_2 \simeq (2 + N_0/N)T$. We can see that the ratio of the two temperatures is $T_1/T_2 \simeq m_2/m_1$. We are in the presence of two distinct gases (*e.g.*, ions and electrons), or three distinct gases if we include the neutral atoms, all at their own equilibrium.

Let us consider two fragments with masses $m_{1,2}$, $m_2 \ll m_1$; making use of the energy E_c of their center of mass and the energy E_r of their relative motion we can express the (kinetic) energies of the two fragments as

$$\begin{aligned} E_1 &= \tfrac{m_1}{M}E_c + \tfrac{m_2}{M}E_r + 2\sqrt{\tfrac{\mu}{M}E_cE_r}\cos\alpha \simeq E_c \ , \\ E_2 &= \tfrac{m_2}{M}E_c + \tfrac{m_1}{M}E_r - 2\sqrt{\tfrac{\mu}{M}E_cE_r}\cos\alpha \simeq E_r \ \ , \end{aligned} \tag{6}$$

where $M = m_1 + m_2$ is the total mass, $\mu = m_1m_2/M$ is the reduced mass and α is the angle made by the relative momentum with the center-of-mass momentum. Since $E_{c,r}$ are conserved in elastic collisions, we can see, that, in general, only the angle α (which is a free parameter) may change in collisions; since the center-of-mass momentum is conserved, this implies a rotation of the relative momentum. This change induces an energy re-distribution between the two particles. However, for $m_2 \ll m_1$, the energies of the two particles remain, practically, unchanged, as derived above from equation (5); for high-energy the lighter fragment carries the (higher) relative energy, while the heavier fragment carries the (lower) center-of-mass energy.

Let us assume that a force act between the two fragments, which may lead to a bound state. The energy of the center of mass is conserved, such that the kinetic energy of the heavier fragment is conserved, $E_1 = E_c$. The relative energy E_r is changed, such that the kinetic energy E_2 of the lighter fragment is changed. It becomes

$$E'_2 = \frac{m_2}{M}E_c + E_{kin} = \frac{m_2}{M}E_c + W - Q \simeq W - Q \ \ , \tag{7}$$

where the first term arises from the motion of the lighter particle together with the heavier fragment (common velocity), E_{kin} is the kinetic energy of the lighter particle in the potential well with depth W and $-Q$ is the binding energy. The total energy of the lighter particle is $\mathcal{E}'_1 = E'_1 - W \simeq -Q$. The high kinetic energy of the lighter particle is transferred, approximately, in the high kinetic energy of the lighter particle in the bound state; the potential well ensures the binding energy of this particle. The kinetic energy of the bound state remains the low kinetic energy of the heavier particle.