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2/27/2020
Ion Energy Analysis - Using Ch. 1 of Atomic Collisions by Earl W. McDaniel to derive the fractional energy loss of the primary electron during ionization of a gas molecule

Here we model the electron-ion collision in ionization as a hard collision between smooth elastic spheres. That is, we imagine two spheres that only interact at the instant of contact and no energy goes into rotation. Figure below diagrams the collision and denotes the coordinate system and all relevant angles and vectors.

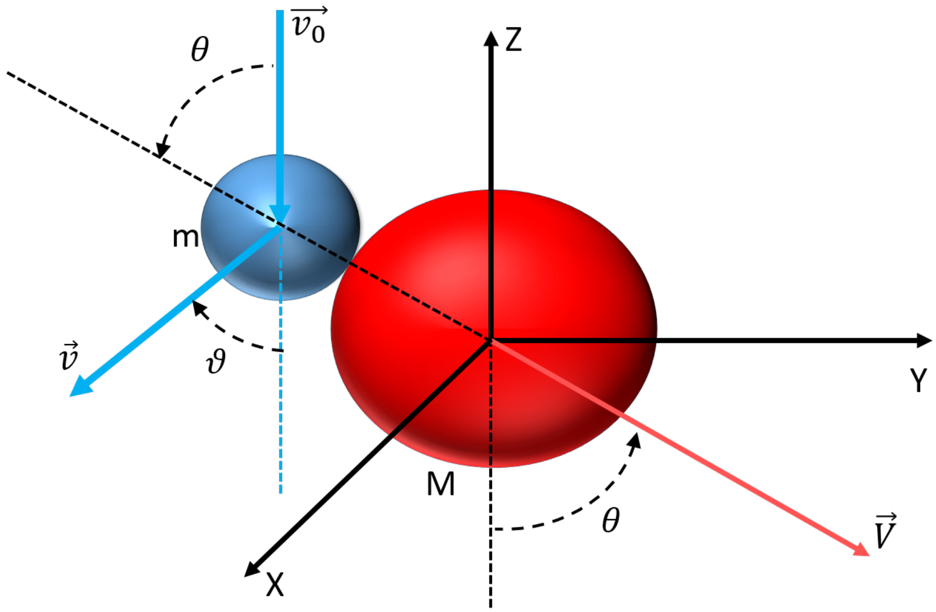

Figure 1: Diagram of Electron-Ion Collision

The primary electron is modeled as a sphere of mass m with initial velocity $\vec{v}_0$ in the $-z$ direction. The primary electron elastically scatters off a target molecule of mass M, which is initially at rest, at an incident angle θ. After the collision, the primary electron scatters with velocity $\vec{v}$ at an angle ϑ. Without loss of generality, the collision occurs only in the yz-plane (there is no constraint *a priori* which plane the collision takes place)

Since there are no external forces on the system, momentum is conserved and we can write down the momentum conservation equations

$$\begin{aligned}
\vec{P}_{tot,i} &= \vec{P}_{tot,f} \\
\vec{p}_{m,i} + \vec{p}_{M,i} &= \vec{p}_{m,f} + \vec{p}_{M,f} \\
\langle 0, 0, -mv_0 \rangle + \langle 0, 0, 0 \rangle &= \langle 0, -mv\sin\vartheta, mv\cos\vartheta \rangle + \langle 0, MV\sin\theta, MV\cos\theta \rangle \\
mv\sin\vartheta &= MV\sin\theta \qquad (1) \\
-mv_0 &= mv\cos\vartheta + MV\cos\theta \qquad (2)
\end{aligned}$$

Since the collision is elastic, kinetic energy is conserved:

$$\begin{aligned}
K_{m,i} + K_{M,i} &= K_{m,f} + K_{M,f} \\
\frac{mv_0^2}{2} &= \frac{mv^2}{2} + \frac{MV^2}{2} \rightarrow mv_0^2 = mv^2 + MV^2 \qquad (3)
\end{aligned}$$

We can solve equations 1 and 2 and get an expression for v^2 in terms of m, M, v_0, V, and θ by squaring equations (1) and (2) and adding them together:

$$\begin{aligned} m^2 v^2 \sin^2 \vartheta &= M^2 V^2 \sin^2 \theta \\ m^2 v^2 \cos^2 \vartheta &= (m v_0 + M V \cos\theta)^2 \\ m^2 v^2 &= m^2 v_0^2 + 2 m M v_0 V \cos\theta + M^2 V^2 \\ v^2 &= v_0^2 + \frac{2M}{m} v_0 V \cos\theta + \frac{M^2}{m^2} V^2 \end{aligned} \tag{4}$$

From eq. (3),

$$v^2 = \frac{m v_0^2 - M V^2}{m} \tag{5}$$

Equating (4) and (5) yields:

$$\begin{aligned} v_0^2 + \frac{2M}{m} v_0 V \cos\theta + \frac{M^2}{m^2} V^2 &= \frac{m v_0^2 - M V^2}{m} \\ m v_0^2 + 2 M v_0 V \cos\theta + \frac{M^2}{m} V^2 &= m v_0^2 - M V^2 \\ 2 M v_0 V \cos\theta + \frac{M^2}{m} V^2 &= -M V^2 \\ 2 v_0 \cos\theta + \frac{M V}{m} &= -V \\ 2 v_0 \cos\theta &= -V\left(1 + \frac{M}{m}\right) \\ 2 m v_0 \cos\theta &= -V\,(m - M) \\ V &= -\frac{2 m v_0 \cos\theta}{m + M} \end{aligned} \tag{6}$$

McDaniel gives V as

$$V = \frac{2 m v_0 \cos\theta}{m + M} \tag{7}$$

i.e. without the minus sign, though I'm too lazy to figure out who's right.

Let $p(\theta)\,d\theta$ be the probability that the incident angle occurs between $[\theta, \theta + d\theta]$. The total effective area presented for m colliding with M is πD^2 where D is the distance between the centers of m and M. Consider the cone defined by the angles within $[\theta, \theta + d\theta]$. The area of this surface element is $2\pi D \sin\theta D d\theta$, though the collision can only take place for a fraction of incident angles along Z; in this case it is $\cos\theta$. Thus $p(\theta)\,d\theta$ is

$$p(\theta)\,d\theta = \begin{cases} \dfrac{2\pi D^2 \sin\theta \cos\theta d\theta}{\pi D^2} = \sin 2\theta d\theta & \theta \in \left[0, \dfrac{\pi}{2}\right] \\ 0 & \theta \in \left(\dfrac{\pi}{2}, \pi\right] \end{cases} \tag{8}$$

The fractional loss of energy of m, $\Delta(\theta)$, is given by

$$\Delta(\theta) = \frac{K_{m,i} - K_{m,f}}{K_{m,i}} = \frac{v_0^2 - v^2}{v_0^2} \tag{9}$$

(Note that $v_0 > v$, so absolute value signs in the numerator are not not necessary). Plugging in eq. (5) yields:

$$\Delta(\theta) = \frac{v_0^2 - \left(v_0^2 - \frac{M}{m} V^2\right)}{v_0^2} = \frac{M V^2}{m v_0^2} = \frac{K_{M,f}}{K_{m,i}} \tag{10}$$

as we'd expect from eq. (3). The mean fractional loss of energy over all incident angles is given by

$$\overline{\Delta(\theta)} = \frac{\int_0^{\pi/2} p(\theta)\,\Delta(\theta)\,d\theta}{\int_0^{\pi/2} p(\theta)\,d\theta} \tag{11}$$

I'll evaluate the numerator and denominator separately. For the numerator:

$$\int_0^{\pi/2} p(\theta)\,\Delta(\theta)\,d\theta = \int_0^{\pi/2} \sin 2\theta d\theta \frac{MV^2}{mv_0^2}$$

Using eq. (7) for V, this becomes

$$\begin{aligned}
\int_0^{\pi/2} p(\theta)\,\Delta(\theta)\,d\theta &= \left(\frac{M}{mv_0^2}\right)\left(\frac{2mv_0}{m+M}\right)^2 \int_0^{\pi/2} \sin 2\theta \cos^2\theta d\theta \\
&= \frac{4Mm}{(m+M)^2}\left(\frac{1}{2}\right) \\
&= \frac{2Mm}{(m+M)^2}
\end{aligned}$$

For the denominator,

$$\int_0^{\pi/2} p(\theta)\,d\theta = \int_0^{\pi/2} \sin 2\theta d\theta = 1$$

Thus,

$$\Delta = \overline{\Delta(\theta)} = \frac{2Mm}{(m+M)^2} \tag{12}$$

In the case of electron-ion collision, $m \ll M$, $\Delta \approx \frac{2m}{M}$ and $V \approx \frac{2m}{M} v_0 \cos\theta$. Now, θ and ϑ are related by $\theta \approx \frac{\pi}{2} - \frac{\vartheta}{2}$. Plugging these into eq. (10) yields

$$\begin{aligned}
\Delta(\vartheta) &= \frac{MV^2}{mv_0^2} = \frac{M}{mv_0^2}\frac{4m^2v_0^2}{M^2}\cos^2\left(\frac{\pi}{2} - \frac{\vartheta}{2}\right) \\
&= \frac{4m}{M}\left(\frac{1}{2}(1-\cos\vartheta)\right) \\
\Delta(\vartheta) &= \frac{2m}{M}(1-\cos\vartheta) \qquad (13)
\end{aligned}$$

where we used the identity $\cos^2\left(\frac{\pi}{2} - x\right) = \sin^2 x = \frac{1}{2}(1-\cos 2x)$. As $\vartheta \to 0$, $\Delta(\vartheta) \to 0$, corresponding to the case of a grazing collision with little to no energy loss. On the other hand, a head-on collision corresponds to $\vartheta = \pi$ in which the electron back-scatters with $\Delta(\pi) = \frac{4m}{M}$. As M increases, Δ decreases, meaning that the electron loses little to no energy regardless of the incident angle. In the case of Hydrogen gas, $\frac{m}{M} \approx 0.03\%$. If an electron with kinetic energy of 130keV backscatters off a hydrogen gas molecule, then the ion receives ~ 156eV of kinetic energy