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Electron-Ion Momentum Calculation for Ionization Code

1 Purpose/Intro

Calculate and predict the momenta of the primary electron, ion, and secondary electron before and after ionization, assuming the ion is initially at rest and there are no external forces on the system. The collision we are considering is:

$$e_{p_i} + I_i \rightarrow e_{p_f} + I_f + e_s$$

where i and f refer to before and after ionization respectively. The primary electron collides with a gas molecule and ionizes it, producing an ion and secondary electron (the primary electron scatters away after the collision). We willassume the problem to be non-relativistic initially and then extend it to the relativistic case. In order to simplify the problem, we will initially solve the 2-body problem where we consider the ion and secondary electron as one target molecule, which is assumed to be at rest initially, and then solve for the final momentum of the primary electron. By conservation of momentum, the change in momentum of the primary electron is independent of the final momenta of the ion and secondary electron. Thus, if we know the energy/momentum of the secondary electron, we can solve for the energy/momentum of the ion.

2 2-Body Derivation

2.1 Momentum Conservation

To solve for the final momentum of the primary electron, we will consider only the momentum and kinetic energy of the primary electron and the target molecule. Later, the energy and momentum of the target will be split into the energy and momentum of the ion and the secondary electron. Let $\vec{p}_e$ be the primary electron momentum and $\vec{p}_{tar}$ be the target molecule momentum before the collision. We'll assume that there are no external forces on the system so that momentum is conserved. We can simplify the problem by considering the center-of-mass coordinate system. In this case, the total momentum in the center of mass frame is equal to zero.

$$\vec{p}_{cm} = (m_e + m_{tar})\,\vec{v}_{cm} = m_e\vec{v}_e + m_{tar}\vec{v}_{tar} \tag{1}$$

$$\vec{v}_{cm} = \frac{m_e}{m_e + m_{tar}}\vec{v}_e + \frac{m_{tar}}{m_e + m_{tar}}\vec{v}_{tar} \tag{2}$$

We can now write down the individual momenta in the center of mass frame:

$$\vec{v}_{e,cm} = \vec{v}_e - \vec{v}_{cm}$$

$$\vec{v}_{tar,cm} = \vec{v}_{tar} - \vec{v}_{cm}$$

$$\vec{p}_{e,cm} = \vec{p}_e - m_e\vec{v}_{cm} = m_e\vec{v}_e - m_e\left(\frac{m_e}{m_e + m_{tar}}\vec{v}_e + \frac{m_{tar}}{m_e + m_{tar}}\vec{v}_{tar}\right)$$

$$\vec{p}_{e,cm} = \frac{m_e m_{tar}}{m_e + m_{tar}}\left(\vec{v}_e - \vec{v}_{tar}\right) = \mu_{2body}\left(\vec{v}_e - \vec{v}_{tar}\right) \tag{3}$$

$$\vec{p}_{tar,cm} = \vec{p}_{tar} - m_{tar}\vec{v}_{cm} = \mu_{2body}\left(\vec{v}_{tar} - \vec{v}_e\right) \tag{4}$$

$$\mu_{2body} = \frac{m_e m_{tar}}{m_e + m_{tar}} \tag{5}$$

where μ_{2body} is the reduced mass of the system ("2body" is to distinguish it from the reduced masses defined in the 3-body problem). Clearly $\vec{p}_{e,cm} + \vec{p}_{tar,cm} = \vec{0}$, implying that $\vec{p}_{e,cm} = -\vec{p}_{tar,cm}$, meaning that in the center of mass frame, the electron and target molecule collide and return with momentum of the same magnitude, but in opposite directions, as expected.

2.2 Change in momentum

We can consider the momentum change to the electron and target molecule as a result of the collision. Since a change in momentum is invariant under a Galilean (non-relativistic) transformation, we can write down the change in momenta and velocity for the electron and target molecule in the lab frame:

$$\Delta\vec{p}_e = \Delta\vec{p}_{e,cm} = 2\mu_{2body}\left(\vec{v}_{tar} - \vec{v}_e\right) \tag{6}$$

$$\Delta\vec{p}_{tar} = \Delta\vec{p}_{tar,cm} = 2\mu_{2body}\left(\vec{v}_e - \vec{v}_{tar}\right) \tag{7}$$

$$\Delta\vec{v}_e = \frac{\Delta\vec{p}_e}{m_e} = 2\frac{m_{tar}}{m_e + m_{tar}}\left(\vec{v}_{tar} - \vec{v}_e\right) \tag{8}$$

$$\Delta\vec{v}_{tar} = \frac{\Delta\vec{p}_{tar}}{m_{tar}} = 2\frac{m_e}{m_e + m_{tar}}\left(\vec{v}_e - \vec{v}_{tar}\right) \tag{9}$$

If we assume that the target molecule is initially at rest ($\vec{v}_{tar} = 0$), then the final velocity of the primary electron is

$$\vec{v}_e' = \left(1 - \frac{2m_{tar}}{m_e + m_{tar}}\right)\vec{v}_e = \left(\frac{m_e - m_{tar}}{m_e + m_{tar}}\right)\vec{v}_e \tag{10}$$

where the prime indicates the momentum/velocity after the collision. Since $m_e < m_{tar}$, $v_e' < 0$, implying that the primary electron scatters backward, as expected.

3 3-Body Derivation

We can make a similar derivation in the 3-body case where we now consider the ion and secondary electron separately. In this case: $m_{tar} = m_I + m_e$ where m_I and m_e are the masses of the ion and secondary electron respectively. In order to differentiate between the two electrons, $\vec{P}_{e_p}$ and $\vec{P}_{e_s}$ denote the primary and secondary electrons respectively. We'll write out the momenta and velocities of the three particles initially and then use initial conditions to solve the problem. In order to differentiate the velocities and momenta from the above derivation, I'll use $\vec{P}$ and $\vec{V}$ to denote the momentum and velocity respectively.

3.1 Conservation of Momentum

Again, considering the center of mass reference frame, we can write down the center of mass momentum and velocity:

$$\vec{P}_{cm} = \left(m_{e_p} + m_I + m_{e_s}\right)\vec{V}_{cm} = m_{e_p}\vec{V}_{e_p} + m_I\vec{V}_I + m_{e_s}\vec{V}_{e_s} \tag{11}$$

$$\vec{V}_{cm} = \frac{m_{e_p}}{m_{e_p} + m_I + m_{e_s}}\vec{V}_{e_p} + \frac{m_I}{m_{e_p} + m_I + m_{e_s}}\vec{V}_I + \frac{m_{e_s}}{m_{e_p} + m_I + m_{e_s}}\vec{V}_{e_s} \tag{12}$$

The individual center of mass momenta are:

$$\begin{aligned}
\vec{V}_{e_p,cm} &= \vec{V}_{e_p} - \vec{V}_{cm} && (13)\\
\vec{V}_{I,cm} &= \vec{V}_{I} - \vec{V}_{cm} && (14)\\
\vec{V}_{e_s,cm} &= \vec{V}_{e_s} - \vec{V}_{cm} && (15)\\
\vec{P}_{e_p,cm} &= \vec{P}_{e_p} - m_{e_p}\vec{V}_{cm}\\
&= m_{e_p}\vec{V}_{e_p} - m_{e_p}\left(\frac{m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} + \frac{m_I}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I + \frac{m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_s}\right)\\
&= \frac{m_{e_p}\left(m_{e_p}+m_I+m_{e_s}\right)}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} - \left(\frac{m_{e_p}^2}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} + \frac{m_I m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I + \frac{m_{e_p} m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_s}\right)\\
&= \frac{m_{e_p}^2}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} + \frac{m_{e_p} m_I}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} + \frac{m_{e_p} m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} - \frac{m_{e_p}^2}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p}\\
&\quad - \frac{m_I m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I - \frac{m_{e_p} m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_s}\\
&= \frac{m_{e_p} m_I}{m_{e_p}+m_I+m_{e_s}}\left(\vec{V}_{e_p} - \vec{V}_I\right) + \frac{m_{e_p} m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\left(\vec{V}_{e_p} - \vec{V}_{e_s}\right)\\
\vec{P}_{e_p,cm} &= \mu_{e_p,I}\left(\vec{V}_{e_p} - \vec{V}_I\right) + \mu_{e_p,e_s}\left(\vec{V}_{e_p} - \vec{V}_{e_s}\right) && (16)\\
\vec{P}_{I,cm} &= \vec{P}_I - m_I\vec{V}_{cm}\\
&= \frac{m_I\left(m_{e_p}+m_I+m_{e_s}\right)}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I - \left(\frac{m_I m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} + \frac{m_I^2}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I + \frac{m_I m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_s}\right)\\
&= \frac{m_I m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I + \frac{m_I^2}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I + \frac{m_I m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I - \frac{m_I m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p}\\
&\quad - \frac{m_I^2}{m_{e_p}+m_I+m_{e_s}}\vec{V}_I - \frac{m_I m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_s}\\
&= \frac{m_I m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\left(\vec{V}_I - \vec{V}_{e_p}\right) + \frac{m_I m_{e_s}}{m_{e_p}+m_I+m_{e_s}}\left(\vec{V}_I - \vec{V}_{e_s}\right)\\
\vec{P}_{I,cm} &= \mu_{e_p,I}\left(\vec{V}_I - \vec{V}_{e_p}\right) + \mu_{I,e_s}\left(\vec{V}_I - \vec{V}_{e_s}\right) && (17)\\
\vec{P}_{e_s,cm} &= \mu_{e_p,e_s}\left(\vec{V}_{e_s} - \vec{V}_{e_p}\right) + \mu_{I,e_s}\left(\vec{V}_{e_s} - \vec{V}_I\right) && (18)\\
\vec{P}_{e_p,cm} + \vec{P}_{I,cm} + \vec{P}_{e_s,cm} &= \mu_{e_p,I}\left(\vec{V}_{e_p} - \vec{V}_I\right) + \mu_{e_p,e_s}\left(\vec{V}_{e_p} - \vec{V}_{e_s}\right) + \mu_{e_p,I}\left(\vec{V}_I - \vec{V}_{e_p}\right) && (19)\\
&\quad + \mu_{I,e_s}\left(\vec{V}_I - \vec{V}_{e_s}\right) + \mu_{e_p,e_s}\left(\vec{V}_{e_s} - \vec{V}_{e_p}\right) + \mu_{I,e_s}\left(\vec{V}_{e_s} - \vec{V}_I\right) && (20)\\
\mu_{e_p,e_s} &= \frac{m_{e_p} m_{e_s}}{m_{e_p}+m_I+m_{e_s}} && (21)\\
\mu_{I,e_s} &= \frac{m_I m_{e_s}}{m_{e_p}+m_I+m_{e_s}} && (22)\\
\mu_{e_p,I} &= \frac{m_I m_{e_p}}{m_{e_p}+m_I+m_{e_s}} && (23)
\end{aligned}$$

Note that $m_{e_p} = m_{e_s} = m_e$. In our case, the target molecule is at rest initially, so $\vec{V}_I = \vec{V}_{e_s} = 0$ and so the center of mass momenta become:

$$\begin{aligned}
\vec{P}_{e_p,cm} &= \left(\mu_{e_p,I} + \mu_{e_p,e_s}\right)\vec{V}_{e_p} && (24)\\
\vec{P}_{I,cm} &= -\mu_{e_p,I}\vec{V}_{e_p} && (25)\\
\vec{P}_{e_s,cm} &= -\mu_{e_p,e_s}\vec{V}_{e_p} && (26)
\end{aligned}$$

Clearly $\vec{P}_{e_p,cm} + \vec{P}_{I,cm} + \vec{P}_{e_s,cm} = \vec{0}$. Note that this equation holds true both before and after the collision.

3.2 Energy Conservation

Neglecting any source of potential energy (Coulomb potential, e.g.), total kinetic energy is conserved. This assumption is valid for fast collisions, where the contribution of kinetic energy to the total energy of each particle is much greater than that of potential energy. Thus, in the center of mass frame, we have

$$\begin{aligned} K_{e_p,cm} + K_{I,cm} + K_{e_s,cm} &= K'_{e_p,cm} + K'_{I,cm} + K'_{e_s,cm} \\ \frac{P^2_{e_p,cm}}{2m_e} + \frac{P^2_{I,cm}}{2m_I} + \frac{P^2_{e_s,cm}}{2m_e} &= \frac{P'^2_{e_p,cm}}{2m_e} + \frac{P'^2_{I,cm}}{2m_I} + \frac{P'^2_{e_s,cm}}{2m_e} \end{aligned} \tag{27}$$

Note that $\vec{P} \cdot \vec{P} = P^2$. Plugging in the squares of (24)-(26) into (27) yields:

$$\begin{aligned} \frac{\left(\mu_{e_p,I} + \mu_{e_p,e_s}\right)^2}{2m_e} V^2_{e_p} + \frac{\mu^2_{e_p,I}}{2m_I} V^2_{e_p} + \frac{\mu^2_{e_p,e_s}}{2m_e} V^2_{e_p} &= \frac{\left(\mu_{e_p,I} + \mu_{e_p,e_s}\right)^2}{2m_e} V'^2_{e_p,cm} + \frac{\mu^2_{e_p,I}}{2m_I} V'^2_{I,cm} + \frac{\mu^2_{e_p,e_s}}{2m_e} V'^2_{e_s,cm} \\ \left[\frac{\left(\mu_{e_p,I} + \mu_{e_p,e_s}\right)^2 + \mu^2_{e_p,e_s}}{2m_e} + \frac{\mu^2_{e_p,I}}{2m_I}\right] V^2_{e_p} &= \frac{\left(\mu_{e_p,I} + \mu_{e_p,e_s}\right)^2}{2m_e} V'^2_{e_p,cm} + \frac{\mu^2_{e_p,I}}{2m_I} V'^2_{I,cm} + \frac{\mu^2_{e_p,e_s}}{2m_e} V'^2_{e_s,cm} \end{aligned} \tag{28}$$

To conserve momentum and energy, we must have that the final momentum of the primary electron is negative the original momentum

$$\vec{P}_{e_p,cm} = -\vec{P}'_{e_p,cm} \tag{29}$$

The ion and secondary electron are initially "together" before the collision, so the total final momentum of the ion and secondary electron is negative the original momentum:

$$\vec{P}_{I,cm} + \vec{P}_{e_s,cm} = -\left(\vec{P}'_{I,cm} + \vec{P}'_{e_s,cm}\right) \tag{30}$$

From (29) and (30), the momentum changes are

$$\Delta\vec{P}_{e_p,cm} = -2\vec{P}_{e_p,cm} \tag{31}$$

$$\Delta\vec{P}_{I,cm} + \Delta\vec{P}_{e_s,cm} = -2\left(\vec{P}_{I,cm} + \vec{P}_{e_s,cm}\right) = 2\vec{P}_{e_p,cm} \tag{32}$$

$$\Delta\vec{P}_{e_p,cm} = -\left(\Delta\vec{P}_{I,cm} + \Delta\vec{P}_{e_s,cm}\right) \tag{33}$$

as expected. Using the invariance of momentum change and eqs. (13)-(15)

$$\begin{aligned}
\Delta\vec{P}_{e_p,cm} &= \Delta\vec{P}_{e_p} = -2\left(\mu_{e_p,I}+\mu_{e_p,e_s}\right)\vec{V}_{e_p} \\
m_e\vec{V}'_{e_p,cm} - m_e\vec{V}_{e_p,cm} &= -2\left(\mu_{e_p,I}+\mu_{e_p,e_s}\right)\vec{V}_{e_p} \\
m_e\vec{V}'_{e_p,cm} &= m_e\left(\vec{V}_{e_p}-\vec{V}_{cm}\right) - 2\left(\mu_{e_p,I}+\mu_{e_p,e_s}\right)\vec{V}_{e_p} \\
&= m_e\left(1-\frac{m_e}{2m_e+m_I}\right)\vec{V}_{e_p} - 2\left(\mu_{e_p,I}+\mu_{e_p,e_s}\right)\vec{V}_{e_p} \\
&= \left(m_e - \frac{m_e^2}{2m_e+m_I} - 2\mu_{e_p,I} - 2\mu_{e_p,e_s}\right)\vec{V}_{e_p} \\
&= \left(m_e - \frac{m_e^2}{2m_e+m_I} - 2\frac{m_I m_e}{2m_e+m_I} - \frac{2m_e^2}{2m_e+m_I}\right)\vec{V}_{e_p} \\
&= \left(m_e - \frac{3m_e^2}{2m_e+m_I} - 2\frac{m_I m_e}{2m_e+m_I}\right)\vec{V}_{e_p} \\
&= \left(\frac{2m_e^2+m_e m_I}{2m_e+m_I} - \frac{3m_e^2}{2m_e+m_I} - 2\frac{m_I m_e}{2m_e+m_I}\right)\vec{V}_{e_p} \\
&= \left(\frac{-m_e^2-m_e m_I}{2m_e+m_I}\right)\vec{V}_{e_p} \\
\vec{V}'_{e_p,cm} &= -\left(\frac{m_e+m_I}{2m_e+m_I}\right)\vec{V}_{e_p} \qquad (34) \\
\Delta\vec{P}_{e_s,cm} &= \Delta\vec{P}_{e_s} \\
m_e\vec{V}'_{e_s,cm} &= m_e\vec{V}_{e_s,cm} + m_e\vec{V}'_{e_s} \\
\vec{V}'_{e_s,cm} &= \vec{V}'_{e_s} - \frac{m_e}{2m_e+m_I}\vec{V}_{e_p} \qquad (35) \\
\vec{P}'_{I,cm} &= \vec{P}'_{e_p,cm} - \vec{P}'_{e_s,cm} \\
m_I\vec{V}'_{I,cm} &= m_e\left(\vec{V}'_{e_p,cm} - \vec{V}'_{e_s,cm}\right) \\
\vec{V}'_{I,cm} &= \frac{m_e}{m_I}\left(-\left(\frac{m_e+m_I}{2m_e+m_I}\right)\vec{V}_{e_p} - \vec{V}'_{e_s} + \frac{m_e}{2m_e+m_I}\vec{V}_{e_p}\right) \\
&= -\frac{m_e}{m_I}\left(\frac{m_I}{2m_e+m_I}\vec{V}_{e_p} + \vec{V}'_{e_s}\right) \\
\vec{V}'_{I,cm} &= -\left(\frac{m_e}{2m_e+m_I}\vec{V}_{e_p} + \frac{m_e}{m_I}\vec{V}'_{e_s}\right) \qquad (36) \\
\Delta\vec{P}_{I,cm} &= \Delta\vec{P}_I \\
m_I\vec{V}'_{I,cm} - m_I\vec{V}_{I,cm} &= m_I\vec{V}'_I + m_I\vec{V}_I \\
\vec{V}'_{I,cm} &= \vec{V}'_I - \frac{m_{e_p}}{m_{e_p}+m_I+m_{e_s}}\vec{V}_{e_p} \qquad (37) \\
\vec{V}'_I &= -\left(\frac{m_e}{2m_e+m_I}\vec{V}_{e_p} + \frac{m_e}{m_I}\vec{V}'_{e_s}\right) - \frac{m_e}{2m_e+m_I}\vec{V}_{e_p} \\
\vec{V}'_I &= -\left(\frac{2m_e}{2m_e+m_I}\vec{V}_{e_p} + \frac{m_e}{m_I}\vec{V}'_{e_s}\right) \qquad (38)
\end{aligned}$$

To summarize our results:

$$\vec{V}'_{e_P} = -\frac{m_I}{2m_e + m_I}\vec{V}_{e_p} \tag{39}$$

$$\vec{P}_{e_p,cm} = m_e\vec{V}_{e_p,cm} = \left(\mu_{e_p,I} + \mu_{e_p,e_s}\right)\vec{V}_{e_p} \tag{40}$$

$$\vec{P}'_{e_p,cm} = m_e\vec{V}'_{e_p,cm} = \left(\frac{-m_e^2 - m_e m_I}{2m_e + m_I}\right)\vec{V}_{e_p} \tag{41}$$

$$\vec{V}'_I = -\left(\frac{2m_e}{2m_e + m_I}\vec{V}_{e_p} + \frac{m_e}{m_I}\vec{V}'_{e_s}\right) \tag{42}$$

$$\vec{V}'_{I,cm} = -\left(\frac{m_e}{2m_e + m_I}\vec{V}_{e_p} + \frac{m_e}{m_I}\vec{V}'_{e_s}\right) \tag{43}$$

$$\vec{V}'_{e_s,cm} = \vec{V}'_{e_s} - \frac{m_e}{2m_e + m_I}\vec{V}_{e_p} \tag{44}$$

$\vec{V}_{e_p}$ and $\vec{V}'_{e_s}$ (and by extension $\vec{V}_I$ and $\vec{V}_{e_s}$) are known. $\vec{V}'_{e_p}$ and $\vec{V}'_I$ are given by eqs. (39) and (42) respectively and are based on known values.