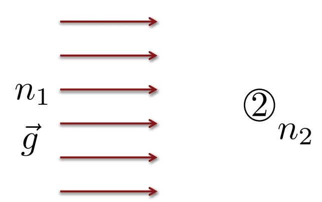
Collision Theory

General Definition of a Collision Cross-Section



Cross-sections can be defined for a large number of "events due to collision: simple scattering, excitation to some energy level, ionization, etc.
To understand the definition of a cross-section, consider first a simple situation where a population of "field particles ② are effectively at rest, and are subjected to a shower of "test particles ① (a particle beam with a flux $\vec{\Gamma}_{12} = n_1\vec{g}$). The collisions between the two populations produce a certain "event at a rate R_{12} (per unit time, per unit volume), which, of course, is proportional to n_2,

$$R_{12} = n_2\nu_{12}$$

The rate is also proportional to the incoming flux $n_1\vec{g}$, and the cross-section for that event is defined as,

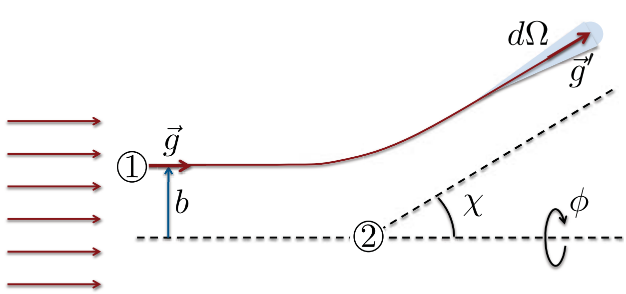
$$\sigma_{12} = \frac{\#\text{ of events per particle ② per second}}{\text{Incident flux of particles ①}} \tag{1}$$

Dimensionally:

$$[\sigma_{12}] \equiv \frac{t^{-1}}{(L^{-3})(Lt^{-1})} \equiv L^2 \quad \text{(an area)}$$

Experimentally, detectors in the lab frame would count the events ν_{12} and the flux $\vec{\Gamma}_{12}$. For some "events the rate ν_{12} will be affected by the fact that the particles ② are, in general, also moving, and the cross-section definition must then specify the frame of reference used. It will turn out that the most useful definition for all rate calculations is when the relative frame is used, i.e., the frame in which a particular particle ② is taken to be at rest. Laboratory measurements must then be corrected to that frame. We will return to this later.

The Differential Scattering Cross-Section



For simple scattering (elastic), an "event is defined as the deflection of particle ① into a range $d\Omega$ of solid angles about some observation direction $\vec{\Omega}$. Using Polar coordinates,

$$d\Omega = \sin\chi d\chi d\phi \tag{2}$$

or if there is symmetry, for all ϕ,

$$d\Omega = 2\pi\sin\chi d\chi \tag{3}$$

The differential scattering cross-section is then defined as,

$$\sigma_{12}(\chi) = \frac{\#\text{ of particles ① scattered per second into } d\Omega}{n_1 g} \tag{4}$$

Notice that, in general, for a particular interaction potential $V(r)$ between the particles, the scattering angle χ depends on relative velocity g and "impact parameter b (miss distance). If g is fixed, the number of particles scattered into the solid angle (ring) $2\pi\text{sin}\chi d\chi$ is the same as that arriving within the ring $2\pi bdb$, provided $\chi = \chi(b)$:

$$\sigma_{12}(\chi)\text{sin}\chi d\chi \;=\; bdb \tag{5}$$

or,

$$\sigma_{12}(\chi) \;=\; \frac{b}{\text{sin}\chi}\left|\frac{db}{d\chi}\right| \tag{6}$$

where the absolute value is used because the same argument applies whether χ increases or decreases with b.

Total Scattering Cross-Section

Considering all possible impact parameters that lead to an interaction (notice that a cutoff distance might be invoked), the total scattering cross-section is,

$$Q_{12}^{tot}(g) \;=\; \int_0^{b_{max}} 2\pi bdb \;=\; \pi(b_{max}^2) \tag{7}$$

or,

$$Q_{12}^{tot}(g) \;=\; 2\pi\int_0^{\pi} \sigma_{12}(g,\chi)\text{sin}\chi d\chi \tag{8}$$

Momentum-Transfer Cross-Section

As noted, the definition of Q_{12}^{tot} is generally divergent, unless a clear cutoff b_{max} can be identified. A more useful total cross section results from consideration of the momentum transferred during the collision. A more precise argument would require transformation of the equations to the relative frame of ② (which we will do later); for now, we notice that the forward momentum of ① before collision is $m_1 g$, while after collision (accepting that in an elastic collision the magnitude of the velocity does not change, i.e., $g' = g$), it is $m_1 g\text{cos}\chi$. The momentum loss by ① (or gain by ②) is then,

$$\Delta p_1 \;=\; m_1 g\,(1 - \text{cos}\chi) \tag{9}$$

The more complete argument (see later) would yield,

$$\Delta p_1 \;=\; \mu_{12} g\,(1 - \text{cos}\chi) \qquad \text{with} \qquad \mu_{12} \;=\; \frac{m_1 m_2}{m_1 + m_2} \tag{10}$$

We now multiply both sides of Eq. (4) times Δp_1 and integrate for all deflections χ (including the solid angle element $d\Omega = 2\pi\text{sin}\chi d\chi$),

$$2\pi\int_0^{\pi} \sigma_{12}(g,\chi)\Delta p_1 \text{sin}\chi d\chi \;=\; \frac{\text{rate of momentum loss by all ① due to one ②}}{n_1 g}$$

and if we choose to represent the momentum loss rate as the momentum flux $\mu_{12} n_1 g^2$ times a cross-section, we must define that cross-section as,

$$Q^*_{12}(g) \;=\; 2\pi \int_0^\pi \sigma_{12}(g,\chi)\sin\chi(1-\cos\chi)d\chi \tag{11}$$

or, alternatively,

$$Q^*_{12}(g) \;=\; 2\pi \int_0^\infty b\,[1-\cos\chi(b)]\,db \tag{12}$$

where we now can extend the range of b to ∞, since the factor $1-\cos\chi(b)$, which becomes very small for large b (small χ) ensures convergence in general (although not always!).
As a general rule, Q^* and Q^{tot} are comparable for nearly isotropic types of scattering (e.g., electron-neutrals at low energy, or neutral-neutral), but Q^* is clearly lower than Q^{tot} (by up to 50%) for high-energy collisions, which tend to be more forward-biased.

Classical Elastic Collision Theory

Since collisions occur at atomic distance, their rigorous analysis requires Quantum Mechanics. Specifically, this is so whenever the distance of closest approach, (of the order of $\sqrt{Q^*}$) is comparable to or less than the Broglie wavelength for the relative momentum $\hbar/p$. Putting $p \sim \mu\sqrt{kT/\mu} = \sqrt{\mu kT}$, quantum effects dominate when,

$$Q^* \;<\; \left(\frac{\hbar^2}{\mu kT}\right) \tag{13}$$

For n-n collisions, $\mu > m_H = 1.7 \times 10^{-27} kg$, and at $T = 3000K$ this requires $Q^* < 10^{-22} m^2 \ll$ actual Q^*. So for this type of collision, classical dynamics can be used. For e-n collisions, $\mu \sim m_e \sim 10^{-30} kg$, and taking $T \sim 10eV \sim 10^5 K$, the condition is $Q^*_{en} < 8 \times 10^{-21} m^2$. Typical Q^*_{en} values tend to be $\sim 10^{-19} m^2$, so even in this case we have some grounds for using classical dynamics. But in detail, many features of e-n collision behavior are traceable to Quantum effects (such as the Ramsauer deep minimum in Q^* at energies where electrons resonate with the atoms potential well).
In what follows, we use Classical Mechanics for estimating some cross-sections, and then also for calculating overall collisional effects using these cross-sections. In practical use, the cross-sections are themselves obtained by laboratory measurements (or sometimes by precise quantum computations), but since momentum and energy conservation are common to both theories, the use of Classical Mechanics given the cross-section is on firm grounds.

Reduction to Relative Coordinates

Define,

$$\begin{aligned}
\vec{w}_1 &\equiv \text{velocity of particle ① in lab frame, before collision} \\
\vec{w}_2 &\equiv \text{velocity of particle ② in lab frame, before collision} \\
\vec{w}_1' &\equiv \text{velocity of particle ① in lab frame, after collision} \\
\vec{w}_2' &\equiv \text{velocity of particle ② in lab frame, after collision}
\end{aligned}$$

Instead of the pair $(\vec{w}_1, \vec{w}_2)$ the collision will be analyzed using the pair,

$$\begin{aligned} \vec{G} &= \frac{m_1\vec{w}_1 + m_2\vec{w}_2}{m_1 + m_2} \\ \vec{g} &= \vec{w}_1 - \vec{w}_2 \end{aligned} \tag{14}$$

Solving for $\vec{w}_1$ and $\vec{w}_2$,

$$\begin{aligned} \vec{w}_1 &= \vec{G} + \frac{m_2}{m_1 + m_2}\vec{g} \\ \vec{w}_2 &= \vec{G} - \frac{m_1}{m_1 + m_2}\vec{g} \end{aligned} \tag{15}$$

Let $\vec{F}_{21}(r)$ be the force exerted by ② on ①, which is assumed to be a function of $r = |\vec{r}_1 - \vec{r}_2|$, and to be along the $\vec{r}_1 - \vec{r}_2$ vector. Then,

$$\begin{aligned} m_1\frac{d\vec{w}_1}{dt} &= \vec{F}_{21} \\ m_2\frac{d\vec{w}_2}{dt} &= -\vec{F}_{21} \end{aligned} \tag{16}$$

From (16),

$$\frac{d\vec{G}}{dt} = 0 \tag{17}$$

So the c.m. velocity $\vec{G}$ is not changed by the interaction. Also, from (16),

$$\frac{d\vec{g}}{dt} = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)\vec{F}_{21} = \frac{m_1 + m_2}{m_1 m_2}\vec{F}_{21}$$

or,

$$\mu_{12}\frac{d\vec{g}}{dt} = \vec{F}_{21} \tag{18}$$

where μ_{12} is the Reduced Mass,

$$\mu_{12} = \frac{m_1 m_2}{m_1 + m_2} \tag{19}$$

(notice if $m_1 << m_2$, $\mu_{12} \approx m_1$, while if $m_1 = m_2$, $\mu_{12} = m_1/2$).
Comparing (18) to (16) we see that the relative motion of particle ① (as seen from the accelerated frame of ②), under their mutual force, is as if ② were at rest, except that the mass m_1 is to be replaced by the smaller mass μ_{12}. All dynamical properties known for motion about a fixed center of force can be applied now. In particular, the angular momentum,

$$\vec{L} = \mu_{12}\vec{r} \times \vec{g} \tag{20}$$

is a constant vector, which shows the motion is planar and that within this plane (using polar coordinates),

$$L = \mu_{12} r^2 \dot{\theta} \equiv \text{constant} \tag{21}$$

The total kinetic energy in the lab frame is (with $m = m_1 + m_2$),

$$K = \frac{1}{2}m_1 w_1^2 + \frac{1}{2}m_2 w_2^2$$

or,

$$K = \frac{m}{2}G^2 + \frac{\mu_{12}}{2}g^2 \tag{22}$$

whereas the overall momentum is,

$$\vec{p} \;=\; m_1\vec{w}_1 + m_2\vec{w}_2 \;=\; m\vec{G} \tag{23}$$

We already know that $\vec{G}$ is constant. If, in addition, the collision is elastic, then K is constant as well, and then Eq. (22) shows that,

$$|\vec{g}| \;=\; g \;\equiv\; \text{constant} \tag{24}$$

So, the relative velocity vector $\vec{g}$ is only rotated by the interaction.
It is of some interest to investigate the possible use of a different set of velocities for analysis. We retain $\vec{G}$ as one of them, but take as the other the velocity of ① relative to the center of mass,

$$\vec{w}_1^G \;=\; \vec{w}_1 - \vec{G} \tag{25}$$

From (14),

$$\vec{w}_1^G \;=\; \vec{w}_1 - \frac{m_1\vec{w}_1 + m_2\vec{w}_2}{m_1+m_2} \;=\; \frac{m_2}{m_1+m_2}\left(\vec{w}_1 - \vec{w}_2\right) \;=\; \frac{m_2}{m}\vec{g} \tag{26}$$

(and it follows that $\vec{w}_2^G = \vec{w}_2 - \vec{G} = -m_1\vec{g}/m$). We see from (26) that the velocity with regard to the center of mass is just a scaled version of that with regard to particle ②. It follows that the rotation χ of $\vec{g}$ is also that of $\vec{w}_1^G$, and therefore that the differential scattering cross-section could be calculated in either frame.

Energy and Momentum Transfer in Elastic Collisions

The momentum increase of ① (decrease for ②) in the collision is,

$$\Delta\vec{P}_1 \;=\; m_1\vec{w}_1' - m_1\vec{w}_1$$

or,

$$\Delta\vec{P}_1 \;=\; \frac{m_1 m_2}{m}\left(\vec{g}' - \vec{g}\right) \tag{27}$$

which justifies a result we advanced in a previous section.
Similarly, the increase in energy of ① (decrease for ②) is,

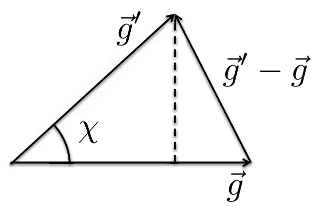
$$\Delta E_1 \;=\; \frac{1}{2}m_1 w_1'^2 - \frac{1}{2}m_1 w_1^2$$

Hence, since $g' = g$,

$$\Delta E_1 \;=\; \mu_{12}\left(\vec{g}' - \vec{g}\right)\cdot\vec{G} \;=\; \Delta\vec{P}_1\cdot\vec{G} \tag{28}$$

Important observation:

Even though the collision is elastic, and no total energy is lost, there is an exchange of energy between the particles, unless their c.m. is at rest.



In some cases, particle ② can be regarded as effectively at rest, $\vec{w}_2 = 0$ (for example, if ① is an electron and ② is a heavy particle). In that case we have,

$$\vec{G} = \frac{m_1}{m}\vec{g} = \frac{m_1}{m}\vec{w}_1$$

and since,

$$(\vec{g}' - \vec{g}) \cdot \left(\frac{\vec{g}}{g}\right) = -g\,(1 - \cos\chi)$$

then we have,

$$\Delta\vec{P}_1 \cdot \frac{\vec{g}}{g} = -\mu_{12} g\,(1 - \cos\chi) = -\mu_{12} w_1\,(1 - \cos\chi)$$

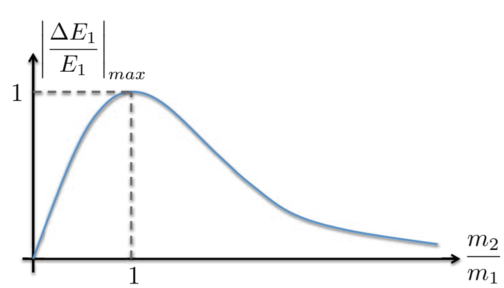
Also (for $\vec{w}_2 = 0$), $\vec{G}$ is along $\vec{g}/g$, so,

$$\Delta E_1 = -\mu_{12}\frac{m_1}{m}\,(1 - \cos\chi)\,w_1^2$$

$$\frac{\Delta E_1}{E_1} = -\frac{2\mu_{12}}{m}\,(1 - \cos\chi) \tag{29}$$

This is maximum for $\chi = \pi$ (a head-on collision), yielding,

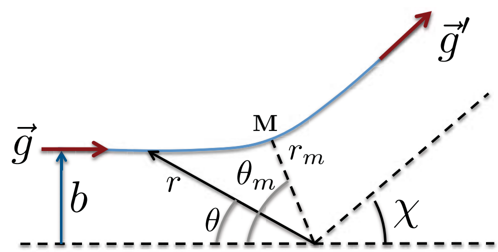
$$\left(\frac{\Delta E_1}{E_1}\right)_{max} = -\frac{4\mu_{12}}{m} = -4\frac{m_1 m_2}{(m_1 + m_2)^2} = -4\frac{m_2/m_1}{\left[1 + (m_2/m_1)\right]^2} = -4\frac{m_1/m_2}{\left[1 + (m_1/m_2)\right]^2}$$



which is largest if $m_1 = m_2$ ($\left(\frac{\Delta E_1}{E_1}\right)_{max} = 1$ in that case). But for $m_1/m_2 \ll 1$ (electron-heavy collision),

$$\left|\frac{\Delta E_1}{E_1}\right|_{max} \approx 4\frac{m_1}{m_2} \ll 1$$

which shows a very poor energy transfer efficiency between light and heavy particles, but a good one for like-mass particles. This is why heavy particles easily thermalize among themselves, but electrons can end up decoupled thermally from the rest of the gas.



Let $V(r)$ be the interaction potential energy, such that,

$$\vec{F} = \nabla V \tag{30}$$

Then, by conservation of total energy,

$$\frac{1}{2}\mu_{12}\left(\dot{r}^2 + r^2\dot{\theta}^2\right) + V(r) = \frac{1}{2}\mu_{12}g^2 \tag{31}$$

and by conservation of angular momentum,

$$r^2\dot{\theta} = gb \tag{32}$$

Eliminating $\dot{\theta}$ and writing $\mu = \mu_{12}$,

$$\dot{r}^2 + r^2\frac{g^2b^2}{r^4} + \frac{2V}{\mu} = g^2$$

or,

$$\dot{r} = \pm g\sqrt{1 - \frac{b^2}{r^2} - \frac{2V(r)}{\mu g^2}} \tag{33}$$

Time can be eliminated by dividing (33) by $\dot{\theta} = gb/r^2$,

$$\frac{dr}{d\theta} = \pm\frac{r^2}{b}\sqrt{1 - \frac{b^2}{r^2} - \frac{2V(r)}{\mu g^2}} \tag{34}$$

Here the $(+)$ sign applies past the point **M** of closest approach, while the $(-)$ applies before **M**. At **M**, the distance r_m follows from $dr/d\theta = 0$, or,

$$1 - \frac{b^2}{r_m^2} - \frac{2V(r_m)}{\mu g^2} = 0 \tag{35}$$

Turning (34) upside down, and integrating from $(r = \infty, \theta = 0)$, with the $(-)$ sign, to $(r = r_m, \theta = \theta_m)$, we obtain,

$$\theta_m = -\int_\infty^{r_m} \frac{(b/r^2)dr}{\sqrt{1 - \frac{b^2}{r^2} - \frac{2V(r)}{\mu g^2}}}$$

or using $\xi = b/r$, we can write (35) as,

$$1 - \xi_m^2 - \frac{2V(b/\xi_m)}{\mu g^2} = 0 \tag{36}$$

and therefore,

$$\theta_m = \int_0^{\xi_m} \frac{d\xi}{\sqrt{1 - \xi^2 - \frac{2V(b/\xi)}{\mu g^2}}} \tag{37}$$

From the geometry,

$$\chi = \pi - 2\theta_m \tag{38}$$

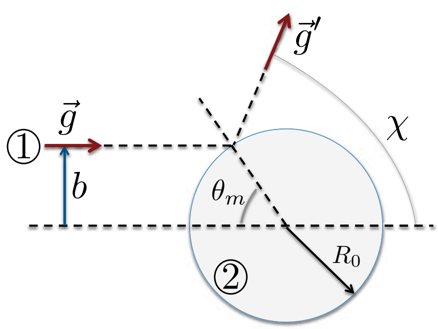
hence,

$$\begin{aligned} 1 - \cos\chi &= 2\cos^2\theta_m \\ \sin\chi &= 2\sin\theta_m\cos\theta_m \end{aligned}$$

and one can then complete the differential scattering cross-section using (6) and the total and momentum transfer cross-sections using (8) and (11), or (12).

<u>The hard sphere model</u>

If each molecule behaves as a hard sphere (R_1 for ① , R_2 for ②), the interaction can be replaced by that of a point mass ① with a field particle ② of effective radius $R_0 = R_1 + R_2$, as in the figure.



This can be seen as the limit of a smooth potential (as we will see below), or it can be dealt with directly. From the geometry,

$$\sin\theta_m = \frac{b}{R_0} \quad \text{and} \quad \cos^2\theta_m = 1 - \frac{b^2}{R_0^2}$$

and from (38),

$$\sin\chi = \sin 2\theta_m = 2\sin\theta_m\cos\theta_m$$

$$1 - \cos\chi = 1 + \cos 2\theta_m = 2\cos^2\theta_m = 2\left(1 - \frac{b^2}{R_0^2}\right)$$

We can now use Eq. (12) for the momentum transfer cross-section,

$$Q_{12}^* = 2\pi \int_0^{R_0} 2b\left(1 - \frac{b^2}{R_0^2}\right) db = 4\pi R_0^2\left(\frac{1}{2} - \frac{1}{4}\right) = \pi R_0^2 = \pi\left(R_1 + R_2\right)^2 \tag{39}$$

We can also calculate the simple total cross-section from (7),

$$Q_{12}^{tot} = 2\pi \int_0^{R_0} bdb = \pi R_0^2 = \pi\left(R_1 + R_2\right)^2 \tag{40}$$

which, in this case, turns out to be the same as Q_{12}^*. An important observation is that neither of them depends on g. All other interaction potentials yield cross-sections that do depend on g.

<u>Power law potentials</u>

Consider interaction forces of the general type $F(r) = \pm\alpha/r^s$, leading to,

$$V(r) = \int_r^\infty F(r)dr = \frac{\pm\alpha}{(s-1)r^{s-1}}$$

In terms of $\xi = b/r$, we have,

$$V(\xi) \;=\; \pm\frac{\alpha\xi^{s-1}}{(s-1)b^{s-1}} \tag{41}$$

Attractive potentials carry the $(-)$ sign, repulsive ones the $(+)$ sign. The relative velocity influences cross-sections (Eq. 37) through the group,

$$\frac{2V}{\mu g^2} \;=\; \pm\frac{2}{\mu g^2}\frac{\alpha\xi^{s-1}}{(s-1)b^{s-1}}$$

and defining a characteristic impact parameter,

$$b_0 \;=\; \left(\frac{\alpha}{\mu g^2}\right)^{\frac{1}{s-1}} \tag{42}$$

$$\frac{2V}{\mu g^2} \;=\; \pm\frac{2}{s-1}\frac{\xi^{s-1}}{(b/b_0)^{s-1}} \tag{43}$$

Define now $y = b/b_0$, and substitute in (37) and then in (12),

$$Q^*_{12} \;=\; 4\pi b_0^2\int_0^\infty y dy \cos^2\left[\int_0^{\xi_m}\frac{d\xi}{\sqrt{1-\xi^2\mp\frac{2}{s-1}\left(\frac{\xi}{y}\right)^{s-1}}}\right] \tag{44}$$

where ξ_m satisfies,

$$1-\xi_m^2\mp\frac{2}{s-1}\left(\frac{\xi_m}{y}\right)^{s-1} \;=\; 0 \tag{45}$$

The integrals in (42) need generally to be numerically completed. A conventional way to write the result, and some numerical results, are as follows,

$$Q^*_{12} \;=\; \pi b_0^2 2A_1(s,\pm) \tag{46}$$

s	$(+)$ or $(-)$	A_1
2	$\pm$	∞
3	$+$	0.783
5	$+$	0.422
7	$+$	0.385
∞	$+$	0.5

The $s\to\infty$ case is the hard-sphere limit, with $b_0 = R_0 = R_1 + R_2$. The $s = 2$ case corresponds to Coulombic interaction, and it is obvious that the $(1-\cos\chi)$ factor in the integrand for Q^* is not sufficient to produce a finite result. This case will be examined in more detail below. One final comment is the absence of attractive potentials in the table above. The integrations must be carried out very carefully in that case, because there are ranges of $(b_1 g)$ which lead to capture in some cases.

The Case of Coulomb Collisions

This is a particular case of a power-law potential with,

$$\alpha \;=\; \frac{z_1 z_2 e^2}{4\pi\epsilon_0} \qquad \text{and} \qquad s = 2 \tag{47}$$

(z_1, z_2 are the charge numbers of the particles; $z = -1$ for electrons, $+n$ for an n^{th}-charged positive ion). From this, the characteristic impact parameter is,

$$b_0 \;=\; \frac{z_1 z_2 e^2}{4\pi\epsilon_0 \mu g^2} \tag{48}$$

which can be positive (repulsion) or negative (attraction). Notice that for the case of electron-electron collisions, $\mu_{ee} = m_e/2$, whereas for electron-ion, $\mu_{ei} \approx m_e$. Hence,

$$b_{0_{ee}} \;=\; 2\,|b_{0_{ei}}| \tag{49}$$

Since $b > 0$, the quantity $y = b/b_0$ can be positive or negative, so both cases are represented by (from (37)),

$$\theta_m \;=\; \int_0^{\xi_m} \frac{d\xi}{\sqrt{1 - \xi^2 - 2\xi/y}} \tag{50}$$

where $\xi_m^2 + 2\xi_m/y - 1 = 0$, i.e.,

$$\xi_m \;=\; -\frac{1}{y} \pm \sqrt{\frac{1}{y^2} + 1} \tag{51}$$

In order to have $\xi_m = b/r_m > 0$, the (+) side must be adopted for either attraction or repulsion in (51).
Eq. (50) can be integrated explicitly to,

$$\theta_m = \sin^{-1}\left(\frac{\xi + 1/y}{\sqrt{1 + 1/y^2}}\right)_0^{\xi_m} = \sin^{-1}(1) - \sin^{-1}\left(\frac{1}{\sqrt{1+y^2}}\right) = \cos^{-1}\left(\frac{1}{\sqrt{1+y^2}}\right) \tag{52}$$

or,

$$\cos^2\theta_m \;=\; \sin^2\frac{\chi}{2} \;=\; \frac{1}{1+y^2} \qquad \text{leading to} \qquad y \;=\; \cot\frac{\chi}{2} \tag{53}$$

or,

$$b \;=\; b_0 \cot\frac{\chi}{2} \tag{54}$$

For attraction, both b_0 and χ are negative, so b is still positive.
We can now calculate the differential scattering cross-section from (6) and,

$$\frac{db}{d\chi} \;=\; -\frac{b_0}{2}\frac{1}{\sin^2\chi/2} \qquad \text{and} \qquad \sin\chi \;=\; 2\sin\frac{\chi}{2}\cos\frac{\chi}{2}$$

$$\sigma \;=\; \frac{b_0^2}{4\sin^4(\chi/2)} \tag{55}$$

which was first derived by Rutherford. This is clearly very forward-biased (strong decrease of $\sigma(\chi)$ as χ increases from zero).

In terms of b, using,

$$\sin^2\frac{\chi}{2} = \frac{1}{1+y^2}$$

$$\sigma = \frac{b_0^2}{4}\left(1+\frac{b^2}{b_0^2}\right)^2 \tag{56}$$

The momentum transfer cross-section is then,

$$Q^* = 4\pi\int_0^\infty b_0^2 \cos^2\theta_m y dy = 4\pi\int_0^\infty \frac{ydy}{1+y^2} = 2\pi b_0^2 \ln\left(1+y^2\right)_0^\infty \to \infty \tag{57}$$

Here, even the factor $2\cos^2\theta_m = (1-\cos\chi)$ is not enough to eliminate the divergence that happens at large b (small χ). Clearly, that is because of the strong singularity of $\sigma(\chi)$ at $\chi = 0$. The divergence is weak (logarithmic) and should not arise for any potential that is less spread-out than the Coulomb potential.
Physically, we know that the plasma has a strong tendency to shield away any region of concentrated charge. We make a small detour here to show that this modifies the Coulomb potential of an isolated charge (ze) in an essential way, and we will then use this result to complete the calculation above.

Consider a plasma where electrons have (as a fluid) negligible inertia, so that only pressure gradients and electric fields matter, $\nabla P_e \approx -en_e\vec{E}$.
With constant T_e, using $P_e = n_e kT_e$ and $\vec{E} = -\nabla\phi$,

$$\frac{\nabla n_e}{n_e} = \frac{e\nabla\phi}{kT_e} \quad \to \quad n_e = n_{e0} e^{\frac{e\phi}{kT_e}} \tag{58}$$

where n_{e_0} is the electron density where $\phi = 0$. Consider now an isolated ion of charge (ze) and assume the ion density in its neighborhood is undisturbed (equal to n_{e_0}) due to their large inertia, while the electron density may locally increase (in a statistical sense) due to the ions attraction. The net charge density is then $-e(n_e - n_{e_0})$, and from Poissons equation in spherical coordinates,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi}{dr}\right) = \frac{en_{e0}}{\epsilon_0}\left(e^{\frac{e\phi}{kT_e}} - 1\right) \tag{59}$$

Not very near the ion, $\phi << kT_e/e$, so expand the exponential to 1st order,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi}{dr}\right) \approx \frac{en_{e0}}{\epsilon_0}\frac{e}{kT_e}\phi$$

The group $\frac{e^2 n_{e0}}{\epsilon_0 kT_e}$ is $1/\lambda_D^2$ (λ_D = Debye's length). Also, put $\phi = \psi/r$. Substituting and simplifying,

$$\frac{d^2\psi}{dr^2} - \frac{\psi}{\lambda_D^2} = 0$$

the solution that does not explode as $r \to \infty$ is,

$$\psi \;=\; Ce^{-r/\lambda_D} \qquad \text{or} \qquad \phi \;=\; \frac{C}{r}e^{-r/\lambda_D} \tag{60}$$

Near the ion ($r \ll \lambda_D$) this behaves as $\phi \sim C/r$, so C must be $ez/4\pi\epsilon_0$,

$$\phi \;=\; \frac{ez}{4\pi\epsilon_0 r}e^{-r/\lambda_D} \tag{61}$$

This shows that the ions potential is Coulombic only inside its Debye sphere, while it decays much faster (exponentially) outside. This screened Coulomb potential should be used in Eq. (37), but this would require numerical integrations. Instead, a simple device is to exclude in the impact parameter integration (57) all values of b larger than one Debye length. Given the weakness of the integral's divergence, this should be adequate. We therefore return to (57) and set the upper limit of the integral equal to λ_D/b_0,

$$Q^* \;\approx\; 2\pi b_0^2 \ln\left(1+y^2\right)_0^{\lambda_D/b_0} \;=\; 2\pi b_0^2 \ln\left(1+\frac{\lambda_D^2}{b_0^2}\right) \tag{62}$$

The quantity,

$$\Lambda \;=\; \sqrt{1+\frac{\lambda_D^2}{b_0^2}} \tag{63}$$

is called the "Coulomb logarithm, and our result can be written,

$$Q^* \;=\; 4\pi b_0^2 \ln\Lambda \tag{64}$$

According to (48),

$$b_0 \;=\; \frac{z_1 z_2 e^2}{4\pi\epsilon_0 \mu g^2}$$

which shows $Q^* \sim 1/g^4$, which implies that Coulomb collisions are most important at low energies. Inside the logarithm, it is sufficient to use the average value of μg^2 , from,

$$\left\langle \frac{1}{2}\mu g^2 \right\rangle \;=\; \frac{3}{2}kT_e \quad \to \quad \mu\left\langle g^2\right\rangle \;=\; 3kT_e$$

so that,

$$\frac{\lambda_D}{b_0} \;=\; \sqrt{\frac{\epsilon_0 kT_e}{e^2 n_e}}\frac{12\pi\epsilon_0 kT_e}{z_1 z_2 e^2} \;=\; \frac{12\pi}{z_1 z_2}\frac{(\epsilon_0 kT_e)^{3/2}}{e^3 n_e^{1/2}} \tag{65}$$

This ratio is related to the average number of electrons inside the Debye sphere,

$$N_D \;=\; \frac{4}{3}\pi\lambda_D^3 n_e \;=\; \frac{4\pi}{3}\left(\frac{\epsilon_0 kT_e}{e^2 n_e}\right)^{3/2} n_e \tag{66}$$

Comparing (65) and (66) we see that,

$$\frac{\lambda_D}{b_0} \;=\; 9N_D \tag{67}$$

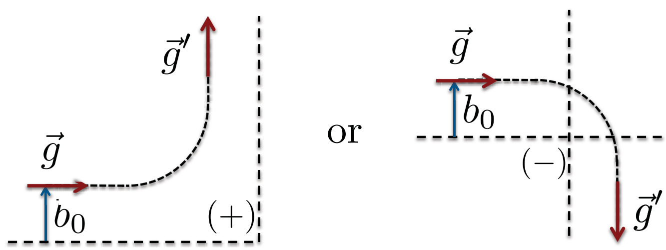
For validity of our statistical treatment of the ion's neighborhood, we should have $N_D \gg 1$ (and hence $\Lambda \gg 1$). For verification, assume $T_e = 1eV = 11600K$, $n_e = 10^{18}m^{-3}$, $z_1 = z_2 = 1$. We calculate $\lambda_D = 7.4 \times 10^{-6}m$ and $b_0 = 4.8 \times 10^{-10}m$,

$$\frac{\lambda_D}{b_0} \approx 1.5 \times 10^4 \gg 1$$

and so, to a good approximation, (63) becomes simply,

$$\Lambda \approx \frac{\lambda_D}{b_0} \tag{68}$$

For our example, $\ln\Lambda = \ln(1.5 \times 10^4) \approx 9.6$. For most plasmas of interest, $\ln\Lambda$ ranges only from about 5 to about 20.
The parameter b_0 has in this case a simple interpretation.

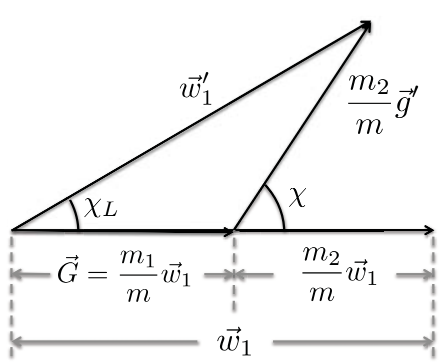


From (54), $b = b_0\cot(\chi/2)$, so that $b = b_0$ implies $\chi = \pm 90°$. b_0 is called the Landau impact parameter, or "90° deflection parameter".

Relationship to Lab-Frame Quantities

Data leading to the experimental determination of cross-sections are invariably taken by instruments rooted in the laboratory frame, and then converted to the relative (or center of mass) frame. The general reduction is fairly tedious, but it is useful to consider the simpler case where particles of kind ② are much slower than those of kind ① (say, heavy particles vs. electrons), in which case we can take $\vec{w}_2 = 0$. From Eqs. (14) then $\vec{G} = m_1\vec{w}_1/m$ and $\vec{g} = \vec{w}_1$. From (15), expressed after collision,

$$\vec{w}_1' = \vec{G} + \frac{m_2}{m}\vec{g}' = \frac{m_1}{m}\vec{w}_1 + \frac{m_2}{m}\vec{g}'$$



These relationships are best viewed graphically in the figure.
The lab-frame deflection of ① is the rotation χ_L of $\vec{w}_1$ as it becomes $\vec{w}_1'$. We have,

$$\tan\chi_L = \frac{\frac{m_2}{m}w_1\sin\chi}{\frac{m_2}{m}w_1\cos\chi + \frac{m_1}{m}w_1}$$

or,

$$\tan\chi_L = \frac{\sin\chi}{\cos\chi + \frac{m_1}{m_2}} \tag{69}$$

In the simple case $m_1/m_2 = 1$, this gives $\chi_L = \chi/2$, and in general $\chi_L < \chi$, due to the recoil of particle ② (notice we only assumed $\vec{w}_2 = 0$, but not $\vec{w}_2' = 0$).
Suppose now a detector measures the number of particles scattered into unit solid angle $2\pi\sin\chi_L d\chi_L$ in the lab frame, and this is used to determine the differential scattering cross-section $\sigma_L(\chi_L)$. As long as χ and χ_L are interrelated through (69), we can also express the number in terms of relative frame quantities, so that,

$$\sigma\sin\chi d\chi = \sigma_L\sin\chi_L d\chi_L \tag{70}$$

We can then use (69) to calculate $d\chi_L/d\chi$ and $\chi(\chi_L)$. The result, after some algebra, is,

$$\sigma_L \ = \ \sigma\frac{\left(1 + r^2 + 2r\cos\chi\right)^2}{1 + r\cos\chi} \quad \text{with} \quad r = \frac{m_1}{m_2} \tag{71}$$

or, perhaps more directly useful,

$$\sigma \ = \ \sigma_L\frac{\left(\sqrt{1 - r^2\sin^2\chi_L} + r\cos\chi_L\right)\sqrt{1 - r^2\sin^2\chi_L}}{\left[r^2 - 1 + 2\sqrt{1 - r^2\sin^2\chi_L}\left(\sqrt{1 - r^2\sin^2\chi_L} + r\cos\chi_L\right)\right]^{3/2}} \tag{72}$$

Because of (70), the total cross-section Q^{tot} will be the same when computed in either frame; but since the factors $1 - \cos\chi$ and $1 - \cos\chi_L$ are not accounted for, the momentum transfer cross-section will be different. But Q^* is only useful in the relative (or c.m.) frame. In fact, the momentum transfer from ① to ② is not $\mu_{12}w_1(1 - \cos\chi_L)$, because $w_1' \neq w_1$.

So the process is:

1. Measure $\sigma_L(\chi_L)$
2. Calculate $\sigma(\chi)$
3. Integrate to $Q^* = 2\pi\int_0^\pi \sigma(\chi)(1 - \cos\chi)\sin\chi d\chi$

Application: Thompson's calculation of ionization cross-section by electron impact

Ionization occurs when a free e imparts more than $E_\infty - E_n$ to a bound electron in the n^{th} state. Assume this e is <u>at rest</u> and <u>free</u>.

$$\Delta E_2 \;=\; -\Delta E_1 \;=\; \mu(1-\cos\chi)\frac{m_1}{m}w_1^2 \;=\; \frac{m_e}{2}(1-\cos\chi)\frac{\cancel{m_e}}{2\cancel{m_e}}w_1^2 \;=\; \frac{1}{4}(1-\cos\chi)m_e w_1^2$$

For this to be more than $\Delta E = E_\infty - E_n$ (the ionization energy),

$$1-\cos\chi > \frac{4(E_\infty - E_n)}{m_e w_1^2} \quad \text{or} \quad \chi > \cos^{-1}\left[1 - \frac{4(E_\infty - E_n)}{m_e w_1^2}\right]$$

The cross section for ionization is then $Q_i = 2\pi\int_{\chi_{min}}^{\pi}\sigma(\chi)\sin\chi d\chi$, where, for the Coulomb interaction,

$$\sigma(\chi) = \frac{b_0^2/4}{\sin^4\frac{\chi}{2}} \quad\rightarrow\quad b_0 = \frac{e^2}{4\pi\epsilon_0\mu g^2} = \frac{e^2}{2\pi\epsilon_0 m_e w_1^2}$$

$$Q_i \;=\; \cancel{2}\pi\int_{\chi_{min}}^{\pi}\frac{b_0^2/\cancel{4}}{\sin^4\frac{\chi}{2}}\cancel{2}\sin\frac{\chi}{2}\underbrace{\cos\frac{\chi}{2}d\chi}_{2d(\sin\frac{\chi}{2})} \;=\; 2\pi b_0^2\int_{\sin\frac{\chi_{min}}{2}}^{1}\frac{ds}{s^3} \;=\; \pi b_0^2\left(\frac{1}{\sin^2\frac{\chi_{min}}{2}} - 1\right)$$

and,

$$\sin^2\frac{\chi_{min}}{2} = \frac{1-\cos\chi_{min}}{2} = \frac{2\Delta E}{m_e w_1^2}$$

therefore,

$$Q_i = \pi b_0^2\left(\frac{m_e w_1^2}{2\Delta E} - 1\right)$$

Now define,

$$u \;\equiv\; \frac{\frac{1}{2}m_e w_1^2}{\Delta E} \quad\rightarrow\quad \pi b_0^2 = \cancel{\pi}\frac{e^4}{16\pi^{\cancel{2}}\epsilon_0^2(\Delta E)^2u^2}$$

In terms of the Bohr radius,

$$\frac{e^2}{4\pi\epsilon_0 a_0^{\cancel{2}}} = \frac{m_e v^2}{\cancel{a_0}} \quad \text{and} \quad m_e v a_0 = \hbar \;\rightarrow\; a_0 \;=\; \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$$

and the H atom ionization energy (from $n=1$ to $n=\infty$),

$$E_i^H \;=\; \frac{e^2}{8\pi\epsilon_0 a_0} \quad \text{recall that in bound orbits} \quad \left|E_i^H\right| \;=\; \frac{|V(a_0)|}{2} \;=\; \frac{1}{2}\left(\frac{e^2}{4\pi\epsilon_0 a_0}\right)$$

then writing,

$$\pi b_0^2 = \frac{e^4}{16\pi\epsilon_0^2(\Delta E)^2u^2} = \frac{e^4}{64\pi^2\varepsilon_0^2 a_0^2}\frac{4\pi a_0^2}{(\Delta E)^2u^2} \;=\; \left(E_i^H\right)^2\frac{4\pi a_0^2}{(\Delta E)^2u^2}$$

Therefore,

$$\pi b_0^2 \;=\; 4\pi a_0^2\left(\frac{E_i^H}{\Delta E}\right)^2\frac{1}{u^2}$$

and the ionization cross section is,

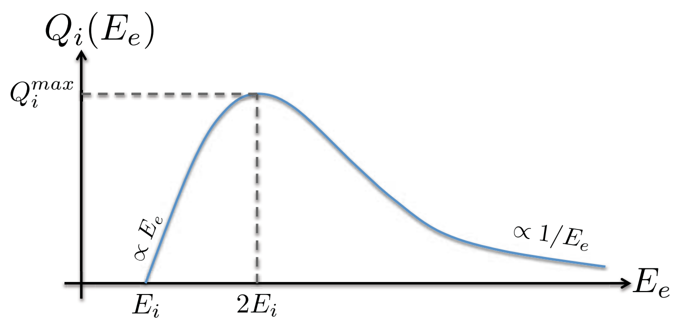
$$Q_i \;=\; 4\pi a_0^2\left(\frac{E_i^H}{E_i}\right)^2\frac{u-1}{u^2} \quad \text{with} \quad u \;=\; \frac{E_e}{E_i}$$

where, for instance, E_e is the energy of an incident electron and E_i is the ionization energy of the target particle in the n^{th} state. We observe that,

$$\left(\frac{u-1}{u^2}\right)_{max} \;=\; \frac{1}{4} \quad \text{when} \quad u=2$$

Finally,

$$Q_i^{max} \;=\; \pi a_0^2\left(\frac{E_i^H}{E_i}\right)^2$$



For H this would predict,

$$Q_i(\text{in } \mathring{A}^2) = 3.52\frac{u-1}{u^2} \qquad \text{with} \qquad u = \frac{E_e(\text{in } eV)}{13.6}$$

This gives $Q_i^{max} = 0.88\mathring{A}^2$ at $E_e = 27.2eV$ (actual is $0.7\mathring{A}^2$ at $70eV$). It also gives $Q_i(200eV) = 0.22\mathring{A}^2$, actual is $0.44\mathring{A}^2$.

For helium, it would predict $Q_i^{max} = 0.88(13.6/24.6)^2 = 0.27\mathring{A}^2$ at $49.2eV$. Actual is $0.36\mathring{A}^2$ at $90eV$.

<u>Note:</u>The cross sections were for a <u>stationary target</u>, and as such contain relative speed g and reduced mass μ. To account for the motion of the target, we need the velocity distribution function f, and will treat that later.
For the Coulomb case, it turns out (1st order Chapman-Enskog theory) that the effective momentum transfer cross-section (to be associated with the mean thermal speed) in $6\pi^2 p_0^2 \ln\Lambda$ instead of $4\pi^2 p_0^2 \ln\Lambda$.

<u>Discussion:</u>

Notice that in a Coulomb orbit $K = -\frac{1}{2}V$ and $E_{tot} = K + V = -K$, i.e., the electron K is numerically equal to the ionization potential from its orbit. Now, this is the <u>least</u> energy in impairing electron can have if it is to produce ionization; therefore, the energy of the bound electron is always less than that of the ionizing electron, and this partially justifies Thompson's assumption of neglecting the bound electron motion. The other assumption, namely, that the electron is effectively free, has a similar justification, since $|V| = -2K$, so that $|V|$ is at most 2 times the energy of the impinging electron, and so the assumptions are expected to be good at several times the ionization potential, and moderately good near the threshold.

<u>More refined cross-section models</u> (see Mitchner-Kruger, pp. 26-29)

<u>Drawin:</u> $Q^{(k\to\lambda)}(E) \;=\; 2.66\pi a_0^2\left(\frac{E_{1\lambda}^H}{E_{k\lambda}}\right)^2 \xi_k\beta_1 g(u)$

$$g(u) \;=\; \frac{u-1}{u^2}ln(1.25\beta_2 u) \quad , \quad u \;=\; \frac{E}{E_{k\lambda}}$$

$$\xi \;=\; \text{number of equivalent electrons in } k^{th}\text{level}$$

$$\beta_1,\beta_2 \simeq 1 \qquad \text{For } \beta_2 = 0.8,\ g_{max} = 0.2603 \text{ at } u = u_m = 4.244$$

<u>Gryzinski:</u> $Q_{GR}(E,E_{k\lambda};\Delta E)$ = Cross section for transfer of energy $> \Delta E$ by electron at E to electron in level k

$$Q_{GR} = 4\pi a_0^2\left(\frac{E_{1\lambda}^H}{\Delta E}\right)^2 \xi_k g(u,v) \quad ; \quad u = \frac{E}{\Delta E}\ ,\ V = \frac{E_{k_\lambda}}{\Delta E}$$

$$g(u_1 v) \;=\; \frac{u-1}{u^2}\left(\frac{u}{u+v}\right)^{3/2}\left(1-\frac{1}{u}\right)^{\frac{v}{v+1}}\left\{1+\frac{2v}{3}\left(1-\frac{1}{2u}\right)\ln\left[e+\left(\frac{u-1}{v}\right)^{1/2}\right]\right\}$$

For ionization, $\Delta E \;=\; E_{k\lambda} \qquad (v = 1)$
For a $k \;\to\; l$ transition, difference between $Q's$ for $\Delta E \;=\; l+1$ and for $\Delta E \;=\; l$

<u>Estimate of 3-body recombination rate</u> (Thompson)

Applies for $T_e \lessapprox E_i$, because at high T_e it is hard to arrange that any e loses so much energy as to be captured.

$R \equiv$ Rate of $e-i$ recombination (3 body, electron 3rd body) in a gas at T_e.

$$R = R_1 p_{ee}$$

$R_1 \;\equiv$ Number of times per second that an electron will pass within an ion's "sphere of influence" (SOI),

$$r_0 \sim \frac{e^2}{4\pi\epsilon_0\frac{3}{2}kT_e}$$

$p_{ee} \equiv$ Probability of an e-e collision while the 1st electron is within the ion's SOI

Strictly speaking, the e-e collision would have to be such that one of the electrons would afterward have negative total energy and be captured (both have initially positive total energies before being accelerated into the ion's field, and one of them should surrender enough K to the other, so that its own K is now less than the magnitude of its (negative) potential energy in the field of the ion). But since e-e collisions are effective for energy transfer, the fraction of all possible e-e collisions satisfying this is of order 1 (for low T_e).

Now,

$$R_1 \simeq n_e n_i \bar{c}_e \pi r_0^2 \qquad \text{and} \qquad P_{ee} = 1 - e^{-r_0/\lambda_{ee}} \simeq \frac{r_0}{\lambda_{ee}} = r_0 n_e Q_{ee} \qquad \text{with} \qquad Q_{ee} \sim \pi r_0^2$$

$$R \simeq n_e n_i \bar{c}_e \pi r_0^2 r_0 n_e \pi r_0^2 \qquad R \simeq n_e^2 n_i \underbrace{\pi^2 r_0^5 \bar{c}_e}_{\alpha} \qquad \alpha = \pi^2 \sqrt{\frac{8}{\pi}\frac{kT_e}{m_e}} \left(\frac{e^2}{6\pi\epsilon_0 kT_e}\right)^5 = \frac{1.04 \times 10^{-20}}{T_e^{9/2}}$$

The more rigorous value (Hinnov-Hirschberg) is,

$$R = \frac{1.09 \times 10^{-20}}{T_e^{9/2}} n_e^2 n_i$$

Notice we did not need screening considerations here, since $r_0 \ll \lambda_D$ ($\Lambda \gg 1$) in cases of interest. In other words, all of this happens <u>within</u> a Debye sphere.

Experimentally, Bates' law gives

$$\frac{R}{n_e n_i} \sim \frac{1.64 \times 10^{-20}}{T_e^{9/2}} n_e$$

So, good within an order of magnitude, and has the right trends in it.