Transport & Coupling

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Contents

Chapter 1

Coulomb scattering

1.1 Particle equations

Consider two particles, with positions $\mathbf{r}_1 = \mathbf{r}_1(t)$ and $\mathbf{r}_2 = \mathbf{r}_2(t)$, velocities $\mathbf{v}_1 = \mathbf{v}_1(t)$ and $\mathbf{v}_2 = \mathbf{v}_2(t)$, charges q_1 and q_2, and masses m_1 and m_2, respectively. Their positions and velocities are governed by the following equations

$$\frac{d\mathbf{r}_1}{dt} = \mathbf{v}_1, \tag{1.1}$$

$$\frac{d\mathbf{r}_2}{dt} = \mathbf{v}_2, \tag{1.2}$$

$$m_1\frac{d\mathbf{v}_1}{dt} = -\frac{q_1q_2}{4\pi\epsilon}\frac{\mathbf{r}_2-\mathbf{r}_1}{|\mathbf{r}_2-\mathbf{r}_1|^3}, \tag{1.3}$$

$$m_2\frac{d\mathbf{v}_2}{dt} = -\frac{q_1q_2}{4\pi\epsilon}\frac{\mathbf{r}_1-\mathbf{r}_2}{|\mathbf{r}_1-\mathbf{r}_2|^3}. \tag{1.4}$$

We note that the above system consists of twelve equations for twelve unknowns. We now introduce the center-of-mass position $\mathbf{R} = \mathbf{R}(t)$, the center-of-mass velocity $\mathbf{V} = \mathbf{V}(t)$, the shifted position $\mathbf{r} = \mathbf{r}(t)$ and the shifted velocity $\mathbf{v} = \mathbf{v}(t)$ as follows

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1+m_2} \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2,$$

$$\mathbf{V} = \frac{m_1\mathbf{v}_1 + m_2\mathbf{v}_2}{m_1+m_2} \qquad \mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2$$

Thus, in terms of these new four variables, the particle equations can be written as

$$\frac{d\mathbf{R}}{dt} = \mathbf{V}, \tag{1.5}$$

$$\frac{d\mathbf{V}}{dt} = 0, \tag{1.6}$$

$$\frac{d\mathbf{r}}{dt} = \mathbf{v}, \tag{1.7}$$

$$\frac{d\mathbf{v}}{dt} = \frac{q_1q_2}{4\pi\epsilon_0 m_r}\frac{\mathbf{r}}{r^3}, \tag{1.8}$$

where the reduced mass m_r is given by

$$\frac{1}{m_r} = \frac{1}{m_1} + \frac{1}{m_2}. \tag{1.9}$$

The first two equations above give the trivial solution $\mathbf{V} =$ constant and $\mathbf{R} = \mathbf{R}(0) + \mathbf{V}t$. Thus, we have reduced the problem from twelve unknowns to six unknowns, namely $\mathbf{r}$ and $\mathbf{v}$.

1.2 Conservation of energy and momentum

Dotting eq. (1.8) by $\mathbf{v}$ gives

$$\begin{aligned}
\mathbf{v}\cdot\frac{d\mathbf{v}}{dt} &= \frac{q_1 q_2}{4\pi\epsilon_0 m_r}\mathbf{v}\cdot\frac{\mathbf{r}}{r^3} \\
&= \frac{q_1 q_2}{4\pi\epsilon_0 m_r}\frac{d\mathbf{r}}{dt}\cdot\frac{\mathbf{r}}{r^3} \\
&= \frac{q_1 q_2}{4\pi\epsilon_0 m_r}\frac{1}{2}\frac{dr^2}{dt}\frac{1}{r^3} \\
&= \frac{q_1 q_2}{4\pi\epsilon_0 m_r}\frac{1}{r^2}\frac{dr}{dt} \\
&= -\frac{q_1 q_2}{4\pi\epsilon_0 m_r}\frac{d}{dt}\left(\frac{1}{r}\right).
\end{aligned}$$

For the left hand side above we have

$$\mathbf{v}\cdot\frac{d\mathbf{v}}{dt} = \frac{1}{2}\frac{dv^2}{dt},$$

and thus we obtain the following expression for conservation of energy

$$\frac{d}{dt}\left(\frac{1}{2}m_r v^2 + \frac{q_1 q_2}{4\pi\epsilon_0}\frac{1}{r}\right) = 0.$$

Crossing eq. (1.8) by $\mathbf{r}$ gives

$$\mathbf{r}\times\frac{d\mathbf{v}}{dt} = \frac{q_1 q_2}{4\pi\epsilon_0 m_r}\frac{\mathbf{r}\times\mathbf{r}}{r^3} = 0,$$

and thus

$$\frac{d}{dt}\left[m_r\left(\mathbf{r}\times\mathbf{v}\right)\right] = 0.$$

That is, angular momentum is conserved. A consequence of this is that the vector $\mathbf{r}\times\mathbf{v}$ is always pointing in the same direction. Thus, if $\mathbf{r}(0)$ and $\mathbf{v}(0)$ form a plane, then $\mathbf{r}(t)$ and $\mathbf{v}(t)$ need to reside within that same plane for all times t so that $\mathbf{r}(t)\times\mathbf{v}(t)$ points in the same direction as $\mathbf{r}(0)\times\mathbf{v}(0)$. Therefore, the evolution of the position and velocity are confined to a plane and the problem can be reduced from six unknowns to four unknowns. This planar encounter is depicted in fig. 1.1.

If we refer to the plane shown in fig. 1.1 as the $x-y$ plane, then one can tell that the angular-momentum vector points in the negative z direction. We will denote the magnitude of the conserved angular momentum by L, and thus we can write

$$m_r\left(\mathbf{r}\times\mathbf{v}\right) = -L\hat{\mathbf{z}}. \tag{1.10}$$

A consequence of both conservation of energy and momentum is as follows. Consider the two limiting states of particle 1—the initial state v_i, b_i and the final state v_f, b_f. Assuming the potential energy is very low at sufficiently early and late times, conservation of energy gives

$$\frac{1}{2}m_r v_i^2 = \frac{1}{2}m_r v_f^2, \tag{1.11}$$

that is, $v_i = v_f$ (note that for other scattering processes, e.g. Compton scattering, this is not necessarily the case). For the angular momentum of the initial state we have

$$\begin{aligned}
m_r\left(\mathbf{r}_i\times\mathbf{v}_i\right) = m_r\sin(-\theta_i)r_i v_i\hat{\mathbf{z}} = -m_r\sin(\theta_i)r_i v_i\hat{\mathbf{z}} &= -m_r\sin(\pi-\varphi_i)r_i v_i\hat{\mathbf{z}} \\
&= -m_r\sin(\varphi_i)r_i v_i\hat{\mathbf{z}} = -m_r b_i v_i\hat{\mathbf{z}}
\end{aligned} \tag{1.12}$$

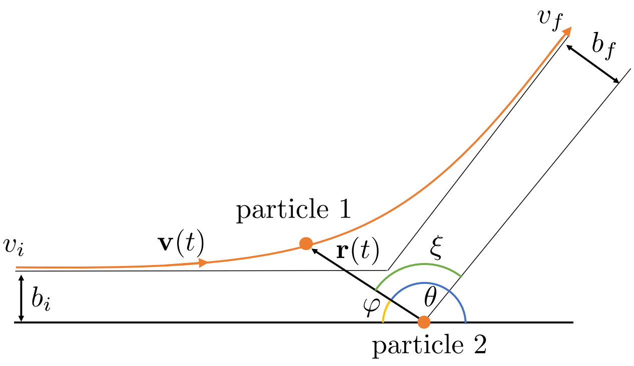

Figure 1.1: Depiction of Coulomb scattering.

Similarly, for the angular momentum of the final state we have

$$m_r\left(\mathbf{r}_f \times \mathbf{v}_f\right) = m_r \sin(-\xi_f) r_f v_f \hat{\mathbf{z}} = -m_r \sin(\xi_f) r_f v_f \hat{\mathbf{z}} = -m_r b_f v_f \hat{\mathbf{z}}. \tag{1.13}$$

Equating the last two relationships gives $m_r b_i v_i = m_r b_f v_f$. Since $v_i = v_f$, we finally have $b_i = b_f = b$. Using eq. (1.10) in eq. (1.12), we can also write

$$L = m_r b v_i. \tag{1.14}$$

1.3 Polar coordinates

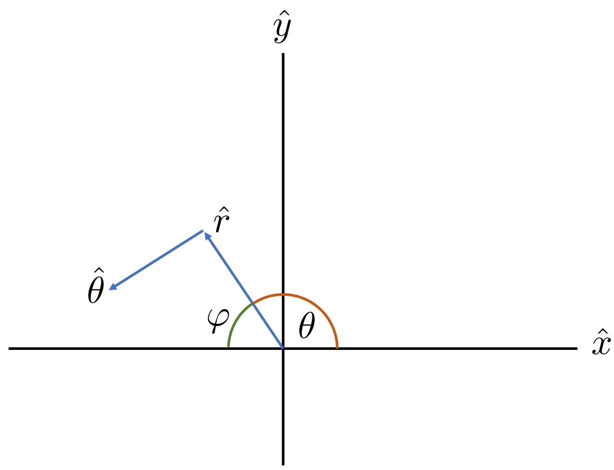

Figure 1.2: Polar coordinates in plane of interaction.

Using polar coordinates, as shown in fig. 1.2, we get

$$r_x = r\cos\theta = r\cos(\pi - \varphi) = -r\cos\varphi,$$

$$r_y = r\sin\theta = r\sin(\pi - \varphi) = r\sin\varphi.$$

Also, since $\mathbf{r} = r\hat{\mathbf{r}}$, we have

$$\begin{aligned}\mathbf{v} =& \frac{d\mathbf{r}}{dt} = \frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\hat{\mathbf{r}}}{dt} \\ &= \frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\hat{\mathbf{r}}}{d\theta}\frac{d\theta}{dt} \\ &= \frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\theta}{dt}\hat{\boldsymbol{\theta}},\end{aligned}$$

and

$$\begin{aligned}\frac{d\mathbf{v}}{dt} &= \frac{d^2r}{dt^2}\hat{\mathbf{r}} + \frac{dr}{dt}\frac{d\hat{\mathbf{r}}}{dt} + \frac{d}{dt}\left(r\frac{d\theta}{dt}\right)\hat{\boldsymbol{\theta}} + r\frac{d\theta}{dt}\frac{d\hat{\boldsymbol{\theta}}}{dt} \\ &= \frac{d^2r}{dt^2}\hat{\mathbf{r}} + \frac{dr}{dt}\frac{d\hat{\mathbf{r}}}{d\theta}\frac{d\theta}{dt} + \frac{d}{dt}\left(r\frac{d\theta}{dt}\right)\hat{\boldsymbol{\theta}} + r\frac{d\theta}{dt}\frac{d\hat{\boldsymbol{\theta}}}{d\theta}\frac{d\theta}{dt} \\ &= \frac{d^2r}{dt^2}\hat{\mathbf{r}} + \frac{dr}{dt}\frac{d\theta}{dt}\hat{\boldsymbol{\theta}} + \frac{d}{dt}\left(r\frac{d\theta}{dt}\right)\hat{\boldsymbol{\theta}} - r\left(\frac{d\theta}{dt}\right)^2\hat{\mathbf{r}}.\end{aligned}$$

The radial component of eq. (1.8) thus becomes

$$\frac{d^2r}{dt^2} - r\left(\frac{d\theta}{dt}\right)^2 = \frac{q_1q_2}{4\pi\epsilon_0 m_r}\frac{1}{r^2}.$$

Since $\theta = \pi - \varphi$, we have

$$\frac{d^2r}{dt^2} - r\left(\frac{d\varphi}{dt}\right)^2 = \frac{q_1q_2}{4\pi\epsilon_0 m_r}\frac{1}{r^2}. \tag{1.15}$$

For the angular momentum we have

$$m_r\mathbf{r}\times\mathbf{v} = m_r r\hat{\mathbf{r}}\times\left(\frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\theta}{dt}\hat{\boldsymbol{\theta}}\right) = m_r r^2\frac{d\theta}{dt}\hat{\mathbf{z}}$$

Using eq. (1.10), we can write the above as

$$m_r r^2\frac{d\varphi}{dt} = L. \tag{1.16}$$

1.4 Particle trajectory

The goal is to find the radial position of the particle as a function of its angular orientation. That is, we want to find $\tilde{r} = \tilde{r}(\tilde{\varphi})$ such that

$$r(t) = \tilde{r}(\varphi(t)). \tag{1.17}$$

To simplify the math, we introduce $\tilde{u} = \tilde{u}(\tilde{\varphi})$ such that $\tilde{u} = 1/\tilde{r}$. Thus

$$\frac{d\tilde{u}}{d\tilde{\varphi}} = -\frac{1}{\tilde{r}^2}\frac{d\tilde{r}}{d\tilde{\varphi}},$$

or, after re-arranging

$$\frac{d\tilde{r}}{d\tilde{\varphi}} = -\frac{1}{\tilde{u}^2}\frac{d\tilde{u}}{d\tilde{\varphi}}. \tag{1.18}$$

We now proceed as follows. Taking the derivative of r, we get

$$\begin{aligned}
\frac{dr}{dt} &= \left(\frac{d\tilde{r}}{d\tilde{\varphi}}\right)_{\tilde{\varphi}=\varphi(t)} \frac{d\varphi}{dt} && [eq.\ (1.17)] \\
&= \left(-\frac{1}{\tilde{u}^2}\frac{d\tilde{u}}{d\tilde{\varphi}}\right)_{\tilde{\varphi}=\varphi(t)} \frac{d\varphi}{dt} && [eq.\ (1.18)] \\
&= \left(-\frac{1}{\tilde{u}^2}\frac{d\tilde{u}}{d\tilde{\varphi}}\right)_{\tilde{\varphi}=\varphi(t)} \frac{L}{m_r r^2} && [eq.\ (1.16)] \\
&= \left(-\frac{1}{\tilde{u}^2}\frac{d\tilde{u}}{d\tilde{\varphi}}\frac{L}{m_r \tilde{r}^2}\right)_{\tilde{\varphi}=\varphi(t)} && [eq.\ (1.17)] \\
&= \left(-\frac{d\tilde{u}}{d\tilde{\varphi}}\frac{L}{m_r}\right)_{\tilde{\varphi}=\varphi(t)} && (1.19)
\end{aligned}$$

Taking the derivative of the above, we get

$$\begin{aligned}
\frac{d}{dt}\frac{dr}{dt} &= \left[\frac{d}{d\tilde{\varphi}}\left(-\frac{d\tilde{u}}{d\tilde{\varphi}}\frac{L}{m_r}\right)\right]_{\tilde{\varphi}=\varphi(t)} \frac{d\varphi}{dt} \\
&= \left(-\frac{d^2\tilde{u}}{d\tilde{\varphi}^2}\frac{L}{m_r}\right)_{\tilde{\varphi}=\varphi(t)} \frac{L}{m_r r^2} && [eq.\ (1.16)] \\
&= \left(-\frac{d^2\tilde{u}}{d\tilde{\varphi}^2}\frac{L}{m_r}\frac{L}{m_r \tilde{r}^2}\right)_{\tilde{\varphi}=\varphi(t)} && [eq.\ (1.17)] \\
&= \left(-\frac{d^2\tilde{u}}{d\tilde{\varphi}^2}\frac{L^2\tilde{u}^2}{m_r^2}\right)_{\tilde{\varphi}=\varphi(t)} && (1.20)
\end{aligned}$$

Plugging the last relation into eq. (1.15) gives

$$\left[-\frac{d^2\tilde{u}}{d\tilde{\varphi}^2}\frac{L^2\tilde{u}^2}{m_r^2} - \frac{1}{\tilde{u}}\left(\frac{L\tilde{u}^2}{m_r}\right)^2\right]_{\tilde{\varphi}=\varphi(t)} = \left(\frac{q_1 q_2}{4\pi\epsilon_0 m_r}\tilde{u}^2\right)_{\tilde{\varphi}=\varphi(t)},$$

which, upon re-arranging and dropping the $\varphi(t)$ dependance, becomes

$$\frac{d^2\tilde{u}}{d\tilde{\varphi}^2} + \tilde{u} = -\frac{q_1 q_2 m_r}{4\pi\epsilon_0 L^2} \tag{1.21}$$

Using eq. (1.14) we write the evolution equation for $\tilde{u}$ as

$$\frac{d^2\tilde{u}}{d\tilde{\varphi}^2} + \tilde{u} = -\frac{q_1 q_2}{4\pi\epsilon_0 m_r b^2 v_i^2}. \tag{1.22}$$

Introducing the notation

$$b_{90} = \frac{q_1 q_2}{4\pi\epsilon_0 m_r v_i^2}, \tag{1.23}$$

the evolution equation for $\tilde{u}$ can be simply expressed as

$$\frac{d^2\tilde{u}}{d\tilde{\varphi}^2} + \tilde{u} = -\frac{b_{90}}{b^2}. \tag{1.24}$$

The boundary conditions for eq. (1.24) are as follows

$$\text{as } \varphi(t) \to 0, \quad r(t) \to \infty \tag{1.25}$$

$$\text{as } \varphi(t) \to 0, \quad \frac{dr(t)}{dt} \to -v_i \tag{1.26}$$

Given eq. (1.17), eq. (1.25) can only be satisfied if as $\tilde{\varphi} \to 0$, $\tilde{r} \to \infty$. Thus, we also have, as $\tilde{\varphi} \to 0$, $\tilde{u} \to 0$. Similarly, given eq. (1.19), eq. (1.26) can only be satisfied if as $\tilde{\varphi} \to 0$

$$\frac{d\tilde{u}}{d\tilde{\varphi}} \frac{L}{m_r} \to v_i.$$

Using eq. (1.14) we rewrite the above as

$$\frac{d\tilde{u}}{d\tilde{\varphi}} \to \frac{1}{b}.$$

The general solution to eq. (1.24) is

$$\tilde{u} = A \cos \tilde{\varphi} + B \sin \tilde{\varphi} - \frac{b_{90}}{b^2}.$$

Applying the boundary conditions, we get

$$\tilde{u} = \frac{b_{90}}{b^2} \cos \tilde{\varphi} + \frac{1}{b} \sin \tilde{\varphi} - \frac{b_{90}}{b^2},$$

which we finally re-write as

$$\frac{1}{\tilde{r}} = \frac{1}{b} \sin \tilde{\varphi} + \frac{b_{90}}{b^2} \left(\cos \tilde{\varphi} - 1\right). \tag{1.27}$$

1.5 The scattering angle

We now drop the tilde notation for the sake of simplicity. That is, for the radial location of an incident particle, we have

$$\frac{1}{r} = \frac{1}{b} \sin \varphi + \frac{b_{90}}{b^2} \left(\cos \varphi - 1\right), \tag{1.28}$$

where φ is the independent variable and $r = r(\varphi)$. We want to know the value of φ as r goes to infinity. Using eq. (1.28), and labeling this angle as φ_s, we have

$$0 = \sin \varphi_s + \frac{b_{90}}{b} \left(\cos \varphi_s - 1\right).$$

We express the above in terms of the scattering angle $\theta_s = \pi - \varphi_s$,

$$0 = \sin(\pi - \theta_s) + \frac{b_{90}}{b} \left[\cos\left(\pi - \theta_s\right) - 1\right].$$

or

$$0 = \sin \theta_s + \frac{b_{90}}{b} \left(-\cos \theta_s - 1\right).$$

Re-writing the above as

$$\frac{\cos \theta_s + 1}{\sin \theta_s} = \frac{b}{b_{90}},$$

and using the trig identity $\cot(\theta/2) = (\cos \theta + 1)/\sin \theta$, we get

$$\cot\left(\frac{\theta_s}{2}\right) = \frac{b}{b_{90}}. \tag{1.29}$$

1.6 The differential cross section

The differential cross section for Coulomb scattering can be computed by making use of a formula derived in my introductory notes, namely

$$\frac{d\sigma_\theta}{d\Omega} = \frac{b}{\sin\theta_s}\left|\frac{db}{d\theta_s}\right|. \tag{1.30}$$

From eq. (1.29) we get,

$$\frac{db}{d\theta} = -\frac{b_{90}}{2}\frac{1}{\sin^2(\theta_s/2)}, \tag{1.31}$$

which, plugging in eq. (1.30), gives

$$\frac{d\sigma_\theta}{d\Omega} = \left[b_{90}\frac{\cot(\theta_s/2)}{\sin\theta_s}\right]\left[\frac{b_{90}}{2}\frac{1}{\sin^2(\theta_s/2)}\right].$$

Using the trig identities $\cot(\theta) = \cos(\theta)/\sin(\theta)$ and $\sin(\theta) = 2\sin(\theta/2)\cos(\theta/2)$ we get

$$\frac{d\sigma_\theta}{d\Omega} = \frac{b_{90}^2}{4}\frac{1}{\sin^4(\theta_s/2)}. \tag{1.32}$$

1.7 Collision integral

$$\Omega^{(lk)}_{\alpha\beta} = \sqrt{\frac{k_BT}{2\pi M_{\alpha\beta}}}\int_0^\infty e^{-g^2}g^{2k+3}\phi^{(l)}_{\alpha\beta}\,dg. \tag{1.33}$$

In the above $M_{\alpha\beta}$ is the reduced mass, given by

$$M_{\alpha\beta} = \frac{M_\alpha M_\beta}{M_\alpha + M_\beta}, \tag{1.34}$$

and $\phi^{(l)}_{\alpha\beta}$ is the collision cross section for a given velocity, and is computed as

$$\phi^{(l)}_{\alpha\beta} = 2\pi\int_0^\infty\left(1-\cos^l\chi_{\alpha\beta}\right)b\,db. \tag{1.35}$$

The scattering angle $\chi_{\alpha\beta}$ is given by

$$\chi_{\alpha\beta} = \pi - 2\int_{r^{\min}_{\alpha\beta}}^\infty \frac{b}{r^2\left[1-\frac{b^2}{r^2}-\frac{V_{\alpha\beta(r)}}{g^2k_BT}\right]^{1/2}}\,dr. \tag{1.36}$$

For a Coulombic interaction between ions, we can define the natural scale fore the cross-sectional area as

$$\phi^{(0)}_{\alpha\beta} = \frac{\pi\left(Z_\alpha Z_\beta e^2\right)^2}{(2k_BT)^2}. \tag{1.37}$$

Given this definition, we express the collision integral as

$$\Omega_{\alpha\beta} = \sqrt{\frac{\pi}{M_{\alpha\beta}}}\frac{(Z_\alpha Z_\beta e^2)^2}{(2k_BT)^{3/2}}\mathcal{F}^{lk}_{\alpha\beta}, \tag{1.38}$$

where

$$\mathcal{F}^{(lk)}_{\alpha\beta} = \frac{1}{2\phi_0}\int_0^\infty e^{-g^2}g^{2k+3}\phi^{(l)}_{\alpha\beta}\,dg \tag{1.39}$$

We note that $\mathcal{F}^{(lk)}_{\alpha\beta} = 4\mathcal{K}_{lk}(g_{\alpha\beta})$, where $\mathcal{K}_{lk}(g_{\alpha\beta})$ is the notation from the Stanton-Murillo paper.

Chapter 2

Transport coefficients

Chapter 3

Coupling coefficients

3.1 Momentum exchange collision frequency ν_{ei}

3.2 Electron-ion thermal coupling w_{ei}