12.3.5 Ion-atom scattering; general binary collision dynamics

A collision between two particles that have an interaction potential $V(r)$ and which collide with an *impact parameter p* is shown in Figure 12.6. It is desired to find the orbit of two particles in an elastic collision and to relate the interaction potential to the differential cross section $\sigma(E, \theta)$.

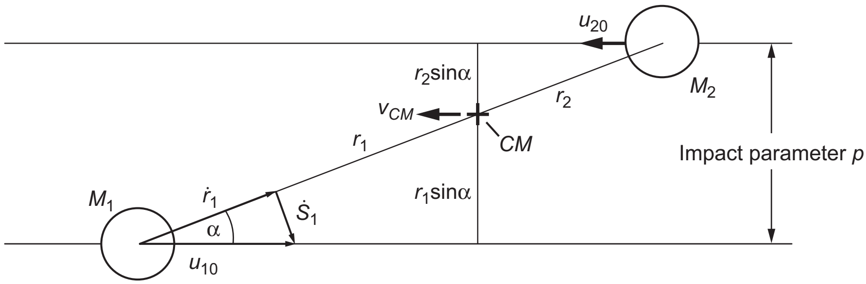

FIGURE 12.6: ***Geometry for derivation of elastic collision between an energetic ion and a stationary atom, interacting by a potential V(r).***

In the system considered, a particle mass M_1 is moving initially with kinetic energy E toward an initially stationary particle mass M_2. The center of mass (CM) is located on the line joining the two masses at a distance

$$r_1 = \frac{M_2}{M_1 + M_2} r \quad \text{and} \quad r = r_1 + r_2 \tag{12.28}$$

from the mass M_1. The initial velocity of particle 1 in the center-of-mass system, u_{10}, is decomposed into two perpendicular components $\dot{r}_1$ and $\dot{S}_1$, such that $\vec{u}_{10} = \vec{\dot{S}}_1 + \vec{\dot{r}}_1$. The line between the particles makes an angle α with the initial direction of the particles in the CM system. Only the initial kinetic energy in the CM system is convertible to potential energy, and this is written

$$E_{CM} = \frac{1}{2}(M_1 + M_2)v_{CM}^2 \quad , \tag{12.29}$$

and using Equation (12.3):

$$E_{CM} = \frac{M_1}{M_1 + M_2} E = \frac{M_1}{M_1 + M_2}\left[\frac{M_1 v_{10}^2}{2}\right] \tag{12.30}$$

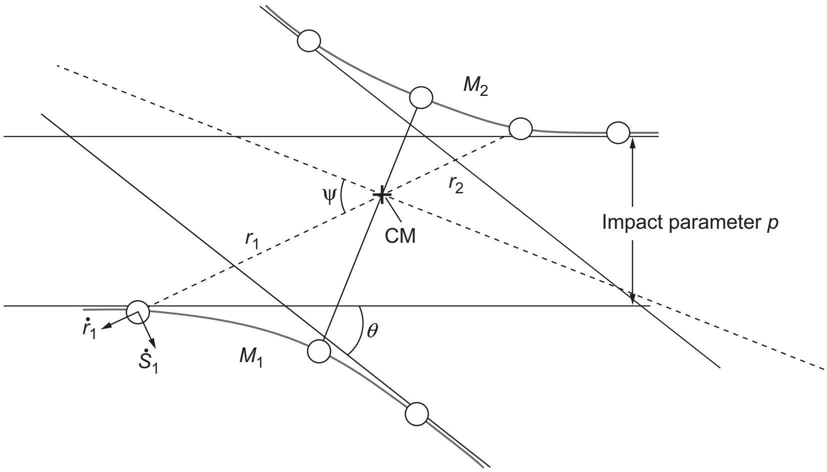

FIGURE 12.7: ***Geometry during the collision in center-of-mass coordinates.***

where E is the initial kinetic energy of particle 1 in the laboratory frame. Now using conservation of energy and angular momentum during the collision, it is possible to derive a relationship between the scattering angle in the center of mass θ and the impact parameter p. The trajectory of the particles as they interact and are deflected by angle θ are shown in Figure 12.7.

Conservation of energy

As the two energetic particles approach each other, they convert kinetic energy into potential energy, $V(r)$, so that at the distance of closest approach, the kinetic energy is minimized. Conservation of energy for the system is

$$E_{CM} = V(r) + \frac{1}{2}M_1 u_{10}^2 + \frac{1}{2}M_2 u_{20}^2 = V(r) + \frac{1}{2}M_1(\dot{r}_1^2 + \dot{S}_1^2) + \frac{1}{2}M_2(\dot{r}_2^2 + \dot{S}_2^2) \quad . \tag{12.31}$$

The tangential speed $\dot{S}$ is equal to $r\dot{\psi}$, so Equation (12.31) is

$$E_{CM} = V(r) + \frac{1}{2}M_1(\dot{r}_1^2 + r_1^2\dot{\psi}^2) + \frac{1}{2}M_2(\dot{r}_2^2 + r_2^2\dot{\psi}^2) \quad , \tag{12.32}$$

and using the definition of the energy of the center of mass,

$$E_{CM} = V(r) + \frac{1}{2}\left(\frac{M_1 M_2}{M_1 + M_2}\right)(\dot{r}^2 + r^2\dot{\psi}^2) \tag{12.33}$$

along with
$$\dot{r}^2 = \left(\frac{dr}{d\psi}\frac{d\psi}{dt}\right)^2 = \left(\frac{dr}{d\psi}\right)^2 \dot{\psi}^2 \tag{12.34}$$

yields
$$E_{CM} = V(r) + \frac{1}{2}\left(\frac{M_1 M_2}{M_1 + M_2}\right)\left(\left[\frac{dr}{d\psi}\right]^2 + r^2\right)\dot{\psi}^2 \quad . \tag{12.35}$$

Conservation of angular momentum

The angular momentum of a mass M about an axis is $\vec{r} \times (M\vec{u}) = rMu \sin\alpha = rM\dot{S}$, where r is the distance between the particle and the axis, u is the velocity, and α is the angle between r and u. Then, the total angular momentum in the CM system is equal to

$$L = r_1 M_1 u_{10} \sin\alpha + r_2 M_2 v_{CM} \sin\alpha \quad . \tag{12.36}$$

The tangential velocity $\dot{S}$ is equal to $r\dot{\psi}$; thus,

$$L = L_1 + L_2 = M_1\dot{S}_1 r_1 + M_2\dot{S}_2 r_2 = M_1 r_1^2\dot{\psi} + M_2 r_2^2\dot{\psi} \quad . \tag{12.37}$$

Using the definition of CM velocity in Equation (12.36) and equating to Equation (12.37)

$$\begin{aligned} L &= \frac{M_1 M_2}{M_1 + M_2} v_{10}(r_1 \sin\alpha + r_2 \sin\alpha) = \frac{M_1 M_2}{M_1 + M_2} v_{10} p \\ &= M_1 r_1^2\dot{\psi} + M_2 r_2^2\dot{\psi} \end{aligned} \tag{12.38}$$

where p is the impact parameter. Using Equations (12.28) in Equation (12.38), we obtain an equation for $\dot{\psi}$

$$\dot{\psi} = v_{10} p / r^2 \quad , \tag{12.39}$$

which can be eliminated in Equation (12.38)

$$E_{CM} = V(r) + \frac{1}{2}\left(\frac{M_1 M_2}{M_1 + M_2}\right)\left(\left[\frac{dr}{d\psi}\right]^2 + r^2\right)\left(\frac{v_{10} p}{r^2}\right)^2 \quad . \tag{12.40}$$

Using Equation (12.30) to eliminate v_{10},

$$\frac{d\psi}{dr} = \frac{p}{r^2}\frac{1}{\left[1 - \frac{V(r)}{E_{CM}} - \frac{p^2}{r^2}\right]^{1/2}} \quad . \tag{12.41}$$

When the particles are at their closest, $r = r_o$ and $\psi = \pi/2$, and when $r \to \infty$, $\psi \to \theta/2$. Integrating Equation (12.41) between these limits:

$$\int_{\theta/2}^{\pi/2} d\psi = \frac{\pi}{2} - \frac{\theta}{2} \quad , \tag{12.42}$$

produces the *Classical Scattering Integral*

$$\theta = \pi - 2\int_{r_o}^{\infty} \frac{p\,dr}{r^2\left[1 - \frac{V(r)}{E_{CM}} - \frac{p^2}{r^2}\right]^{1/2}} \quad . \tag{12.43}$$

Equation (12.43) relates the impact parameter p to the scattering angle in the center of mass θ. At the distance of closest approach, $dr/d\psi = 0$ and

$$1 - \frac{V(r_o)}{E_{CM}} - \frac{p^2}{r_o^2} = 0 \quad . \tag{12.44}$$

Equation (12.44) can be solved for the distance of closest approach as a function of impact parameter. In a head-on collision, $p = 0$ and Equation (12.44) reduces to $V(r_o) = E_{CM}$, which, using Equation (12.27), yields the distance of closest approach in a head-on collision.