Beginning with Rutherford scattering, collisions, between atoms or between charged particles and atoms / molecules, have provided us enormous insights into the structure and dynamics of many-body systems. They have also provided Key information on the evolution of a bound state to a continuum state. The problem is relatively easy to formulate, formally, but usually impossible to solve without making approximations.

Classically, collisions between two particles are entirely determined by their relative velocity (v) and the impact parameter (b) (the distance at which they would pass each other if they did not interact). In quantum mechanics the problem cannot be posed in terms of v ~~ab~~ and b, because the concept of a definite path for a definite velocity are mutually incoststent owing to the uncertainty principle. We can only speak of the probability that an incident particle deviates or scatters through a certain angle, as a result of the collision. Such collisions are called elastic collisions - in which the particles remain unchanged, or if they are composite particles (e.g. atoms), their internal structure remains unchanged. There can also be inelastic collisions - collisions in which the particles themselves or their internal structure changes as a result of the collision.

The problem of collision of two bodies can be reduced to the problem of the scattering of a single body of reduced mass $m = m_1 m_2 / (m_1+m_2)$ moving under the action of a field $U(r)$ of a fixed centre of force (centred on the c-o-m.) The scattering angle in the centre of mass system θ is related to the angles of deviation of the two particles in the laboratory frame by the relationship

$$\tan\theta_1 = (m_2 \sin\theta) / (m_1 + m_2 \cos\theta) \quad ; \quad \theta_2 = (\pi - \theta_1)/2$$

if $m_1 = m_2$, $\theta_1 = \theta/2$, $\theta_1 + \theta_2 = \pi/2$

We will work in the c-o-M frame, and take the incident particles along $\hat{z}$. A free particle of definite momentum $\hbar k$ moving along the $+z$ axis is described by a plane wave $\psi = e^{ikz}$. The current density corresponding to this is given by

$$j = \frac{i\hbar}{2m} \left[\psi \nabla\psi^* - \psi^* \nabla\psi\right]$$

$$= \frac{i\hbar}{2m} \left[-ik\, e^{ikz} e^{-ikz} - ik\, e^{-ikz} e^{ikz}\right] = \frac{2\hbar k}{2m} = v$$

At large distances from the scattering centre the amplitude of the scattered wave must fall off as $1/r$ in order to conserve flux
Thus the scattered particles are described by ~~the~~ a spherical wave $f(\theta)e^{ikr}/r$
We can thus say that asymptotically, irrespective of the type of scattering potential, the solution to the Schrödinger equation with the scattering potential $U(r)$, must have the form

$$\psi_{r\ \text{large}} \approx \underset{\substack{\uparrow \\ \text{ingoing}}}{e^{ikz}} + f(\theta)\underset{\substack{\uparrow \\ \text{outgoing}}}{\frac{e^{ikr}}{r}}$$

[relative amplitudes of the two parts is taken care of in $f(\theta)$]

The probability per unit time that the scattered wave will cross a surface area $d\vec{S}$ is given by $\vec{J}_{scatt}\cdot d\vec{S}$. Since we are looking at spherical scattering, $\vec{J}_{scatt} = j_{scatt}\,\hat{r}$ and $d\vec{S} = r^2 d\Omega\,\hat{r}$.

$$\vec{J}_{scatt} = \frac{i\hbar}{2m}\left[\psi_{sc}\,\hat{r}\frac{\partial}{\partial r}\psi^*_{sc} - \psi^*_{sc}\,\hat{r}\frac{\partial}{\partial r}\psi_{sc}\right]$$

where ψ_{sc} is the scattered wave $f(\theta)e^{ikr}/r$

Hence
$$j_{sc} = \frac{\hbar k}{mr^2}|f(\theta)|^2$$
$$= \frac{v}{r^2}|f(\theta)|^2$$

Thus the probability per unit time that the scattered wave crosses an area dS is $(v/r^2)|f(\theta)|^2\,dS$, or $(v/r^2)|f(\theta)|^2 r^2 d\Omega$
The ratio of the scattering probability to the incident current density is simply $|f(\theta)|^2 d\Omega$
The quantity $f(\theta)$ has dimensions of length, so $|f(\theta)|^2 d\Omega$ must have dimensions of area. Hence we can define the quantity

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2$$

as the differential cross-section for scattering through angle θ

Thus the quantum-mechanical problem of determining the scattering cross-section reduces to the problem of determining $f(\theta)$.
The Schrödinger equation for this probem is (for positive energies $E = \frac{\hbar^2 k^2}{2m}$)

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right]\psi_{klm} = \frac{\hbar^2 k^2}{2m}\psi_{klm}$$

(subject to boundary conditions)

The general solution to this equation is of the form

$$\psi_{\cancel{k\ell m}} = \sum_{\ell=0}^{\infty} A_\ell R_{k\ell}(r)\ P_\ell(\cos\theta)$$

There is not ϕ-dependence in the solution due to azimuthal symmetry of the initial condition, $\vec{k} = k\hat{z}$. The radial part of the Schrödinger eqn is

$$\frac{1}{r^2}\frac{d}{dr} r^2 \frac{dR}{dr} - \frac{\ell(\ell+1)}{r^2} R + \frac{2m}{\hbar^2}\left(E - U(r)\right) R = 0$$

IF $U(r)=0$ the solution to this equation for $\ell=0$ is $\frac{\sin kr}{r}$ or $\frac{\cos kr}{r}$ or $\frac{e^{\pm ikr}}{r}$

Of these only $\sin(kr)/r$ is finite at $r=0$ and by recurrence relation we can obtain solutions for $\ell \neq 0$

$$R_{k\ell} = (-)^\ell \frac{2r^\ell}{k^\ell}\left[\left(\frac{1}{r}\frac{d}{dr}\right)^\ell \frac{\sin kr}{r}\right]$$

For large r the Schrö eqn for radial part is

$$\frac{1}{r}\frac{d^2(rR)}{dr^2} + k^2 R = 0$$

and as $r \to \infty$ $\quad R^\infty_{k\ell} \approx \frac{2\sin(kr - \ell\pi/2)}{r}$

IF $U(r) \neq 0$, but $U(r) \to 0$ as $r \to \infty$, then

$$R^\infty_{k\ell} \simeq \frac{2\sin(kr - \ell\pi/2 + \delta_\ell)}{r} = \frac{1}{ir}\left\{(-i)^\ell e^{i(kr+\delta_\ell)} - (i)^\ell e^{-i(kr+\delta_\ell)}\right.$$

The difference between the solutions for the two cases $U(r)=0$ everywhere and $U(r) \to 0$ as $r \to \infty$ leads to a phase shift in the radial solution.

The phase shift has to be determined by requiring that $R_{k\ell}$ remain finite as $r \to 0$ in the presence of $U(r)$. This requires the solution of the exact radial Schrödinger equation (NO GENERAL FORMULA for δ_ℓ)

Thus for large r

$$\psi = \sum_{\ell=0}^{\infty} A_\ell \frac{2\sin(kr - \ell\pi/2 + \delta_\ell)}{r} P_\ell(\cos\theta)$$

we choose $A_\ell = \frac{1}{2k}(2\ell+1)\, i^\ell \exp(i\delta_\ell)$ to match the general form of $\psi\,(r\to\infty)$ for the scattering case. (i.e. $\psi \to e^{ikz} + f(\theta)\, e^{ikr}/r$)

Note that

$$e^{ikz} = \frac{1}{2ikr}\sum_0^\infty (2\ell+1) P_\ell(\cos\theta)\left[(-)^{\ell+1} e^{-ikr} + e^{+ikr}\right]$$

and

$$\psi\,(r\to\infty) = \sum_0^\infty \frac{1}{2k}(2\ell+1)\, i^\ell e^{i\delta_\ell} \cdot \frac{1}{ir}\left\{(-i)^\ell e^{i(kr+\delta_\ell)} - i^\ell e^{-i(kr+\delta_\ell)}\right\} \times P_\ell(\cos\theta)$$

The difference $\psi_{r\to\infty} - e^{ikz}$ has no terms containing e^{-ikr} that is the difference between the outgoing and ~~incoming~~ incident waves has only outgoing radial waves, as expected.

The coeff of e^{ikr}/r in the difference $\psi_{r\to\infty} - e^{ikz}$ is the scattering amplitude $f(\theta)$.

$$f(\theta) = \frac{1}{2ik} \sum_{0}^{\infty} (2l+1)\left[S_l - 1\right] P_l(\cos\theta) \qquad \text{where } S_l = e^{2i\delta_l}$$