12 Scattering in three dimensions

12.1 Cross sections and geometry

Most experiments in physics consist of sending one particle to collide with another, and looking at what comes out.

The quantity we can usually measure is the scattering cross section: by analogy with classical scattering of hard spheres, we assuming that scattering occurs if the particles 'hit' each other. The cross section is the apparent 'target area'. The total scattering cross section can be determined by the reduction in intensity of a beam of particles passing through a region on 'targets', while the differential scattering cross section requires detecting the scattered particles at different angles.

We will use spherical polar coordinates, with the scattering potential located at the origin and the plane wave incident flux parallel to the z direction. In this coordinate system, scattering processes are symmetric about ϕ, so $\frac{d\sigma}{d\Omega}$ will be independent of ϕ.

We will also use a purely classical concept, the impact parameter b which is defined as the distance of the incident particle from the z-axis prior to scattering.

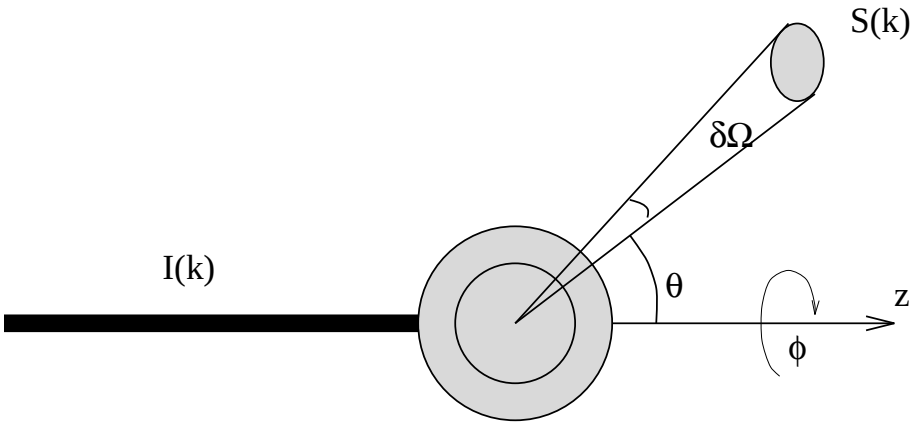

Figure 11: Standard spherical coordinate geometry for scattering

12.2 The Born Approximation

We can use time-dependent perturbation theory to do an approximate calculation of the cross-section. Provided that the interaction between particle and scattering centre is *localised* to the region around $r = 0$, we can regard the incident and scattered particles as free when they are far from the scattering centre. We just need the result that we obtained for a *constant* perturbation, Fermi's Golden Rule, to compute the rate of transitions between the initial state (free particle of momentum $\mathbf{p}$) to the final state (free particle of momentum $\mathbf{p}'$).

The Hamiltonian for a single particle being scattered by a fixed potential as

$$\hat{H} = \hat{H}_0 + \hat{V}(\mathbf{r}) \quad \text{where} \quad \hat{H}_0 = \frac{\hat{\mathbf{p}}^2}{2m}, \text{ the kinetic energy operator}$$

and treat the potential energy operator, $\hat{V}(\mathbf{r})$, as the perturbation inducing transitions between the eigenstates of $\hat{H}_0$, which are plane waves.

If we label the initial and final plane-wave states $\Phi_{in} = \exp(i\mathbf{k}.\mathbf{r} - i\omega t)$ and $\Phi_{scat} = \exp(i\mathbf{k}'.\mathbf{r} - i\omega' t)$ by their respective wave-vectors, then Fermi's Golden Rule for the rate of transitions is

$$R = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle|^2 \, g(E_k)$$

where $g(E_k)$ is the density of final states; $g(E_k)\mathrm{d}E_k$ is the number of final states with energy in the range $E_k \to E_k + \mathrm{d}E_k$.

The quantity $\langle \mathbf{k}'|\hat{V}|\mathbf{k}\rangle$ is known as the *matrix element* of the perturbation and is usually abbreviated thus

$$V_{\mathbf{k}'\mathbf{k}} \equiv \langle \mathbf{k}'|\hat{V}|\mathbf{k}\rangle = \int\int\int u^*_{\mathbf{k}'}(\mathbf{r})\, V(\mathbf{r}) u_{\mathbf{k}}(\mathbf{r})\, \mathrm{d}\tau.$$

The time variation has been suppressed here. For constant potential, the only non-zero terms come from $\omega = \omega'$: elastic scattering. For a time oscillating potential (e.g. $V(\mathbf{r})\sin\omega_0 t$) the non-zero contribution comes from $\omega = \omega' \pm \omega_0$: inelastic scattering where the scattered particle gains/loses a quantum of energy from/to the system providing the potential.

12.3 Box Normalisation and Density of Final States

Plane-wave states have wavefunctions of the form: $u_{\mathbf{k},\omega}(\mathbf{r}) = C\,\exp(i(\mathbf{k}.\mathbf{r} - \omega t))$ with C a normalisation constant. Because plane-wave states are not properly normalisable we employ the trick of normalising them in a large (relative to potential range) cubic box of side L with periodic boundary conditions. We then take the limit $L \to \infty$ at the end of the calculation.

Thus we require that

$$\int\int\int_{\text{box}} u^*_{\mathbf{k},\omega}(\mathbf{r}) u_{\mathbf{k},\omega}(\mathbf{r})\, \mathrm{d}\tau = |C|^2 \int\int\int_{\text{box}} \mathrm{d}\tau = |C|^2\, L^3 = 1$$

giving for the normalised eigenfunctions: $u_{\mathbf{k},\omega}(\mathbf{r}) = L^{-3/2}\,\exp(i\mathbf{k}.\mathbf{r} - \omega t)$

Of course, enclosing the system in a finite box has the consequence that the allowed momentum eigenvalues are no longer continuous but *discrete*. With periodic boundary conditions

$$u(-\frac{L}{2}, y, z) = u(\frac{L}{2}, y, z), \quad \text{etc.}$$

the momentum eigenvalues are forced to be of the form

$$\mathbf{p} \equiv \hbar\mathbf{k} = \frac{2\pi\hbar}{L}(n_x, n_y, n_z), \quad \text{with } n_x,\, n_y,\, n_z = 0, \pm1, \pm2, \ldots$$

For sufficiently large L, we can approximate the continuous spectrum arbitrarily closely.

Any possible final-state wave-vector, $\mathbf{k}$, corresponds to a point in *wave-vector* space with coordinates (k_x, k_y, k_z). The points form a cubic lattice with lattice spacing $2\pi/L$. Thus the volume of k–space per lattice point is $(2\pi/L)^3$, and the number of states in a volume element $\mathrm{d}^3\mathbf{k}$ is

$$\left(\frac{L}{2\pi}\right)^3 \mathrm{d}^3\mathbf{k}' = \left(\frac{L}{2\pi}\right)^3 k^{\,2}\, \mathrm{d}k\, \mathrm{d}\Omega$$

We require $g(E_k)$, the density of states per unit energy, where: $E_k = \hbar^2 k^2/2m$ is the energy corresponding to wave-vector $\mathbf{k}'$. Now, the wave-vectors in the range $\mathbf{k}' \to \mathbf{k}' + \mathrm{d}^3\mathbf{k}'$ correspond to the energy range $E_k \to E_k + \mathrm{d}E_k$, so that

$$g(E_k)\, \mathrm{d}E_k = \left(\frac{L}{2\pi}\right)^3 k^{\,2}\, \mathrm{d}k\, \mathrm{d}\Omega$$

is the number of states with energy in the desired interval and with wave-vector, $\mathbf{k}'$, pointing into the solid angle $\mathrm{d}\Omega$ about the direction (θ, ϕ). Noting that $\mathrm{d}E_k = (\hbar^2 k/m)\ \mathrm{dk}$ yields the final result for the density of states,

$$g(E_k) = \frac{L^3\, mk}{8\pi^3\hbar^2}\, \mathrm{d}\Omega$$

12.4 Incident and Scattered Flux

The box normalisation corresponds to one particle per volume L^3, so that the number of particles crossing unit area perpendicular to the beam per unit time is just given by the magnitude of the incident velocity divided by L^3:

$$\text{incident flux } = \frac{|\mathbf{p}|/m}{L^3} = \frac{\hbar k}{mL^3}$$

Using the Golden Rule, we have that the rate of transitions between the initial state of wave-vector $\mathbf{k}$ and final states whose wave-vectors $\mathbf{k}'$ lie in the element of solid angle $\mathrm{d}\Omega$ about the direction (θ, ϕ) of the wave-vector $\mathbf{k}'$, is given by

$$R = \frac{2\pi}{\hbar} |V_{\mathbf{k}'\mathbf{k}}|^2 \frac{L^3}{8\pi^3} \frac{mk}{\hbar^2} \mathrm{d}\Omega$$

but this is just the number of particles scattered into $\mathrm{d}\Omega$ per unit time. To get the scattered flux we simply divide by $\mathrm{d}\Omega$ to get the number per unit time per unit solid angle.

12.5 The Differential Cross-Section

We now have all the ingredients, the scattered flux and the incident flux, to compute the cross-section:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \equiv \frac{\text{scattered flux}}{\text{incident flux}} = \frac{mL^3}{\hbar k'} \frac{2\pi}{\hbar} |V_{\mathbf{k}'\mathbf{k}}|^2 \frac{L^3}{8\pi^3} \frac{mk}{\hbar^2}$$

Noting that, for *elastic scattering*, $k' = k$, we obtain finally the so-called Born approximation for the differential cross-section:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{m^2}{4\pi^2\hbar^4} L^6 \left| \langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle \right|^2$$

where the matrix element $V_{\mathbf{k}'\mathbf{k}} \equiv \langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle$ is given by

$$\langle \mathbf{k}' | \hat{V} | \mathbf{k} \rangle = \frac{1}{L^3} \int\int\int V(\mathbf{r}) \exp(-i\chi.\mathbf{r}) \, \mathrm{d}\tau$$

with $\chi \equiv \mathbf{k}' - \mathbf{k}$, the so-called *wave-vector transfer*. Thus the required matrix element in the Born approximation is just the 3-dimensional Fourier transform of the potential energy function. The total scattering cross section is simply:

$$\sigma_T = \int \frac{d\sigma}{d\Omega} d\Omega = \int\int \frac{d\sigma}{d\Omega} \sin\theta \, d\theta d\phi$$

Observe that the final result for the differential cross-section is independent of the box size, L, which we used to normalise the plane-wave states.

12.6 Further Simplification to 1D for Conservative, Central Potential

Consider a central potential $V(\mathbf{r}) = V(|\mathbf{r}|)$ where energy is conserved $|\mathbf{k}'|^2 = |\mathbf{k}|^2$. Here χ is a vector of length $2k \sin\frac{\theta}{2}$ where θ is the scattering angle.

We can make some progress with the matrix element integral if we choose a polar coordinate system with χ along the z-axis, so that $\chi.\mathbf{r} = \chi r \cos\theta$. Since we are trying to integrate over all space this change does not affect the limits of the integral.

$$V_{\mathbf{k}'\mathbf{k}} = \int_0^{2\pi} d\phi \int_{-1}^{+1} \int_0^{\infty} V(r) e^{-i\chi r \cos\theta} r^2 dr d(\cos\theta)$$

$$= 2\pi \int_0^{\infty} \frac{e^{-i\chi r} - e^{i\chi r}}{-i\chi r} V(r) r^2 dr = \frac{4\pi}{\chi} \int_0^{\infty} r V(r) \sin(\chi r) dr$$

But since $|\mathbf{k}| = |\mathbf{k}'|$, $|\chi| = 2k\sin\frac{\theta}{2}$, Whence we obtain the most useful form of the Born approximation:

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(k\sin\frac{\theta}{2})^2\hbar^4}\left|\int_0^\infty rV(r)\sin(2kr\sin\frac{\theta}{2})dr\right|^2$$

Thus the scattering cross-section is independent of ϕ (due to cylindrical symmetry of the problem). Note that this shows that the differential cross section does not depend on scattering angle and beam energy independently, but on a single parameter χ. By using a range of energies for the incoming particles, k, this dependence can be used to test whether experimental data can be well described by the Born Approximation.

The most common use of the Born approximation is, of course, in reverse. Having found $\frac{d\sigma}{d\Omega}$ experimentally, a reverse Fourier transform can be used to obtain the form of the potential.

12.7 Example of Born Approximation

Consider scattering of particles interacting via a 3D square well potential: $V(r < a) = V_0$; $V(r > a) = 0$.

The integral required here is then (with $\chi = 2k\sin\frac{\theta}{2}$):

$$\int_0^a rV_0\sin(\chi r)dr = \left[\frac{\sin(\chi r) - \chi r\cos(\chi r)}{\chi^2}\right]_0^a$$

whence:

$$\frac{d\sigma}{d\Omega} = \left[\frac{2\mu V_0}{\chi\hbar^2}\right]^2\left[\frac{\sin(\chi a) - \chi a\cos(\chi a)}{\chi^2}\right]^2$$

Using a Maclaurin expansion, the low energy limit is:

$$\frac{d\sigma}{d\Omega} = \left[\frac{2\mu V_0}{\chi\hbar^2}\right]^2\frac{1}{9}\left[1 - \frac{1}{5}\chi^2a^2\right]$$

From integrating over θ and ϕ the low and high energy limits for the total cross section are

$$\sigma(E\to\infty) = 2\pi\left[\frac{\mu}{\hbar^2}\right]^2\left[\frac{V_0a^3}{ka}\right]^2 \qquad \sigma(E\to 0) = 2\pi\left[\frac{\mu}{\hbar^2}\right]^2\left[\frac{V_0a^3}{ka}\right]^2\frac{8}{9}(k^2a^2 - \frac{2}{5}k^4a^4 + ...)$$

12.8 General Notes on Scattering in the Born Approximation

The square well illustrates some general feature of scattering in the Born approximation:

- Born approximation is based on perturbation theory, so works best for high energy particles.
- Scattering depends on V_0^2, so both attractive and repulsive potentials behave the same.
- At high energy, cross section is inversely proportional to the energy ($E = \hbar^2k^2/2m$)
- Dependence on k and θ arises only through the combination $\chi = 2k\sin\frac{\theta}{2}$. Thus as energy increases, the scattering angle θ is reduced and the scattered beam becomes more peaked in the 'straight on' direction.
- Angular dependence depends on the range of the potential a but not on the strength V_0.
- Total cross section depends on both range a and depth V_0 of the potential.