Scattering

Classical model

As a model for the classical approach to collision, consider the case of a billiard ball colliding with a stationary one. The scattering direction quite clearly depends rather sensitively on *where* the first ball strikes the second. This is traditionally parametrized in terms of b, the 'impact parameter'.

Let b be the distance of closest approach between the trajectory of the *center* of the moving ball and the *center* of the stationary one.

Similarly the direction of the scattering is parametrized by θ, the angle between the asymptotic exiting trajectory and the incoming trajectory. θ is 0° in the absence of collision and 180° if the incoming ball is knocked back along its incoming trajectory.

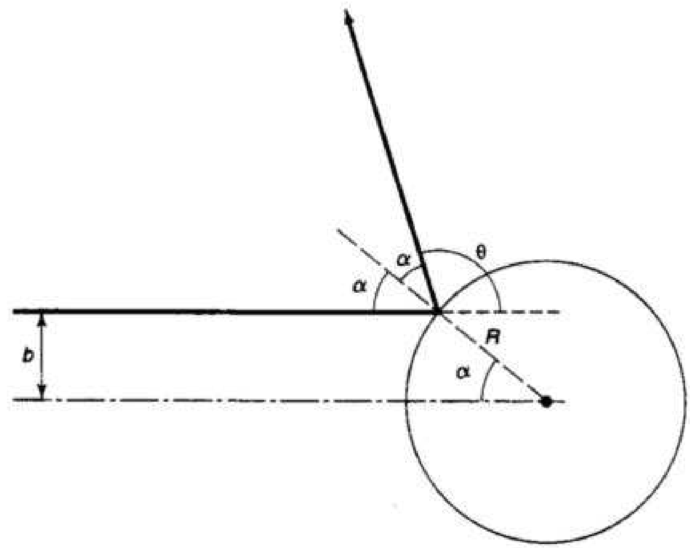

Figure 11.2 - Classical elastic hard-sphere scattering.

Assuming that the stationary ball is so massive that it will not move during the collision, it is a geometry exercise to show that $b = R\cos(\theta/2)$, yielding the scattering angle as a function of impact parameter for what is known as 'hard-sphere scattering'.

More generally, particles incident within an infinitesimal patch of cross-sectional area $d\sigma$ will scatter into a corresponding infinitesimal solid angle $d\Omega$. The ratio of these, which clearly is a function of the location of $d\sigma$, is called the 'differential scattering cross-section', $D(\theta) \equiv d\sigma/d\Omega$.

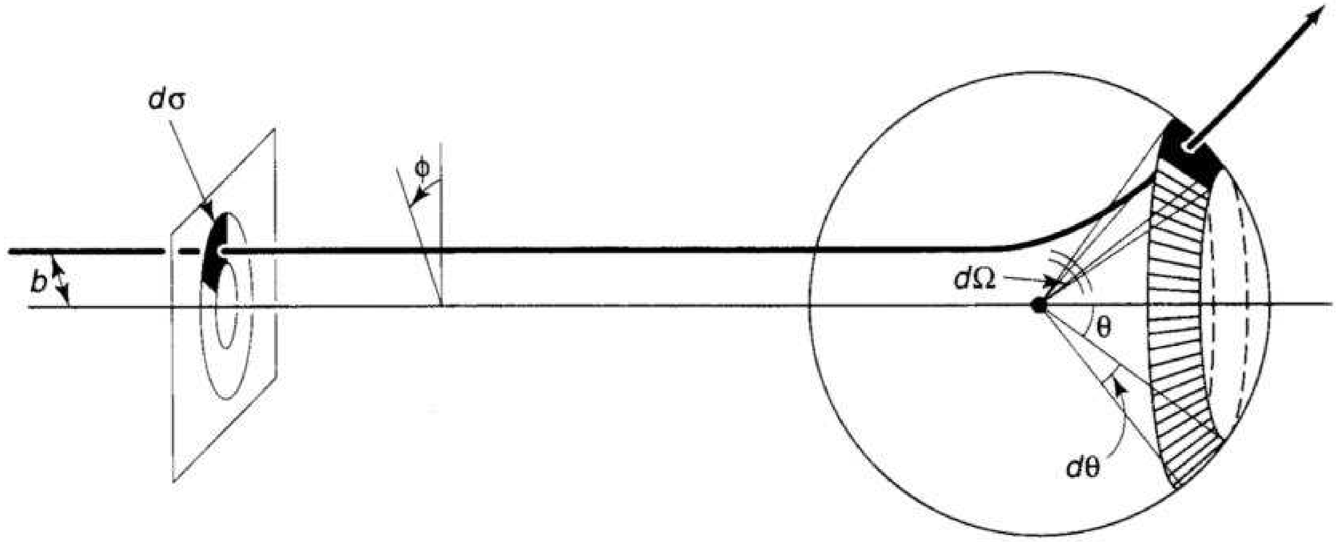

Figure 11.3 - Particles incident in the area $d\sigma$ scatter into the solid angle $/d\Omega$.

Note that D is a function only of θ because the scatterer is symmetric with azimuthal angle ϕ, the only other parameter necessary to specify completely a direction.

On the other hand, $d\Omega = \sin\theta d\theta d\phi$ and $d\sigma = bdbd\phi$, so $D(\theta) = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$. The total scattering cross-section is the integral of D over all angles, $\sigma \equiv \int d\Omega D(\theta)$.

For hard-sphere scattering, $D(\theta) = \frac{R^2}{4}$ and $\sigma = \pi R^2$, a comforting result.

Quantum model

In developing a quantum theory, it is natural to start with a plane wave $\psi(z) = Ae^{ikz}$, traveling in the z direction, incident on a potential which scatters that plane wave, creating an outgoing spherical wave.

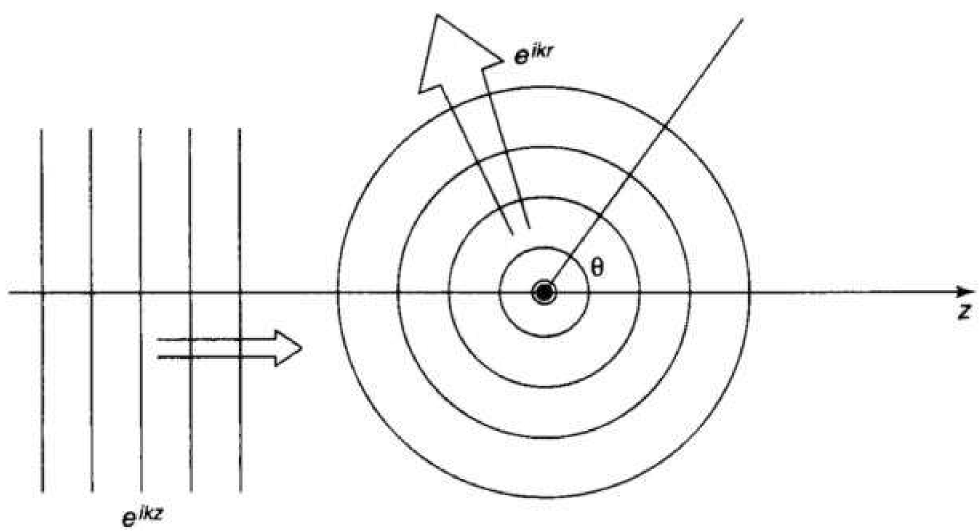

Figure 11.4 - Scattering of waves: incoming plane wave e^{ikz} generates outgoing spherical wave.

This leads to solutions of the Schrödinger equation of the general form $\psi(r,\theta) = A[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}]$, for large r.

We have restricted the scattering potential to have azimuthal symmetry, leading to an azimuthally symmetric scattered wave. Otherwise, $f \to f(\theta, \phi)$.

We have chosen to display the r dependence of the scattered state explicitly; which dependence is required to conserve probability. Finally, $k \equiv \frac{\sqrt{2mE}}{\hbar}$.

We now want to relate the scattering amplitude, f, which is the probability of scattering in a given direction θ, with the differential cross-section. The probability that the incident particle, traveling at speed v, passes through the infinitesimal area $d\sigma$ in time dt is $dP = |\psi_{\text{incident}}|^2 dV = |A|^2 (v dt) d\sigma$.

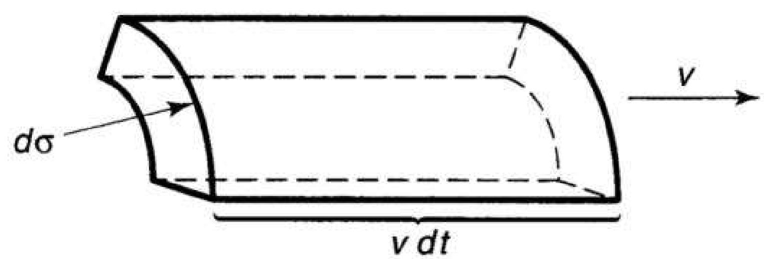

Figure 11.5 - The volume dV of incident beam that passes through area $d\sigma$ in time dt.

But this is equal to the probability that the particle later emerges into the corresponding angle $d\Omega$, *i.e.*,
$dP = |\psi_{\text{scattered}}|^2 dV = \frac{|A|^2 |f|^2}{r^2} (v dt) r^2 d\Omega$.

Equating these two expressions implies $d\sigma = |f|^2 d\Omega$, or $D(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2$. In words, the differential scattering cross-section is determined by the scattering amplitude, obtained by solving the Schrödinger equation.

In the remainder of the chapter, we investigate two techniques for calculating these quantities.

Partial wave analysis

Most useful calculational techniques involve a critical approximation or assumption. In this case, we assume that the scattering potential is localized in space, allowing us to use solutions for the spherically symmetric Schrödinger equation while in the region external to the potential. This approximation would *not* allow us to treat scattering from an unscreened Coulomb potential, for example.

The Schrödinger equation for a spherically symmetric geometry can be solved by assuming a product solution: $\psi(r,\theta,\phi) = R(r)Y_l^m(\theta,\phi)$, where the Y_l^m are the spherical harmonics and $u(r) = rR(r)$ satisfies

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu,$$

with normalization $\int dr\,|u|^2 = 1$.

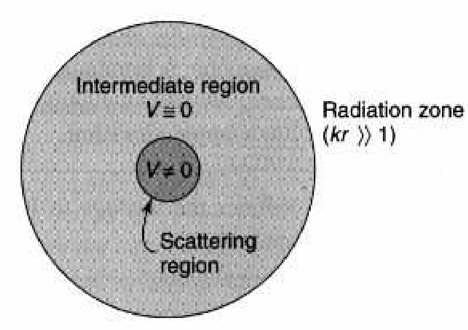

Figure 11.6 - Scattering from a localized potential: the scattering region (shaded dark), the intermediate region (where $V = 0$), and the radiation zone (where $kr \gg 1$).

For *very* large r, both terms in square brackets $\rightarrow 0$, and the differential equation $\rightarrow \frac{d^2u}{dr^2} \approx -k^2 u$ for $E > 0$.

The solutions to this equation are $u(r) = Ce^{ikr} + De^{-ikr}$. Since $\Psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-iEt/\hbar}$, the first term represents an *outgoing* spherical wave, and the second an *incoming* one. $\therefore D = 0$ and $R(r) \approx \frac{e^{ikr}}{r}$, a result which has already been incorporated in the form for a scattered wave. This is the solution for *very* large r (or, more precisely, for $kr \gg 1$), a region corresponding to the 'radiation zone' in optics.

Suppose we are closer to the potential, but still outside its range. Including the centrifugal term, the d.e. becomes $\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u = -k^2u$. The solutions of this equation are the spherical Bessel functions, $j_l(kr)$ and $n_l(kr)$.

If our solutions were plane waves we could choose to use either sin(x) and cos(x) as a complete set of functions, or e^{ix} and e^{-ix}. Similarly, for this d.e. we have a choice between j_l and n_l, or $h_l^{(1)}$ and $h_l^{(2)}$, the spherical Hankel functions. The latter set is better in this instance since, as $r \to \infty$, $h_l^{(1)}(kr) = j_l(kr) + n_l(kr) \to (-i)^{l+1}\frac{e^{ikr}}{kr}$.

Therefore, in the external region where $V(r) = 0$, the solution is

$$\psi(r, \theta, \phi) = A[e^{ikz} + \sum_{l,m} C_{l,m} h_l^{(1)}(kr) Y_l^m(\theta, \phi)].$$

The (potentially infinite) sum over l and m generalizes this w.f. to express the ‘large r’ solution for *any* localized potential.

Comparing this expression for ψ in the limit as $r \to \infty$ with the earlier expression involving f yields

$$f(\theta, \phi) = \frac{1}{k} \sum_{l,m} (-i)^{l+1} C_{l,m} Y_l^m(\theta, \phi).$$

This leads directly to corresponding expressions for D and σ. Somewhat simpler expressions would have resulted if V were independent of ϕ, as is usually the case.

Partial wave analysis proceeds by solving the Schrödinger equation in the interior region, where $V(r)$ is definitely not zero, and then matching this to the exterior solution given above, thereby determining the $C_{l,m}$.

In doing this, it is helpful to expand e^{ikz} in spherical harmonics, leading to

$$\psi(r, \theta, \phi) = A \sum_{l,m} \Big[\delta_{m,0} \sqrt{4\pi(2l+1)} i^l j_l(kr) + C_{l,m} h_l^{(1)}(kr) \Big] \, Y_l^m(\theta, \phi).$$

Integral form of the Schrödinger equation

The Schrödinger equation, $-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$, can be written as $(\nabla^2 + k^2)\psi = Q$, where $k \equiv \frac{\sqrt{2mE}}{\hbar}$ and $Q \equiv \frac{2m}{\hbar^2}V\psi$.

This would be the Helmholtz equation were it not that Q depends in fact on ψ.

Suppose we had a solution, G, to the Helmholtz equation with a δ-function source, $(\nabla^2 + k^2)G(\mathbf{r}) = \delta^3(\mathbf{r})$.

Then we could express ψ as an integral: $\psi(\mathbf{r}) = \int d^3\mathbf{r}' G(\mathbf{r} - \mathbf{r}')Q(\mathbf{r}')$. G is called the *Green's function* for the three-dimensional Helmholtz equation.

Some manipulation, including using Cauchy's integral formula to evaluate contour integrals in complex space, yields in due course $G(\mathbf{r}) = -\frac{e^{ikr}}{4\pi r}$. This is the free-particle Green's function.

Adding a solution of the homogeneous equation to G and incorporating the $\frac{2m}{\hbar^2}$ factor leads to the following integral equation:
$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \int d^3\mathbf{r}'\, g(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')$, where ψ_0 satisfies the free-particle Schrödinger equation and $g(\mathbf{r}) \equiv -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}$.

This equation is completely equivalent to the differential Schrödinger equation.

Schematically, $\psi = \psi_0 + \int gV\psi$.

Iterating, $\psi = \psi_0 + \int gV\psi_0 + \int gVgV\psi_0 + \ldots$.

This series is a sensible approach if V is ‘small’, and is called the ‘Born series’.

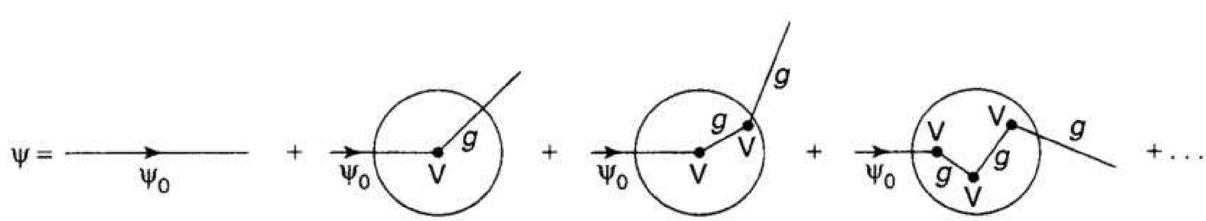

Figure 11.13 - A diagrammatic representation of the Born series.

Born approximation in scattering

The *Born approximation* results when the potential is taken to be so small that only the first power of V in the Born series is important, yielding $\psi \cong \psi_0 + \int gV\psi_0$.

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \int d^3\mathbf{r}'\, g(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi_0(\mathbf{r}')$$

The potential is negligible except near $\mathbf{r}' = 0$. Far away from the scattering center, $r \gg r'$. Then $|\mathbf{r}-\mathbf{r}'| \cong r - \mathbf{r}\cdot\mathbf{r}'/r$ and $\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \cong \frac{e^{ikr}}{r}e^{-i\mathbf{k}\cdot\mathbf{r}'}$, where $\mathbf{k} \equiv k\hat{\mathbf{r}}$.

Let $\psi_0(\mathbf{r}') = Ae^{ikz'} = Ae^{i\mathbf{k}'\cdot\mathbf{r}'}$, where $\mathbf{k}' \equiv k\hat{\mathbf{z}}'$. Note that $\mathbf{k}'$ points in the direction of the incident beam, while $\mathbf{k}$ points toward the detector.

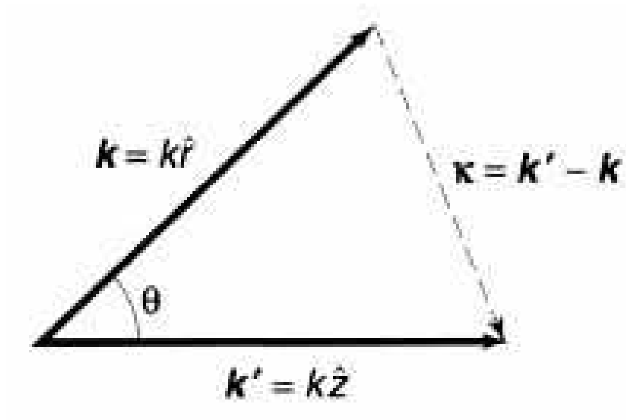

Figure 11.11 - The two wave vectors in the Born approximation: $\mathbf{k}'$ points in the *incident* direction; $\mathbf{k}$ in the *scattered* direction; $\kappa \equiv \mathbf{k}' - \mathbf{k}$.

Comparing the above expression for ψ with the equation involving f yields $f(\theta, \phi) \cong -\frac{m}{2\pi\hbar^2} \int d^3\mathbf{r}'\, e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}'} V(\mathbf{r}')$, plus related expressions.