Chapter 2

Scattering

2.1 Solving the Schrödinger equation for unbound states

We saw in the previous lecture how to solve the Schrödinger equation for bound states, using either the Runge-Kutta or Numerov method. The bound states were characterised by having quantised energies and wavefunctions that went to zero as $r \to \infty$. What then, of unbound states? Here we typically have a continuum of available energy levels, and a finite wavefunction as $r \to \infty$. Obviously, such states do not correspond to electrons in an atom, but are still nevertheless very important. One very important role of such unbound quantum particles is in scattering experiments, where a high energy particle is scattered off some potential barrier, and the measurement of the scattering is used to yield important information about both the scatterer and the scattering centre.

The solution techniques are the same as for bound states, but the analysis of the scattered wavefunction is different. In general, scattering may be either elastic (energy conserving) or inelastic (energy transferred from scattering particle to scattering centre). In this lecture, we shall only consider elastic scattering, and continuing in the same vein as the last lecture, we shall only consider spherically symmetric scattering potentials, whereupon the Schrödinger equation becomes a simple ordinary differential equation for the radial part.

We shall assume the scattering geometry as in figure 2.1. An incoming beam of scattering particles (usually a mono-energetic collimated beam known as a plane-wave) is incident upon a scattering centre, resulting in an outgoing beam that has different intensities in different directions depending on the *spatial angle* $\Omega = (\theta, \phi)$ as shown in the figure. The two key experimental quantities that we want to calculate are the *differential scattering cross section* $\frac{d\sigma}{d\Omega}$ and the *total scattering cross section* σ. The differential cross section describes how the flux of scattered particles (intensity) varies

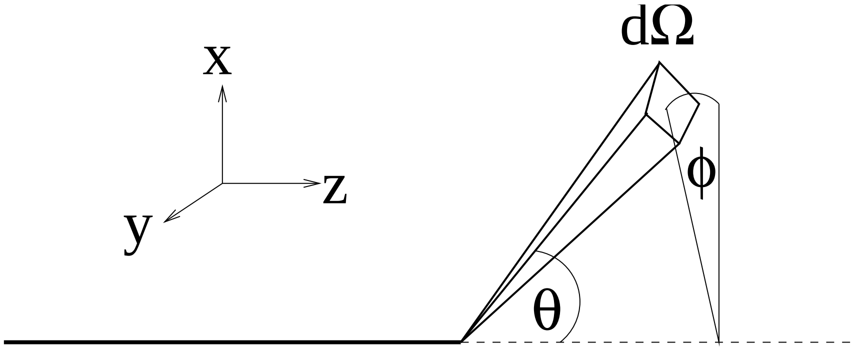

Figure 2.1: Geometry of a scattering process.

with outgoing spatial angle Ω, whereas the total cross section is the integrated flux over all angles. That is,

$$\frac{d\sigma}{d\Omega} = \frac{scattered\,flux\,into\,d\Omega}{total\,incident\,flux} \tag{2.1}$$

It can be proved that, for a spherically symmetric potential, the solution of the Schrödinger equation can always be written as

$$\psi(\mathbf{r}) = \psi(r,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}\frac{\chi_l(r)}{r}Y_{lm}(\theta,\phi) \tag{2.2}$$

where A_{lm} is some normalisation constant, $\chi(r)$ is the solution to the radial equation that we met last lecture, and Y_{lm} is a *spherical harmonic function* which determines the angular variation of the solution (which we ignored in the last lecture) and will obviously be important for calculating $\frac{d\sigma}{d\Omega}$.

If we assume that the scattering centre has a finite range, i.e.

$$V(r) = 0\; r > r_{max} \tag{2.3}$$

then we have two regions of solution. Inside the well there will be a complicated spatial and angular variation, involving the sum of various kinds of *spherical Bessel functions*. Outside the well, we do not need to worry about the exact functional form of the well, and can also work with the asymptotic expansion of these same spherical Bessel functions, which then simplifies things considerably. This is also the experimentally relevant regime - if we consider scattering of α-particles off Au nuclei, then the experimental apparatus will be at a distance of at least 10^{13} times the Au nucleus size (centimetres vs femtometres). In which case, the radial solution to equation 2.2 can be written as

$$\chi_l(r) \propto \sin\left(kr - l\frac{\pi}{2} + \delta_l\right)\; r \gg r_{max} \tag{2.4}$$

where k is known as the *wavenumber* which characterises the momentum of the outgoing wave (and the incoming wave as this is elastic scattering) and is given as

$$k = \sqrt{2E} \tag{2.5}$$

and δ_l is known as the *phase shift.*

Note that as in the case of the hydrogen atom considered in the last lecture, for $l \neq 0$ there will be an additional contribution to the effective potential caused by the centrifugal barrier. Hence the phase shift depends on the angular momentum quantum number l.

2.2 The phase shift

It is the phase shift which is the key quantity in scattering. It arises from the need to match the solutions to the Schrödinger equation at the scattering potential boundary edge. It is called the phase shift, because as we see from equation 2.4, the outgoing wave becomes a pure sine-wave at large distances with a phase dependent on δ_l. Indeed, for $l = 0$, it can be shown that $\chi_0(r)$ is a sine-wave for all $r > r_{max}$. The phase shift depends on the incoming energy E and also the angular momentum l of the incoming particles relative to the scattering centre and as such is a key theoretical quantity which can be used to derive the experimentally observed quantites (cross-sections, etc).

It can be shown, for an incoming plane-wave, that the differential scattering cross-section is related to the phase shift by

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2}\left|\sum_{l=0}^{\infty}(2l+1)\,e^{i\delta_l}\sin(\delta_l)\,P_l(\cos(\theta))\right|^2 \tag{2.6}$$

and to the total cross-section by

$$\begin{aligned}\sigma &= 2\pi\int\frac{d\sigma}{d\Omega}\sin(\theta)\,d\theta \\ &= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin(\delta_l)^2 \end{aligned} \tag{2.7}$$

where $P_l(\cos(\theta))$ is a *Legendre polynomial.*

These expressions, whilst theoretically precise, are not particularly useful in a numerical calculation due to the infinite sums. However, we can use some physical insight to convert this expression into a more useful form. Classically, a particle with angular momentum l and linear momentum k must pass the origin at a distance x such that $kx = l$. In quantum mechanics, we replace l with $\sqrt{l(l+1)}$ and so we see that only particles with angular momentum $l < l_{max}$ where

$$\sqrt{l_{max}\left(l_{max}+1\right)} \simeq k r_{max} \tag{2.8}$$

will "feel" the potential. Any particles with higher angular momentum will pass through unaffected. Therefore we may use this to truncate the infinite sum at a reasonable value to calculate the cross-sections. As a check on the accuracy of the calculation, we should then repeat the calculation using a higher value of l_{max} and ensure that nothing has significantly changed. This use of a numerical cut-off to infinite sums is a common technique in many numerical methods. Note that equation 2.8 implies that it is possible to tune the incoming beam for a given potential such that only $l = 0$ contributes to the scattering, which is then known as *s-wave scattering*.

We can also learn some interesting things directly from δ_l - for example, equation 2.7 shows that if $\delta_l = 0$ then the total scattering cross-section is zero, which implies that there can be no scattering! This is seen, for example in the scattering of electrons by rare-gas atoms - electrons with $E \sim 0.7\,eV$ pass through helium without being scattered - which is known as the *Ramsauer-Townsend effect*. A second interesting phenomena happens when $\delta_l = \frac{\pi}{2}$ which then gives maximum scattering. This corresponds to tuning the incoming beam energy E to cause *resonant scattering* whereupon the total cross-section σ is much greater than the geometrical cross section πr_{max}^2. For example, when scattering neutrons off hydrogen there is a characteristic neutron-proton interaction range $r \sim 2 \times 10^{-15} m$ and yet low-energy $l = 0$ neutrons have an experimental total scattering cross section $\sigma \simeq 20.4 \times 10^{-28} m^2 \sim 162 \times \pi r^2$. For $l \neq 0$ the effective potential may contain an additional barrier which can trap incoming particles for a short time in a *virtual energy level* and enhance the amplitude of the wavefunction inside the scattering region.

2.3 Final comments

A few final points to highlight:

- We can use the same techniques to solve the Schrödinger equation for continuum states as for bound states.
- Any potential will cause scattering of an incoming beam of particles
  - the scattering depends on both the incoming energy and angular momentum
  - in principle the outgoing beam contains an infinite spread of angular momenta
  - in practice only a small number of angular momenta contribute if the potential is short ranged.

- Analysis of the phase shift over a range of energies yields a lot of information about the nature of the scattering potential.

2.4 Further reading

- "Computational Physics" by J.M. Thijssen, Chapter 2