Advanced Quantum Mechanics
Brendon W. Lovett

Part II: Scattering theory

1. **Introduction**
2. **Overview and Definitions**
3. **Green's functions and the Born Approximation**
4. **An Example: Rutherford scattering**
5. **Partial Waves**
6. **Two particles**

2.1 Introduction

One of the most effective (and basic) ways of probing the structure of objects is to fire known particles at the object and look at how they *scatter* from it. For example, experiments at CERN to find the Higgs particle did exactly this kind of experiment - in this case by colliding two beams of protons together and looking at what particles come away from the interaction region. However, this is just one example of many in which a theory of scattering is crucial in physics. For example:

- X-ray scattering leads to crystal structure.
- Atom-atom collisions lead to cooling and ultimately Bose-Einstein condensation – or more straightforwardly to fluorescent lamps.
- Neutron scattering leads to understanding of magnetic ordering in solids.
- In astronomy, scattering is a crucial tool used to observe extra terrestrial objects, and can lead to well known effects such as the aurora borealis.

In general, scattering of particles takes the following form:

$$a(\alpha) + b(\beta) + ... \rightarrow c(\gamma) + d(\delta) + ... \tag{1}$$

where $\{a, b, c, ...\}$ are the names of the particles and $\{\alpha, \beta, \gamma, ...\}$ are their kinematic variables. Particles before the scattering event appear to the left of the arrow, scattered particles to the right.

In general, scattering can alter the distribution of kinetic, potential or internal energy of the particles. Indeed, in relativistic collisions, mass can be generated (hence the Higgs discovery). In this first course on scattering however, we will limit ourselves to non-relativistic *elastic* scattering, in which kinetic energy is conserved, and will assume all particles involved have no internal structure. For most of the course will only consider single particles scattering off a defined potential; we will only touch on two-particle collisions at the end of this part of the course.

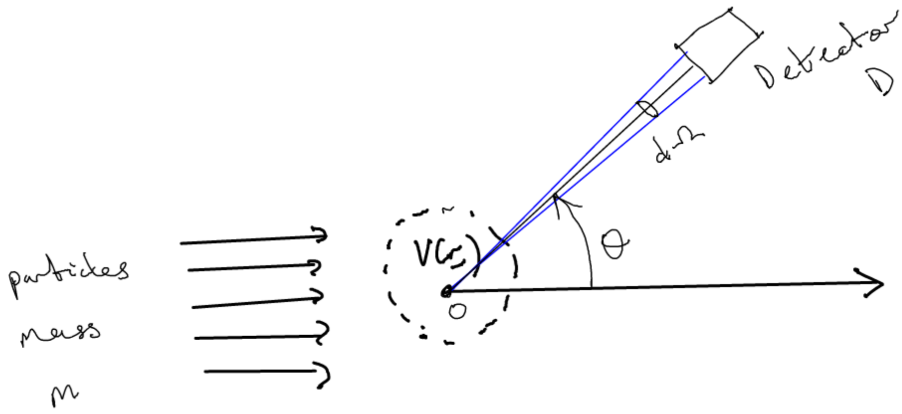

Figure 1: Particles of mass m are elastically scattered by a potential $V(\mathbf{r})$ into a detector subtending solid angle $d\Omega$ at angle θ.

2.2 Overview and Definitions

In Fig. 1 we depict elastic scattering of a beam of particles, each of **mass** m. The scattering is caused by a **potential** $V(\mathbf{r})$ that is centred about the origin O. We assume that the potential goes to zero far from the origin.

The number of particles incident on the potential region per unit time, from a far distance away, per unit area of plane perpendicular to their direction of travel z is the incident **flux** F_i.

A detector is placed a long way 'downstream' of the interaction region, in a direction defined by spherical polar angles θ and ϕ (see Fig. 1). It subtends a **solid angle** $d\Omega$, and the detector will count the **number of particles per unit time** dn incident on it.

We expect dn to be proportional to both $d\Omega$ and F_i and so define

$$dn = F_i \frac{d\sigma(\theta,\phi)}{d\Omega} d\Omega, \tag{2}$$

where $\frac{d\sigma(\theta,\phi)}{d\Omega}$ is called the **differential scattering cross section**. Integrating this quantity over all solid angles leads to the total scattering cross section σ.

We'd like to relate this quantity to the wave function of the scattering particles. In order to do this let's consider the Schrödinger equation of one such particle:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_{\mathbf{k}}(\mathbf{r}) = E\psi_{\mathbf{k}}(\mathbf{r}). \tag{3}$$

We know that far away from the potential region, our particles are in free space and so have plane wave solutions. Such an 'asymptotic' wave function, valid for large $|\mathbf{r}|$ looks like:

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r} = \psi_i(\mathbf{r}) + \psi_{sc}(\mathbf{r}). \tag{4}$$

The first term is the incident wave, which is travelling in the $+z$ direction and has wave vector k, the second term is the scattered wave, which travels radially outwards from the scattering potential. $f(\theta,\phi)$ is the **scattering amplitude**. It does not depend on r: we have included a factor $1/r$ in the second term to account for the fall off in scattering amplitude as r increases. This factor is a consequence of the fact that at a distance r from the origin, the scattering probability current can be spread over a sphere whose surface area is r^2; the square of the wave function is a probability and hence we obtain the $1/r$ factor. We will see this more formally in a moment.

In order to relate $f(\theta, \phi)$ to $\frac{d\sigma(\theta,\phi)}{d\Omega}$ we need to calculate the flux of outgoing particles.[1] Consider first the probability current, in general for a wavefunction $\psi(\mathbf{r})$ it is

$$\mathbf{J} = \frac{\hbar}{2mi} \left(\psi^*(\mathbf{r}) \nabla \psi(\mathbf{r}) - [\nabla \psi(\mathbf{r})]^* \psi(\mathbf{r}) \right). \tag{5}$$

So for the incoming wave we find

$$|\mathbf{J}_i| = \frac{\hbar k}{m}, \tag{6}$$

and for the scattered wave

$$\mathbf{J}_{sc} = \mathbf{e_r} \frac{|f|^2}{r^2} \frac{\hbar k}{m} = \mathbf{e_r} \frac{|f|^2}{r^2} |\mathbf{J}_i|, \tag{7}$$

where $\mathbf{e_r}$ is a unit vector in the direction $\mathbf{r}$ (note the $1/r^2$ factor alluded to above). Now the probability current flows into the solid angle $d\Omega$ at the rate

$$R(d\Omega) = \mathbf{J}_{sc} \cdot \mathbf{e_r} r^2 d\Omega = |f|^2 |\mathbf{J}_i| d\Omega, \tag{8}$$

and the probability current flowing into the interaction region per unit area is just $|\mathbf{J}_i|$. However, it must be the case that the ratio of R and $|\mathbf{J}_i|$ is simply dn/F_i. Thus using Eqs. 2 and 7 we find

$$\frac{dn}{F_i} = \frac{d\sigma}{d\Omega} d\Omega = \frac{R(d\Omega)}{|\mathbf{J}_i|} = |f|^2 d\Omega, \tag{9}$$

and so we arrive at

$$\frac{d\sigma(\theta, \phi)}{d\Omega} = |f(\theta, \phi)|^2. \tag{10}$$

2.3 Green's functions and the Born Approximation

So far we have focussed on looking at general, asymptotic forms of the scattering wave function - but in order to find $f(\theta, \phi)$ in real systems we must find a way of solving the problem more completely. In this section I will introduce *Green's functions*, a tool which has many applications throughout physics.

Let's first rearrange the general Schrödinger equation (Eq. 3) into the following form:

$$\left[\nabla^2 + k^2 \right] \psi_{\mathbf{k}}(\mathbf{r}) = \frac{2m}{\hbar^2} V(\mathbf{r}) \psi_{\mathbf{k}}(\mathbf{r}), \tag{11}$$

where $k^2 = 2mE/\hbar^2$. Clearly, if the RHS of this equation were simply zero, the equation would be easy to solve - our solution in this case, which we'll denote $\psi^0(\mathbf{r})$ would be a plane wave like $\psi^0(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}}$.

Now let us introduce the Green's function $G(\mathbf{r})$ as the solution of the alternative equation

$$\left[\nabla^2 + k^2 \right] G(\mathbf{r}) = \delta^3(\mathbf{r}). \tag{12}$$

[1] Note that we have not discussed normalisation of the wave function in Eq. 4. Since it is composed of plane waves, it cannot be normalised over infinite space, rather we must choose a volume over which to normalise it. It could indeed be normalised such that the integral over a unit volume gives the density of particles, if a direct comparison to the flux and number quantities appearing in Eq. 2 were to be made. However, for simplicity, we will simply leave out any normalisation constant; this will be fine for our purposes since as we shall soon see we will only be considering the ratios of probability currents below.

In fact, if we are able to find $G(\mathbf{r})$ then we are led to an expression for the full solution of Eq. 11: We will now show that this solution is:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \psi^0(\mathbf{r}) + \frac{2m}{\hbar^2}\int G(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}'. \tag{13}$$

To do this substitute Eq. 13 into the LHS of Eq. 11:

$$\left[\nabla^2 + k^2\right]\psi^0(\mathbf{r}) + \frac{2m}{\hbar^2}\int \left[\nabla^2 + k^2\right] G(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}' \tag{14}$$

the first term is zero by the definition of $\psi^0(\mathbf{r})$, and the second can be evaluated by substituting Eq. 12:

$$\frac{2m}{\hbar^2}\int \left[\nabla^2 + k^2\right] G(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}' = \frac{2m}{\hbar^2}\int \delta^3(\mathbf{r}-\mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}' = \frac{2m}{\hbar^2}V(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}), \tag{15}$$

where we have used the fundamental property of Dirac delta functions when they are integrated. The RHS of the above equation is just the RHS of Eq. 11 and so we have proven that Eq. 13 is a general solution of the Schrödinger equation.

The form, Eq. 13 looks promising since the first term on the RHS looks like an incident plane wave, and the second term is dependent on the potential V, and we might try and relate it to the scattered wave. However, we have a difficulty in that the function $\psi_{\mathbf{k}}(\mathbf{r})$ we are trying to solve for also appears in the RHS of the solution, Eq. 13. As we will see shortly we can deal with this using perturbation theory.

First, we now show that a specific form for $G(\mathbf{r})$ is

$$G(\mathbf{r}) = -\frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|}. \tag{16}$$

It is possible to show this directly, but it is easier to use Fourier transforms and *complex analysis*. Let us define the Fourier transform of the Green's function as

$$g(\mathbf{k}') = \frac{1}{(2\pi)^3}\int G(\mathbf{r})e^{-i\mathbf{k}'\cdot\mathbf{r}}d\mathbf{r} \tag{17}$$

with the inverse

$$G(\mathbf{r}) = \int g(\mathbf{k}')e^{i\mathbf{k}'\cdot\mathbf{r}}d\mathbf{k}'. \tag{18}$$

We now take the Fourier transform of both sides of Eq. 12, and use the fact that $\nabla^2 e^{-i\mathbf{k}'\cdot\mathbf{r}} = -k'^2 e^{-i\mathbf{k}'\cdot\mathbf{r}}$ [2] to get

$$\int (k^2 - k'^2)G(\mathbf{r})e^{-i\mathbf{k}'\cdot\mathbf{r}}d\mathbf{r} = \int e^{-i\mathbf{k}'\cdot\mathbf{r}}\delta(\mathbf{r})d\mathbf{r} = 1 \tag{19}$$

or

$$(2\pi)^3(k^2 - k'^2)g(\mathbf{k}') = 1 \tag{20}$$

As always with Fourier transforms, we have reduced a differential equation to an algebraic equation. Hence

$$g(\mathbf{k}') = \frac{1}{(2\pi)^3(k^2 - k'^2)} \tag{21}$$

[2] and recall, that for an Hermitian operator $\hat{L}(\mathbf{r})$, $\int u^*(\mathbf{r})\hat{L}(\mathbf{r})v(\mathbf{r})d\mathbf{r} = \int v(\mathbf{r})\hat{L}(\mathbf{r})u^*(\mathbf{r})d\mathbf{r}$

Now 'all' we need to do is take the inverse transform to find $G(\mathbf{r})$:

$$G(\mathbf{r}) = \frac{1}{(2\pi)^3} \int \frac{1}{(k^2 - k'^2)} e^{i\mathbf{k}'\cdot\mathbf{r}} d\mathbf{k}'. \tag{22}$$

We may do the angular integrals now:

$$\begin{aligned} G(\mathbf{r}) &= -\frac{1}{(2\pi)^3} \int_0^{2\pi} \int_1^{-1} \int_0^{\infty} \frac{1}{(k^2 - k'^2)} e^{ik'r\cos\theta} k'^2 d\phi\, d(\cos\theta)\, dk', & (23) \\ &= \frac{1}{(2\pi)^2} \int_0^{\infty} \frac{k'^2}{(k^2 - k'^2)} \frac{e^{ik'r} - e^{-ik'r}}{ik'r} dk', & (24) \\ &= \frac{1}{(2\pi)^2 ir} \int_{-\infty}^{\infty} k' \frac{e^{ik'r}}{k^2 - k'^2} dk'. & (25) \end{aligned}$$

At this point it looks as though we are in trouble: the integrand has points where it diverges at $k = k'$ and $k = -k'$, and so the integral does not really exist. In order to find a method for doing the integral, we need to view it in a different way. Instead of thinking of k' as an ordinary, real, variable, let us instead consider it to be a complex number. It may then be defined anywhere on the complex plane. We must view the integral then as a *contour integral* along the *real axis* of this plane - see Fig. 2.

We still have the problem of the divergences, since these lay on the real axis. However, we could try move them off that axis slightly by changing the integrand by adding a small complex number to the denominator in the following way:

$$G(\mathbf{r}) = \frac{1}{(2\pi)^2 ir} \int_{-\infty}^{\infty} k' \frac{e^{ik'r}}{k^2 + i\epsilon - k'^2} dk'. \tag{26}$$

In order to evaluate this function, we need the *residue theorem*, derived in the *complex analysis* section of this course:

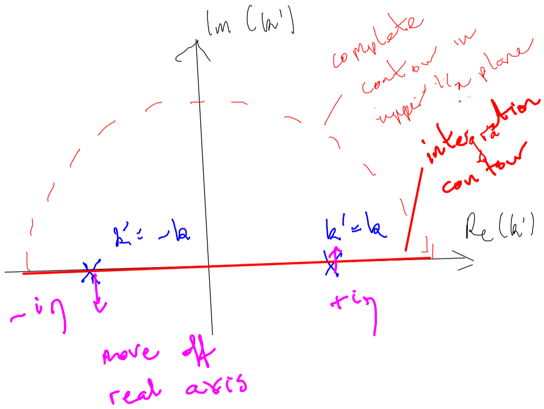

Figure 2: In order to evaluate the integral in Eq. 25 we view the integral in the complex plane of variable k'. We then shift the positions of the poles off the real axis, and complete the contour in the upper half plane. This enables us to apply the residue theorem.

$$\oint f(z)dz = 2\pi i \sum_j R(z_j) \tag{27}$$

where the z_j are the *poles* of the integral and $R(z_j)$ is the *residue* of the pole z_j. We need to find the poles of the integrand in Eq. 26:

$$w(k') = \frac{1}{(2\pi)^2 ir} k' \frac{e^{ik'r}}{k^2 + i\epsilon - k'^2} \tag{28}$$

which are found by setting the denominator of the second fraction (which is the only one to depend on k') to zero:

$$k^2 + i\epsilon - k'^2 = 0. \tag{29}$$

These are simply at points $k' = p$ where

$$\begin{aligned} p &= \pm\sqrt{k^2 + i\epsilon} && (30)\\ &\approx \pm\left(k + \frac{i\epsilon}{2k}\right) \equiv \pm(k + i\eta) && (31) \end{aligned}$$

Then to first order in η, we may write

$$w(k') = \frac{1}{(2\pi)^2 ir} k' \frac{e^{ik'r}}{(k + i\eta - k')(k + i\eta + k')} \tag{32}$$

Now in order to apply the residue theorem we need a closed contour that consists of one section that runs along the real line (that is, after all, the integral we wish to calculate) plus an enclosing contour. We choose such an enclosing contour to be a semi-circle in the upper half plane whose radius tends to infinity (see Fig. 2). If we can work out what the contribution of this semi-circular contour is, and using the residue theorem we know what the entire, closed contour is, then we can infer the value of the real axis integral we need.

Now, if we write k' in polar coordinates ($k' = \rho e^{i\theta}$) then we want the form of the integrand $w(k')$ as $\rho \to \infty$:

$$\lim_{\rho\to\infty} w(k') = \frac{i}{(2\pi)^2 r} \frac{e^{ik'r}}{k'} \tag{33}$$

and so the integral over the semicircle is:

$$\frac{i}{(2\pi)^2 r} \int_{C_\rho} \frac{e^{ik'r}}{k'} = \int_0^\pi e^{i\rho r(\cos\theta + i\sin\theta)} d\theta. \tag{34}$$

This integral vanishes to zero, since the integrand is zero everywhere along the contour due to the presence of the $e^{-\rho r\sin\theta}$ term[3].

We can therefore find the real-axis integral simply by evaluating the residue of the enclosed pole at $p = k + i\eta$:

$$\begin{aligned} R(k + i\eta) &= \lim_{k'\to k+i\eta} (k' - i\eta - k) w(k') && (35)\\ &= \frac{i}{8\pi^2 r} \frac{(k + i\eta) e^{ikr} e^{-\eta r}}{k + i\eta} && (36) \end{aligned}$$

and so

$$G(\mathbf{r}) = \lim_{\eta\to 0} 2\pi i R(k + i\eta) = -\frac{e^{ikr}}{4\pi r} \equiv G_+(\mathbf{r}) \tag{37}$$

[3]Except for at the point at $\theta = 0$, but this contributes an infinitesimal amount

We have defined this Green's function as $G_+(\mathbf{r})$ since it is not unique. If we had instead chosen a small *negative* imaginary shift in the denominator of Eq. 26 then the poles would be at $k - i\eta$ and $-k + i\eta$ (η positive), and then our Green's function would take a different form:

$$G_-(\mathbf{r}) = -\frac{e^{-ikr}}{4\pi r}. \tag{38}$$

Note that $G_+(\mathbf{r})$ takes the same form as a wave that is *outgoing* from the scattering region, and $G_-(\mathbf{r})$ takes the form of a wave that is *incoming* to the scattering region. These two are also known as *retarded* and *advanced* respectively. Which one to choose is motivated by the particular problem at hand: in our case, where we want to study how the pattern of outgoing particles after a scattering event we choose the retarded function $G_+(\mathbf{r})$; note that this is the form of solution we set out to prove from Eq. 16.

2.3.1 Relation to Scattering Cross Section

Let's now use our solution, Eq. 13:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \psi^0(\mathbf{r}) + \frac{2m}{\hbar^2}\int G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}', \tag{13}$$

and use it to obtain an expression for the scattering cross section. In order to do this we must find the form of our Green's function, Eq. 38 at large $|\mathbf{r}|$. To do this we first expand the argument of the exponential of the Green's function:

$$k|\mathbf{r}-\mathbf{r}'| = k\sqrt{r^2 + r'^2 - 2\mathbf{r}\cdot\mathbf{r}'} = kr\left[1 + \left(\frac{r'}{r}\right)^2 - 2\frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right]^{1/2}. \tag{39}$$

Now, the integrand in Eq. 13 is only significant in the region where the potential is non-zero; it can therefore be assumed that $|r| \gg |r'|$ over the whole integral. In that case we may approximate:

$$k|\mathbf{r}-\mathbf{r}'| \approx kr\left(1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right) = kr - k\hat{\mathbf{r}}\cdot\mathbf{r}' = kr - \mathbf{k}_f\cdot\mathbf{r}' \tag{40}$$

where $\hat{\mathbf{r}}$ is the unit vector in the direction $\mathbf{r}$ and so $\mathbf{k}_f$ is the wave vector for the scattered wave. Similarly

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} \approx \frac{1}{r}\left(1 + \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2}\right). \tag{41}$$

Therefore we may write, for the purposes of obtaining an asymptotic solution, that the Green's function is approximately

$$G(\mathbf{r},\mathbf{r}') = -\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|} \approx -\frac{1}{4\pi}\frac{e^{ikr}}{r}e^{-i\mathbf{k}_f\cdot\mathbf{r}'}. \tag{42}$$

Substituting in Eq. 13, and using the plane incident wave solution $\psi^0(\mathbf{r}) = e^{i\mathbf{k}_i\cdot\mathbf{r}}$, with $\mathbf{k}_i$ the incident wave vector yields:

$$\lim_{r\to\infty}\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}_i\cdot\mathbf{r}} - \frac{e^{ikr}}{r}\frac{2m}{4\pi\hbar^2}\int e^{-i\mathbf{k}_f\cdot\mathbf{r}'}V(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}')d\mathbf{r}'. \tag{43}$$

This is not yet a calculable solution, since $\psi_{\mathbf{k}}(\mathbf{r}')$ still appears on the RHS. However, let us now make the *Born approximation*, and substitute the zeroth order approximation (in V) of Eq. 43, $\psi_{\mathbf{k}}(\mathbf{r}) \approx e^{-i\mathbf{k}_i\cdot\mathbf{r}}$ back into the same equation:

$$\lim_{r\to\infty}\psi_{\mathbf{k}}(\mathbf{r}) \approx e^{i\mathbf{k}_i\cdot\mathbf{r}} - \frac{e^{ikr}}{r}\frac{m}{2\pi\hbar^2}\int e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}'}V(\mathbf{r}')d\mathbf{r}', \tag{44}$$

and then, using Eq. 4 we are able to write

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int e^{-i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}'}V(\mathbf{r}')d\mathbf{r}'. \tag{45}$$

If we define

$$\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i \tag{46}$$

as the *momentum transfer* to the particle, then we obtain a remarkably simple expression for the cross section

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int e^{-i\mathbf{q}\cdot\mathbf{r}'}V(\mathbf{r}')d\mathbf{r}'. \tag{47}$$

In other words, the scattering amplitude is simply the *Fourier transform* of the scattering potential, in the Born approximation.

2.3.2 Interpreting the Green's function: Relation to Huygen's Principal

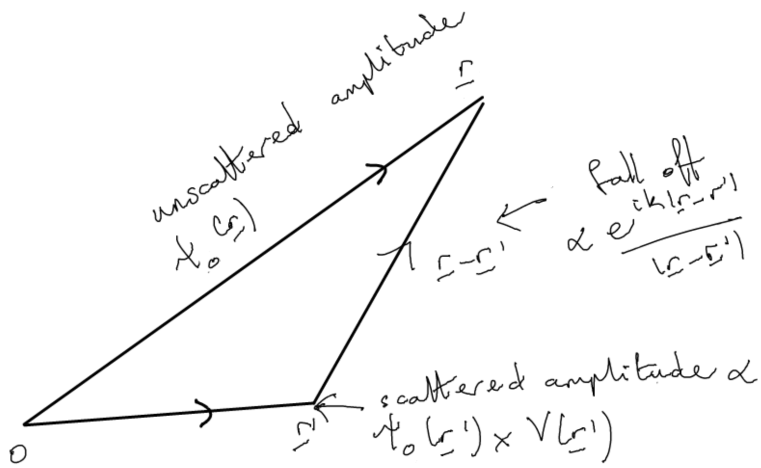

Figure 3: Huygen's construction for a single scattering events.

There is an insightful interpretation of the Green's function solution to the scattering problem (Eq. 12), which is similar to Huygen's principle in optics.

Refer to Fig. 3. In the Born approximation, we have just seen that we may write Eq. 13 as

$$\begin{aligned}\psi_{\mathbf{k}}(\mathbf{r}) &= \psi^0(\mathbf{r}) + \frac{2m}{\hbar^2}\int G(\mathbf{r},\mathbf{r}')V(\mathbf{r}')\psi_0(\mathbf{r}')d\mathbf{r}', \\ &= \psi^0(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(\mathbf{r}')\psi_0(\mathbf{r}')d\mathbf{r}'. \end{aligned} \tag{48}$$

In the figure you can see that the total scattering amplitude at point $\mathbf{r}$ is a sum of the unscattered wave $\psi^0(\mathbf{r})$, which is the first term in Eq. 48, plus a contribution from each singly scattered wave. These latter contributions arise from the potential which scatters the incoming wave. At a point $\mathbf{r}'$ of the potential, the incoming wave amplitude is $\psi_0(\mathbf{r}')$ and it might reasonably be expected to scatter proportional to the strength of the potential at that point, $V(\mathbf{r}')$. Once scattered, it must then propagate to the point $\mathbf{r}$, where is can interfere with all the other scattered waves. We must therefore apply a factor $e^{-ik|\mathbf{r}-\mathbf{r}'|}$ to account for the phase difference of the wave between $\mathbf{r}$ and $\mathbf{r}'$ and a factor $1/|\mathbf{r}-\mathbf{r}'|$ to account for the amplitude fall off discussed earlier, related to the increasing surface area of a sphere centred on $\mathbf{r}'$.

Integrating all the scattered wave contributions would then lead to Eq.48 for the total wave function. This construction also allows us to see that the Born approximation corresponds to *allowing only one* scattering event in the potential. Note that one could go to higher orders by substituting Eq. 13 into itself iteratively, and cutting the series at whichever power of the potential V is desired. These higher powers would correspond to multiple scattering events, but these may be ignored at high incident kinetic energy compared with the potential energy. Thus we see that the Born approximation is valid at high incident energy - we will discuss another technique for dealing with low incident energy in Section 2.5.

2.4 An Example: Rutherford scattering

Having been through some fairly heavy going mathematical machinery to reach the elegant result Eq. 47, we now exploit this hard work by straightforwardly calculating the scattering cross section for a single atomic nucleus. Let's assume it's potential takes the spherically symmetric Yukawa form:

$$V(r) = \frac{ge^{-\mu r}}{r} \tag{49}$$

where g represents the strength of the potential and μ an extra radial fall off (which we can set to zero at the end of the calculation if we wish!).

Now for any spherically symmetric potential $V(r)$ we can simplify Eq. 47 to:

$$\begin{aligned}
f(\theta,\phi) &= \frac{m}{2\pi\hbar^2}\int_0^{2\pi}\int_1^{-1}\int_0^{\infty} e^{-i\mathbf{q}\cdot\mathbf{r}'}r'^2V(r')d(\cos\theta')d\phi' dr', \\
&= \frac{m}{\hbar^2}\int_1^{-1}\int_0^{\infty} e^{-iqr'\cos\theta'}r'^2V(r')d(\cos\theta')dr', \\
&= -\frac{2m}{\hbar^2}\int_0^{\infty}\frac{\sin(qr')}{q}r'V(r')dr' = f(\theta),
\end{aligned} \tag{50}$$

where we have called the angular integration variables θ' and ϕ' to distinguish them from the scattering angles θ and ϕ. θ' is specifically the angle between $\mathbf{q}$ and $\mathbf{r}'$, different from the scattering angle θ. We have also in the final line now made explicit that for a spherical potential there is no dependence of f on ϕ, though there could be a residual θ dependence once we relate q to the initial momentum k.

For the specific form appearing in Eq. 49 we find

$$\begin{aligned}
f(\theta) &= -\frac{2mg}{\hbar^2 q}\int_0^{\infty}\frac{e^{iqr'}-e^{-iqr'}}{2i}e^{-\mu r'}dr', \\
&= -\frac{2mg}{\hbar^2(q^2+\mu^2)}.
\end{aligned} \tag{51}$$

To see how the θ dependence comes about explicitly, we relate q to the initial momentum k_i:

$$|\mathbf{q}|^2 = |\mathbf{k}_f - \mathbf{k}_i|^2 = 2k^2(1-\cos\theta) = 4k^2\sin^2(\theta/2). \tag{52}$$

Substituting Eq. 52 into Eq. 51, and assuming the Yukawa potential is to represent an atomic nucleus of charge Ze interacting with an electron, and $\mu = 0$ yields

$$f(\theta) = \frac{mZe^2}{8\pi\epsilon_0\hbar^2k^2\sin^2(\theta/2)}, \tag{53}$$

and therefore, from relation Eq. 10 we have

$$\frac{d\sigma(\theta,\phi)}{d\Omega} = \frac{m^2 Z^2 e^4}{(8\pi\epsilon_0\hbar^2 k^2)^2 \sin^4(\theta/2)} = \frac{Z^2 e^4}{(16\pi\epsilon_0)^2 E^2 \sin^4(\theta/2)} \tag{54}$$

with the kinetic energy of the incident particle $E = \hbar^2 k^2/2m$.

Eq. 54 is nothing other than the Rutherford scattering formula. Rutherford himself calculated this quantity classically, and this gives precisely the same answer. (N. B. This is a coincidence and not usually the case when considered scattering of quantum particles.)

The cross section peaks rather sharply in the forward direction (corresponding to $\theta = 0$ or $\theta = 2\pi$), as shown in Fig. 4.

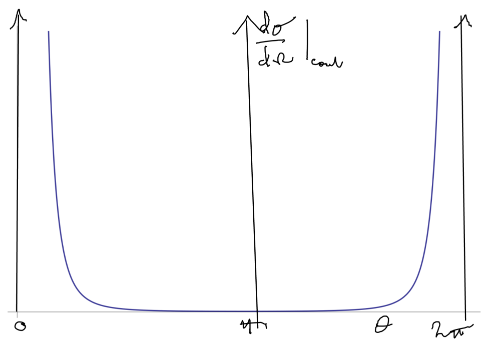

Figure 4: Differential scattering cross section for scattering from a Coulomb potential.

2.5 Partial Waves

The Born approximation works well for a scattering events in which the kinetic energy of incoming particles is much greater than the typical potential energy of the scatterer. In this section, we review an alternative analysis - that using *partial waves* - which works well in the opposite limit of small kinetic energy.

Let's return to the Schrödinger equation (Eq. 11) for a spherically symmetric scattering potential:

$$\left[\nabla^2 + k^2\right]\psi_{\mathbf{k}}(\mathbf{r}) = \frac{2m}{\hbar^2} V(r)\psi_{\mathbf{k}}(\mathbf{r}). \tag{55}$$

We exploit the spherical symmetry of our potential by first writing the ∇^2 operator out in spherical coordinates:

$$\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{\hat{L}^2}{\hbar^2 r^2} + k^2\right]\psi_{\mathbf{k}}(\mathbf{r}) = \frac{2m}{\hbar^2}V(r)\psi_{\mathbf{k}}(\mathbf{r}), \tag{56}$$

with the angular momentum squared operator given by

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right). \tag{57}$$

Since $V(r)$ does not depend on θ and ϕ we can use the separation of variables technique to find that $\psi_{\mathbf{k}}(\mathbf{r})$ can be expanded as a sum of terms of the form $R(r)Y_{l,m}(\theta,\phi)$. In general, we might expect the radial functions $R(r)$ to be different for each of the spherical harmonics $Y_{l,m}(\theta,\phi)$ - we will return to this later. The spherical harmonics are eigenfunctions of $\hat{L}^2$:

$$\hat{L}^2 Y_{l,m}(\theta,\phi) = \hbar^2 l(l+1)Y_{l,m}(\theta,\phi), \tag{58}$$

and therefore we have for the radial equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right)+\left(k^2-\frac{l(l+1)}{r^2}-\frac{2m}{\hbar^2}V(r)\right)R(r)=0. \tag{59}$$

The equation is simplified if we use the substitution $\chi(r)=rR(r)$. Then

$$\frac{d\chi}{dr} = r\frac{dR}{dr}+R \tag{60}$$

$$\frac{d^2\chi}{dr^2} = 2\frac{dR}{dr}+r\frac{d^2R}{dr^2} \tag{61}$$

and so

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)=\frac{2}{r}\frac{dR}{dr}+\frac{d^2R}{dr^2}=\frac{1}{r}\frac{d^2\chi}{dr^2}. \tag{62}$$

Therefore, Eq. 59 is transformed into

$$\frac{d^2\chi}{dr^2}+\left(k^2-\frac{l(l+1)}{r^2}-\frac{2m}{\hbar^2}V\right)\chi=0. \tag{63}$$

In the asymptotic limit of large distances, the equation becomes

$$\frac{d^2\chi}{dr^2}+k^2\chi=0 \tag{64}$$

which has the simple solution

$$\chi=\alpha e^{-ikr}+\beta e^{ikr} \tag{65}$$

α and β are complex coefficients determined by boundary conditions. The first term on the RHS corresponds to an incoming wave, the second to an outcoming wave: thus only the second can contain a scattered component.

Putting together the radial solution (Eq. 65) together with the spherical harmonics gives the complete asymptotic solution:

$$\psi_{\mathbf{k}}(\mathbf{r})=\sum_{l,m}A'_{lm}\frac{1}{r}\left(\alpha e^{-ikr}+\beta e^{ikr}\right)Y_{lm}(\theta,\phi) \tag{66}$$

with the A'_{lm} some set of constants to be determined by boundary conditions. Since we know that the same number of particles come into the scattering region as leave it, we are able to set $|\alpha|^2=|\beta|^2$. Thus α and β must then have the same magnitude but can have a different phase - and this phase can be different for each term in Eq. 66. To account for this we will set $\beta=-\alpha e^{i(2\delta_{lm}-l\pi)}$; we've added in some extra phases and a minus sign here for future convenience. This is exactly the l and m dependence of the radial function I mentioned earlier. Therefore, we have

$$\psi_{\mathbf{k}}(\mathbf{r})=\sum_{l,m}\alpha A'_{lm}\frac{1}{r}\left(e^{-ikr}-e^{i(kr+2\delta_{lm}-l\pi)}\right)Y_{lm}(\theta,\phi). \tag{67}$$

We can absorb α by setting $A_{lm}=\alpha A'_{lm}$ so

$$\psi_{\mathbf{k}}(\mathbf{r})=\sum_{l,m}A_{lm}\frac{1}{r}\left(e^{-ikr}-e^{i(kr+2\delta_{lm}-l\pi)}\right)Y_{lm}(\theta,\phi)=\sum_{l,m}A_{lm}u_{klm}, \tag{68}$$

where u_{klm} is called a *partial wave*:

$$u_{klm}=\frac{1}{r}\left(e^{-ikr}-e^{i(kr+2\delta_{lm}-l\pi)}\right)Y_{lm}(\theta,\phi). \tag{69}$$

The calculation of scattering cross section now proceeds as follows

- Calculate δ_{lm} for a given $V(r)$ for each partial wave.
- From this set of δ_{lm} find $d\sigma(\theta, \phi)/d\Omega$.

The first of these two steps typically needs to be performed numerically on a computer, but we will go through an analytical example in the problem sheet.

We'll tackle the second stage now. We first need to find which parts of our expansion Eq. 66 correspond to the incoming wave and which to the scattered wave. We already know that the e^{-ikr} term is purely due to the incoming wave, though some of the other term could also be contributing to the incoming wave too; we need an expansion of our incoming e^{ikz} plane wave form in terms of partial waves. It can be shown (but we won't go through the proof here) that this plane wave can be written as a sum of Legendre polynomials:

$$e^{ikz} = \sum_{l=0}^{\infty} \frac{(2l+1)}{2kr} i^{2l+1} \left(e^{-ikr} - e^{i(kr-l\pi)} \right) P_l(\cos\theta) \tag{70}$$

where $Y_{l0} = \sqrt{(2l+1)/4\pi} P_l(\cos\theta)$. We note that in this expansion all of the phase shifts δ_{lm} are zero; this is what we want since we have no scattered wave here. Also there is no component for any $m \neq 0$: again this makes sense, our incident wave is symmetric about the z axis and so ϕ will play no role.

Now we may exploit the fact that we know that the e^{-ikr} term in our expansion Eq. 66 contains only the incoming wave, and we can equate the coefficients of that term to our plane wave expansion, Eq. 70. This yields $A_{lm} = 0$ if $m \neq 0$ and

$$A_{l0} = \frac{1}{2k}(2l+1) i^{2l+1} \sqrt{\frac{4\pi}{2l+1}}. \tag{71}$$

Now let us substitute this expression for A_{l0} back into Eq. 68, and absorb the square root factor by writing the result in terms of $P_l(\cos\theta)$. We find:

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_{l} \frac{(2l+1)}{2kr} i^{2l+1} \left(e^{-ikr} - e^{i(kr+2\delta_l-l\pi)} \right) P_l(\cos\theta). \tag{72}$$

where we have now written $\delta_{l0} = \delta_l$ since we know there are no scattered waves except those with $m = 0$.

We can now find the scattered wave by subtracting the incident wave from the total wave function: $\psi_s = \psi_{\mathbf{k}}(\mathbf{r}) - e^{ikz}$, and using Eqs. 70 and 72:

$$\psi_s = \sum_{l} \frac{(2l+1)}{2kr} i^{2l+1} \left(e^{i(kr-l\pi)} - e^{i(kr+2\delta_l-l\pi)} \right) P_l(\cos\theta) \tag{73}$$

$$= \frac{e^{ikr}}{2kr} \sum_{l} (2l+1) i^{2l+1} \left(1 - e^{2i\delta_l} \right) e^{-il\pi} P_l(\cos\theta). \tag{74}$$

Eq. 74 takes the form of the scattered wave definition in Eq. 4 with

$$f(\theta) = \frac{1}{2k} \sum_{l} (2l+1) i^{2l+1} e^{-il\pi} (1 - e^{2i\delta_l}) P_l(\cos\theta) \tag{75}$$

but

$$\frac{1 - e^{2i\delta_l}}{2} = e^{i\delta_l} \frac{e^{-i\delta_l} - e^{i\delta_l}}{2} = -e^{i\delta_l} i \sin\delta_l \tag{76}$$

and

$$-i^{2l+1} e^{-il\pi} i = 1 \tag{77}$$

thus

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta) \tag{78}$$

and therefore for the differential scattering cross section we find

$$\frac{d\sigma(\theta)}{d\Omega} = |f(\theta)|^2 = \frac{1}{k^2}\left|\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta)\right|^2. \tag{79}$$

For the total cross section $\sigma = 2\pi\int_0^\pi \frac{d\sigma(\theta)}{d\Omega}\sin\theta d\theta$, we exploit the orthogonality properties of the $P_l(\cos\theta)$:

$$\int_0^\pi P_l P_{l'}\sin\theta d\theta = 0 \quad \text{if} \quad l \neq l' \quad \text{and} \tag{80}$$

$$\int_0^\pi P_l^2\sin\theta d\theta = \frac{2}{2l+1} \tag{81}$$

and therefore

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l. \tag{82}$$

This is a key result which should be memorised. We have arrived at rather a simple expression for the scattering cross section: It is simply a sum of contributions from partial waves of different angular momentum l. Each phase shift δ_l needs to be determined from $V(\mathbf{r})$; notice that if there is no scattering potential ($V(\mathbf{r}) = 0$) then $\delta_l = 0 \forall l$ and there is no scattered wave.

In a typical experimental situation, $V(r)$ is not known at the outset, and scattering is supposed to help us determine what $V(r)$ is. By looking at the angular dependence of $d\sigma/d\Omega$, we are able to start to determine which phase shifts are non-zero. For example, if we measure a uniform scattering distribution in θ, then we know that there is only an $l = 0$ phase shift, and we'd need to look for potentials which give rise to that. For non-uniform distributions, we know that higher angular momentum states are contributing.

Finally in this section we introduce a further relation for σ. The imaginary part of $f(\theta)$ in the forward scattering direction is, from Eq. 78

$$\Im[f(0)] = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\Im[e^{i\delta_l}]\sin\delta_l = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{83}$$

since $P_l(1) = 1$. Hence

$$\sigma = \frac{4\pi}{k}\Im[f(0)]. \tag{84}$$

This relation is known as the *optical theorem.* It is not too surprising that there's a relationship between the scattering amplitude in the forward direction – which is the direction in which the incident and scattered waves interfere – and the total cross section for scattering everywhere else.

In the next section we'll discuss a simplification of the partial wave analysis.

2.5.1 A Simplification of Partial Wave Analysis

We saw above that, for a given $V(r)$ any of the angular momentum states could contribute to the cross section. However, in a typical experiment at low energies, we are able to limit ourselves to small angular momentum quantum numbers.

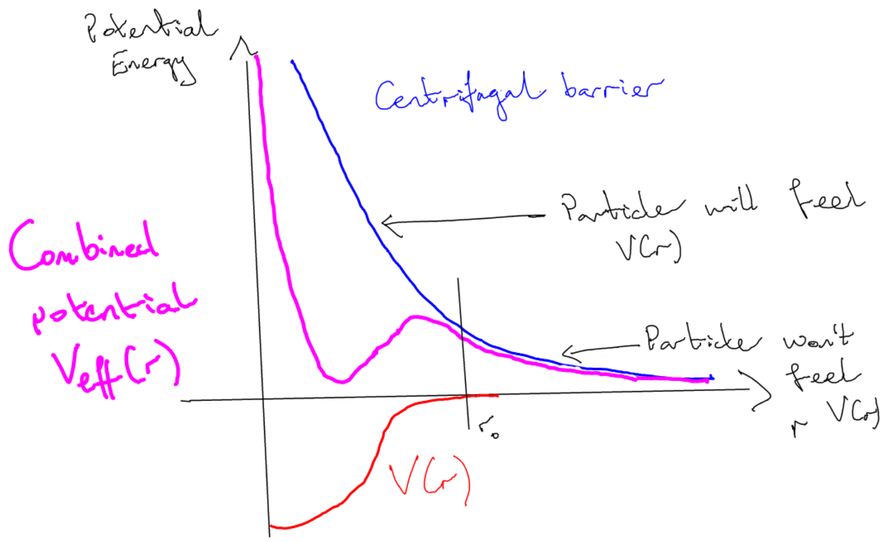

Figure 5: The effective potential for a partial wave of angular moment l consists of the raw potential $V(r)$, plus a 'centrifugal barrier'. Shown also by black arrows are the levels of initial kinetic energy of two incident particles - one at lower energy will be reflected before even reaching a region where $V(r)$ plays a role, whereas those at higher initial energy can penetrate further into the core of the potential.

To see why this is consider again Eq. 63:

$$\frac{d^2\chi}{dr^2} + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2}V(r)\right)\chi = 0. \tag{63}$$

Multiplying by $-\hbar^2/2m$:

$$-\frac{\hbar^2}{2m}\frac{d^2\chi}{dr^2} + \left(\frac{\hbar^2 l(l+1)}{2mr^2} + V(r) - \frac{\hbar^2k^2}{2m}\right)\chi = 0. \tag{85}$$

This looks exactly like the one-dimensional Schrödingier equation, but with a modified potential

$$V_{\text{eff}}(r) = \begin{cases} V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} & r \geq 0 \\ \infty & r < 0 \end{cases} \tag{86}$$

where the effective potential is infinite for $r < 0$ since we know that negative r solutions are not physical. The term $\frac{\hbar^2 l(l+1)}{2mr^2}$ which must be added to $V(r)$ is called the *centrifugal barrier*. See Fig. 5 for a pictorial representation.

Now, consider a particle in a plane wave state approaching the region of significant potential from large r. In the absence of an external potential ($V(r) = 0$) then we might expect that particle to have a 'closest approach' to $r = 0$ when its initial kinetic energy matches the effective potential energy, i.e.

$$\frac{\hbar^2k^2}{2m} = \frac{\hbar^2 l(l+1)}{2mr^2_{\text{min},l}} \tag{87}$$

or

$$r_{\text{min},l} = \frac{l(l+1)}{k}. \tag{88}$$

In other words, only s-waves can get all the way to $r = 0$, higher angular momentum states have increasingly longer distance closest approaches.

If we now imagine we do have an external scattering potential, with a typical range of r_0, then it is reasonable that if $r_0 < r_{\mathrm{min},l}$ then that scattering potential can have no effect on a partial wave with angular momentum l; all waves satisfying this condition have zero phase shifts and can be ignored in the sum, Eq. 82. Indeed, it is often the case that the only partial wave that is significantly scattered is that one with $l = 0$, the s-wave.

2.6 Two particle scattering

In this final section on scattering, we will consider the case of two particles, of equal mass m, at positions $\mathbf{r}_1$ and $\mathbf{r}_2$ which scatter off each other via a mutual potential which only depends on their relative coordinate $V(\mathbf{r}_1 - \mathbf{r}_2)$. (See Fig. 6).

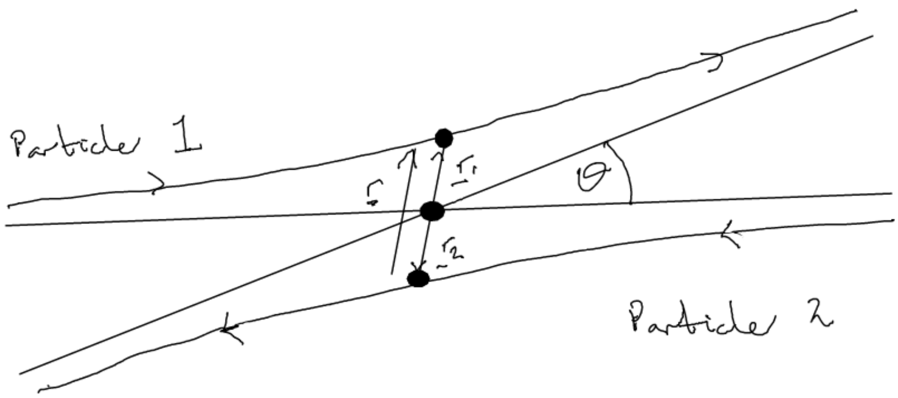

Figure 6: A collision between two particles, where the potential each feels only depends on the relative coordinate $\mathbf{r} - \mathbf{r}_1 - \mathbf{r}_2$. The collision is depicted here in the centre of mass frame.

Imagine that the two particles are initially both travelling along the z axis; we then write, for their initial state

$$\psi_i^{(2)}(z_1, z_2) = e^{ik_1 z_1} e^{ik_2 z_2} \tag{89}$$

where z_1 and z_2 are the position variables of the two particles, and k_1 and k_2 are their wave vectors.[4]

To simplify our problem we rewrite Eq. 89 as follows:

$$\begin{aligned}
\psi_i^{(2)} &= e^{ik_1 z_1} e^{ik_2 z_2} && (90)\\
&= \exp\left[i(k_1 + k_2)\left(\frac{z_1 + z_2}{2}\right)\right] \exp\left[i\left(\frac{(k_1 - k_2}{2}\right)(z_1 - z_2)\right] && (91)\\
&= \psi_i^{\mathrm{CM}}(z_{\mathrm{CM}})\psi_i^{\mathrm{rel}}(z_{\mathrm{rel}}) && (92)
\end{aligned}$$

where 'CM' refers to the centre of mass motion which for equal masses is just defined by the average position coordinate $z_{\mathrm{CM}} = \frac{z_1 + z_2}{2}$. 'rel' refers to the relative coordinate, given by $z_{\mathrm{rel}} = z_1 - z_2$.

[4]again we have not put an explicit normalisation into the plane wave function; as it happens the simple function we have chosen would integrate to unity over a unit volume, and hence the particles can be considered as normalised to a density of one particle per unit volume. In the case of two particles the scattering cross section is proportional to the densities of both types of particle; by using this unity normalisation these factors drop out, and we recover our simple relationship between scattering amplitude and differential cross section. See Shankar for more details.

Now, as we stated above the potential only depends on the relative coordinate. Therefore the CM part of the wave function is unaffected by scattering. On the other hand the relative coordinate will develop a scattered wave. In the asymptotic ($r \to \infty$) limit, we obtain:

$$\psi^{\mathrm{rel}}(z_{\mathrm{rel}}) \to e^{ik_{\mathrm{rel}} z_{\mathrm{rel}}} + f(\theta, \phi) \frac{e^{ik_{\mathrm{rel}} r_{\mathrm{rel}}}}{r_{\mathrm{rel}}} \tag{93}$$

where $k_{\mathrm{rel}} = \frac{k_1 - k_2}{2}$ and $r_{\mathrm{rel}} = r_1 - r_2$.

From now on we will drop the subscript 'rel' in order to simply the notation. The total asymptotic wave function then becomes

$$\psi^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \psi^{\mathrm{CM}}(z_{\mathrm{CM}}) \left(e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r} \right) \tag{94}$$

To simplify the analysis even further, we can simply move into the centre of mass frame, in which $k_1 + k_2 = 0$; then $\psi^{\mathrm{CM}}(z_{\mathrm{CM}}) = 1$ and we *completely remove the centre of mass motion from the problem.* Moreover, since the relative coordinate $\mathbf{r}$ is parallel to both individual coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ in the CM frame, the scattering rate into the solid angle $d\Omega$ of the particle 1 off particle 2, must be the same as that for the fictitious particle described by $\mathbf{r}$ (the angular distribution is just the same - see Fig. 6). Thus, all we need to do now is to solve for $f(\theta, \phi)$ as we did before, but this time writing the Schrödinger equation for the relative coordinate. We then simply square this quantity to find the differential cross section in the CM frame:

$$\left. \frac{d\sigma(\theta, \phi)}{d\Omega} \right|_{\mathrm{CM}} = |f(\theta, \phi)|^2. \tag{95}$$

We should note here that in other frames the scattering cross section will be different, since the incremental solid angle $d\Omega$ will change under a change of frame. This is not difficult to deal with however, and we need not explore it further here.

To conclude, we have found that the differential cross section for a single particle scattering from a potential $V(\mathbf{r})$ is the same as the centre of mass differential cross section for two particles scattering through a relative potential $V(\mathbf{r}_1 - \mathbf{r}_2)$.

2.6.1 Indistinguishable particles

For two indistinguishable particles scattering the picture has to change a little. This is because, depending on whether our scattered particles are bosons or fermions, the overall wave function must be symmetric or antisymmetric under exchange of particles.

Refer back to our expression, Eq. 94. The CM coordinate is $(\mathbf{r}_1 + \mathbf{r}_2)/2$, and so this part of the wave function is obviously unchanged under exchange of particles. However the relative coordinate $\mathbf{r}_1 - \mathbf{r}_2$ flips sign - and so we must symmetrize this part of the wave function for bosons and antisymmetrize it for fermions. If we do this we have

$$\psi^{\mathrm{rel,ind}} = \left(\frac{e^{ikz} + \epsilon e^{-ikz}}{\sqrt{2}} + \left[\frac{f(\theta, \phi) + \epsilon f(\pi - \theta, \phi + \pi)}{\sqrt{2}} \right] \frac{e^{ikr}}{r} \right) \tag{96}$$

where in the final term we have used that the magnitude of r does not change under $\mathbf{r} \to -\mathbf{r}$, but that under the same transformation $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$. The factor ϵ is $+1$ for bosons and -1 for fermions.

What does the symmetrisation mean in terms of our partial wave analysis? Referring back to Eq. 78, we know that the function f is composed of a sum of partial waves whose angular dependence is given by the Legendre polynomials. These have the property that

$$P_l(\cos\theta) + P_l(\cos[\pi - \theta]) = \begin{cases} 2P_l(\cos\theta) & : \ l \text{ even} \\ 0 & : \ l \text{ odd,} \end{cases} \tag{97}$$

and similarly

$$P_l(\cos\theta) - P_l(\cos[\pi - \theta]) = \begin{cases} 0 & : \ l \text{ even} \\ 2P_l(\cos\theta) & : \ l \text{ odd.} \end{cases} \tag{98}$$

Therefore, for bosons only even l partial waves contribute to the total cross section, but for fermions only odd l contribute.

A consequence of this is that a gas of fermions are harder to cool in an atomic gas through evaporative cooling - basically fermions can't scatter at low temperature since there is no s wave contribution.