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Applications of Quantum Mechanics

University of Cambridge Part II Mathematical Tripos

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Recommended Books and Resources

There are many good books on quantum mechanics. Here's a selection that I like:

- Griffiths, *Introduction to Quantum Mechanics*

An excellent way to ease yourself into quantum mechanics, with uniformly clear explanations. For this course, it covers both approximation methods and scattering.

- Shankar, *Principles of Quantum Mechanics*
- James Binney and David Skinner, *The Physics of Quantum Mechanics*
- Weinberg, *Lectures on Quantum Mechanics*

These are all good books, giving plenty of detail and covering more advanced topics. Shankar is expansive, Binney and Skinner clear and concise. Weinberg likes his own notation more than you will like his notation, but it's worth persevering.

This course also contains topics that cannot be found in traditional quantum textbooks. This is especially true for the condensed matter aspects of the course, covered in Sections 3, 4 and 5. Some good books include

- Ashcroft and Mermin, *Solid State Physics*
- Kittel, *Introduction to Solid State Physics*
- Steve Simon, *Solid State Physics Basics*

Ashcroft & Mermin and Kittel are the two standard introductions to condensed matter physics, both of which go substantially beyond the material covered in this course. I have a slight preference for the verbosity of Ashcroft and Mermin. The book by Steve Simon covers only the basics, but does so very well. (An earlier draft can be downloaded from his homepage; see below for a link.)

A number of lecture notes are available on the web. Links can be found on the course webpage: http://www.damtp.cam.ac.uk/user/tong/aqm.html

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Acknowledgements

This course is built on the foundation of previous courses, given in Cambridge by Ron Horgan and Nick Dorey. I'm supported by the Royal Society and Alex Considine Tong.

0. Introduction

Without wishing to overstate the case, the discovery of quantum mechanics is the single greatest achievement in the history of human civilisation.

Quantum mechanics is an outrageous departure from our classical, comforting, common sense view of the world. It is more baffling and disturbing than anything dreamt up by science fiction writers. And yet it is undoubtably the correct description of the Universe we inhabit and has allowed us to understand Nature with unprecedented accuracy. In these lectures we will explore some of these developments.

The applications of quantum mechanics are many and various, and vast swathes of modern physics fall under this rubric. Here we tell only a few of the possible stories, laying the groundwork for future exploration. There are two major topics.

Much of these lectures is devoted to *condensed matter physics* or, more precisely, *solid state physics*. This is the study of "stuff", of how the wonderfully diverse properties of solids can emerge from the simple laws that govern electrons and atoms. We will develop the basics of the subject, learning how electrons glide through seemingly impenetrable solids, how their collective motion is described by a Fermi surface, and how the vibrations of the underlying atoms get tied into bundles of energy known as phonons. We will learn that electrons in magnetic fields can do strange things and start to explore some of the roles that geometry and topology play in quantum physics.

The second major topic is *scattering theory*. In the past century, physicists have developed a foolproof and powerful method to understand everything and anything: you take the object that you're interested in and you throw something at it. This technique was pioneered by Rutherford who used it to understand the structure of the atom. It was used by Franklin, Crick and Watson to understand the structure of DNA. And, more recently, it was used at the LHC to demonstrate the existence of the Higgs boson. In fact, throwing stuff at other stuff is the single most important experimental method known to science. It underlies much of what we know about condensed matter physics and all of what we know about high-energy physics.

In many ways, these lectures are where theoretical physics starts to fracture into separate sub-disciplines. Yet areas of physics which study systems separated by orders of magnitude — from the big bang, to stars, to materials, to information, to atoms and beyond — all rest on a common language and background. The purpose of these lectures is to build this shared base of knowledge.

1. Scattering Theory

The basic idea behind *scattering theory* is simple: there's an object that you want to understand. So you throw something at it. By analysing how that something bounces off, you can glean information about the object itself.

A very familiar example of scattering theory is called "looking at things". In this section we're going to explore what happens when you look at things by throwing a quantum particle at an object.

1.1 Scattering in One Dimension

We start by considering a quantum particle moving along a line. The maths here will be simple, but the physics is sufficiently interesting to exhibit many of the key ideas.

The object that we want to understand is some potential $V(x)$. Importantly, the potential is localised to some region of space which means that $V(x) \to 0$ as $x \to \pm\infty$. An example is shown to the right. We will need the potential to fall-off to be suitably fast in what follows although, for now, we won't be careful about what this means. A quantum particle moving along the line is governed by the Schrödinger equation,

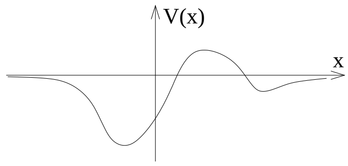


Figure 1:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{1.1}$$

Solutions to this equation are energy eigenstates. They evolve in time as $\psi(x,t) = e^{-iEt/\hbar}\psi(x)$. For any potential, there are essentially two different kinds of states that we're interested in.

- *Bound States* are states that are localised in some region of space. The wavefunctions are normalisable and have profiles that drop off exponentially far from the potential

  $$\psi(x) \sim e^{-\lambda|x|} \quad \text{as} \quad |x| \to \infty$$

  Because the potential vanishes in the asymptotic region, the Schrödinger equation (1.1) relates the asymptotic fall-off to the energy of the state,

  $$E = -\frac{\hbar^2\lambda^2}{2m} \tag{1.2}$$

  In particular, bound states have $E < 0$. Indeed, it is this property which ensures that the particle is trapped within the potential and cannot escape to infinity.

Bound states are rather special. In the absence of a potential, a solution which decays exponentially to the left will grow exponentially to the far right. But, for the state to be normalisable, the potential has to turn this behaviour around, so the wavefunction decreases at both $x \to -\infty$ and $x \to +\infty$. This will only happen for specific values of λ. Ultimately, this is why the spectrum of bound states is discrete, like in the hydrogen atom. It's where the name "quantum" comes from.

- *Scattering States* are not localised in space and, relatedly, the wavefunctions are not normalisable. Instead, asymptotically, far from the potential, scattering states take the form of plane waves. In one dimension, there are two possibilities

$$\text{Right moving:} \quad \psi \sim e^{ikx}$$
$$\text{Left moving:} \quad \psi \sim e^{-ikx}$$

where $k > 0$. To see why these are left or right moving, we need to put the time dependence back in. The wavefunctions then take the form $e^{\pm ikx - iEt/\hbar}$. The peaks and troughs of the wave move to the right with the plus sign, and to the left with the minus sign. Solving the Schrödinger equation in the asymptotic region with $V = 0$ gives the energy

$$E = \frac{\hbar^2 k^2}{2m}$$

Scattering states have $E > 0$. Note that, in contrast, to bound states, nothing special has to happen to find scattering solutions. We expect to find solutions for any choice of k.

This simple classification of solutions already tells us something interesting. Suppose, for example, that the potential looks something like the one shown in the figure. You might think that we could find a localised solution that is trapped between the two peaks, with $E > 0$. But this can't happen because if the wavefunction is to be normalisable, it must have $E < 0$. The physical reason, of course, is quantum tunnelling which allows the would-be bound state to escape to infinity. We will learn more about this situation in Section 1.1.5.

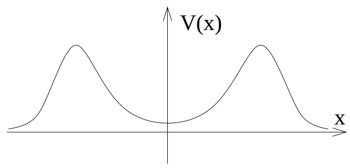


Figure 2:

1.1.1 Reflection and Transmission Amplitudes

Suppose that we stand a long way from the potential and throw particles in. What comes out? This is answered by solving the Schrödinger equation for the scattering states. Because we have a second order differential equation, we expect that there are two independent solutions for each value of k. We can think of these solutions physically as what you get if you throw the particle in from the left or in from the right. Let's deal with each in turn.

Scattering from the Left

We throw the particle in from the left. When it hits the potential, one of two things can happen: it can bounce back, or it can pass straight through. Of course, this being quantum mechanics, it can quite happily do both at the same time. Mathematically, this means that we are looking for a solution which asymptotically takes the form

$$\psi_R(x) \sim \begin{cases} e^{ikx} + re^{-ikx} & x \to -\infty \\ te^{ikx} & x \to +\infty \end{cases} \tag{1.3}$$

We've labelled this state ψ_R because the ingoing wave is *right*-moving. This can be seen in the first term e^{ikx} which represents the particle we're throwing in from $x \to -\infty$. The second term re^{-ikx} represents the particle that is reflected back to $x \to -\infty$ after hitting the potential. The coefficient $r \in \mathbf{C}$ is called the *reflection amplitude*. Finally, the term te^{ikx} at $x \to +\infty$ represents the particle passing through the potential. The coefficient $t \in \mathbf{C}$ is called the *transmission coefficient*. (Note: in this formula t is a complex number that we have to determine; it is not time!) There is no term e^{-ikx} at $x \to +\infty$ because we're not throwing in any particles from that direction. Mathematically, we have chosen the solution in which this term vanishes.

Before we proceed, it's worth flagging up a conceptual point. Scattering is clearly a dynamical process: the particle goes in, and then comes out again. Yet there's no explicit time dependence in our ansatz (1.3); instead, we have a solution formed of plane waves, spread throughout all of space. It's best to think of these plane waves as describing a beam of particles, with the ansatz (1.3) giving us the steady-state solution in the presence of the potential.

The probability for reflection R and transmission T are given by the usual quantum mechanics rule:

$$R = |r|^2 \quad \text{and} \quad T = |t|^2$$

In general, both R and T will be functions of the wavenumber k. This is what we would like to calculate for a given potential and we will see an example shortly. But, before we do this, there are some observations that we can make using general statements about quantum mechanics.

Given a solution $\psi(x)$ to the Schrödinger equation, we can construct a conserved probability current

$$J(x) = -i\frac{\hbar}{2m}\left(\psi^\star \frac{d\psi}{dx} - \psi\frac{d\psi^\star}{dx}\right)$$

which obeys $dJ/dx = 0$. This means that $J(x)$ is constant. (Mathematically, this is the statement that the Wronskian is constant for the two solutions to the Schrödinger equation). For our scattering solution ψ_R, with asymptotic form (1.3), the probability current as $x \to -\infty$ is given by

$$\begin{aligned} J(x) &= \frac{\hbar k}{2m}\Big[\left(e^{-ikx} + r^\star e^{+ikx}\right)\left(e^{ikx} - re^{-ikx}\right) + \left(e^{ikx} + re^{-ikx}\right)\left(e^{-ikx} - r^\star e^{+ikx}\right)\Big] \\ &= \frac{\hbar k}{m}\left(1 - |r|^2\right) \qquad \text{as } \ x \to -\infty \end{aligned}$$

Meanwhile, as $x \to +\infty$, we have

$$J(x) = \frac{\hbar k}{2m}|t|^2 \qquad \text{as } \ x \to +\infty$$

Equating the two gives

$$1 - |r|^2 = |t|^2 \quad \Rightarrow \quad R + T = 1 \tag{1.4}$$

This should make us happy as it means that probabilities do what probabilities are supposed to do. The particle can only get reflected or transmitted and the sum of the probabilities to do these things equals one.

Scattering from the Right

This time, we throw the particle in from the right. Once again, it can bounce back off the potential or pass straight through. Mathematically, we're now looking for solutions which take the asymptotic form

$$\psi_L(x) \sim \begin{cases} t' e^{-ikx} & x \to -\infty \\ e^{-ikx} + r' e^{+ikx} & x \to +\infty \end{cases} \tag{1.5}$$

where we've now labelled this state ψ_L because the ingoing wave, at $x \to +\infty$, is *left*-moving. We've called the reflection and transmission amplitudes r' and t'.

There is a simple relation between the two solutions ψ_R in (1.3) and ψ_L in (1.5). This follows because the potential $V(x)$ in (1.1) is a real function, so if ψ_R is a solution then so is $\psi_R^\star$. And, by linearity, so is $\psi_R^\star - r^\star \psi_R$ which is given by

$$\psi_R^\star(x) - r^\star \psi_R(x) \sim \begin{cases} (1-|r|^2)e^{-ikx} & x \to -\infty \\ t^\star e^{-ikx} - r^\star t e^{ikx} & x \to +\infty \end{cases}$$

This takes the same functional form as (1.5) except we need to divide through by $t^\star$ to make the normalisations agree. (Recall that scattering states aren't normalised anyway so we're quite at liberty to do this.) Using $1 - |r|^2 = |t|^2$, this tells us that there is a solution of the form (1.5) with

$$t' = t \quad \text{and} \quad r' = -\frac{r^\star t}{t^\star} \tag{1.6}$$

Notice that the transition amplitudes are always the same, but the reflection amplitudes can differ by a phase. Nonetheless, this is enough to ensure that the reflection probabilities are the same whether we throw the particle from the left or right: $R = |r|^2 = |r'|^2$.

An Example: A Pothole in the Road

Let's compute r and t for a simple potential, given by

$$V(x) = \begin{cases} -V_0 & -a/2 < x < a/2 \\ 0 & \text{otherwise} \end{cases}$$

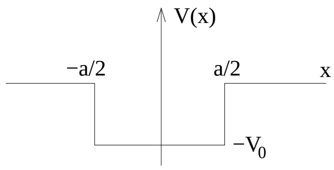


Figure 3:

with $V_0 > 0$. This looks like a pothole in the middle of an, otherwise, flat potential.

Outside the potential, we have the usual plane waves $\psi \sim e^{\pm ikx}$. In the middle of the potential, the solutions to the Schrödinger equation (1.1) take the form

$$\psi(x) = Ae^{iqx} + Be^{-iqx} \qquad x \in [-a/2, a/2] \tag{1.7}$$

where

$$q^2 = \frac{2mV_0}{\hbar^2} + k^2$$

To compute the reflection and transmission amplitudes, r, r' and t, we need to patch the solution (1.7) with either (1.3) or (1.5) at the edges of the potential.

Let's start by scattering from the left, with the solution (1.3) outside the potential. Continuity of the wavefunction at $x = \pm a/2$ tells us that

$$e^{-ika/2} + re^{ika/2} = Ae^{-iqa/2} + Be^{iqa/2} \quad \text{and} \quad te^{ika/2} = Ae^{iqa/2} + Be^{-iqa/2}$$

Meanwhile, matching the derivatives of ψ at $x = \pm a$ gives

$$\frac{k}{q}\left(e^{-ika/2} - re^{ika/2}\right) = Ae^{-iqa/2} - Be^{iqa/2} \quad \text{and} \quad \frac{kt}{q}e^{ika/2} = Ae^{iqa/2} - Be^{-iqa/2}$$

These are four equations with four unknowns: A, B, r and t. One way to proceed is to add and subtract the two equations on the right, and then do the same for the two equations on the left. This allows us to eliminate A and B

$$A = t\left(1 + \frac{k}{q}\right)e^{i(k-q)a/2} = \left(1 + \frac{k}{q}\right)e^{-i(k-q)a/2} + r\left(1 - \frac{k}{q}\right)e^{i(k+q)a/2}$$

$$B = t\left(1 - \frac{k}{q}\right)e^{i(k+q)a/2} = \left(1 - \frac{k}{q}\right)e^{-i(k+q)a/2} + r\left(1 + \frac{k}{q}\right)e^{i(k-q)a/2}$$

We've still got some algebraic work ahead of us. It's grungy but straightforward. Solving these two remaining equations gives us the reflection and transmission coefficients that we want. They are

$$\begin{aligned} r &= \frac{(k^2 - q^2)\sin(qa)e^{-ika}}{(q^2 + k^2)\sin(qa) + 2iqk\cos(qa)} \\ t &= \frac{2iqke^{-ika}}{(q^2 + k^2)\sin(qa) + 2iqk\cos(qa)} \end{aligned} \tag{1.8}$$

Even for this simple potential, the amplitudes are far from trivial. Indeed, they contain a lot of information. Perhaps the simplest lesson we can extract comes from looking at the limit $k \to 0$, where $r \to -1$ and $t \to 0$. This means that if you throw the particle very softly ($k \to 0$), then it won't make it through the potential; it's guaranteed to bounce back.

Conversely, in the limit $k \to \infty$, we have $r = 0$. (Recall that $q^2 = k^2 + 2mV_0/\hbar^2$ so we also have $q \to \infty$ in this limit.) By conservation of probability, we must then have $|t| = 1$ and the particle is guaranteed to pass through. This is what you might expect; if you throw the particle hard enough, it barely notices that the potential is there.

There are also very specific values of the incoming momenta for which $r = 0$ and the particle is assured of passage through the potential. This occurs when $qa = n\pi$ with $n \in \mathbf{Z}$ for which $r = 0$. Notice that you have to fine tune the incoming momenta so that it depends on the details of the potential which, in this example, means V_0 and a.

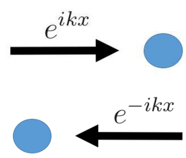
We can repeat the calculation above for scattering from the right. In fact, for our pothole potential, the result is exactly the same and we have $r = r'$. This arises because $V(x) = V(-x)$ so it's no surprise that scattering from the left and right are the same. We'll revisit this in Section 1.1.3.

1.1.2 Introducing the S-Matrix

The *S-matrix* is a convenient way of packaging the information about reflection and transmission coefficients. It is useful both because it highlights new features of the problem, and because it generalises to scattering in higher dimensions.

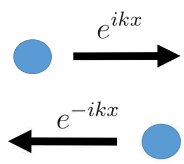
We will start by writing the above solutions in slightly different notation. We have two ingoing asymptotic wavefunctions, one from the left and one from the right

$$\text{Ingoing} \begin{cases} \text{right-moving:} \quad \mathcal{I}_R(x) = e^{+ikx} \quad x \to -\infty \\ \text{left-moving:} \quad \mathcal{I}_L(x) = e^{-ikx} \quad x \to +\infty \end{cases}$$



Similarly, there are two outgoing asymptotic wavefunctions,

$$\text{Outgoing} \begin{cases} \text{right-moving:} \quad \mathcal{O}_R(x) = e^{+ikx} \quad x \to +\infty \\ \text{left-moving:} \quad \mathcal{O}_L(x) = e^{-ikx} \quad x \to -\infty \end{cases}$$



The two asymptotic solutions (1.3) and (1.5) can then be written as

$$\begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} \mathcal{I}_R \\ \mathcal{I}_L \end{pmatrix} + \mathcal{S} \begin{pmatrix} \mathcal{O}_R \\ \mathcal{O}_L \end{pmatrix} \tag{1.9}$$

where

$$\mathcal{S} = \begin{pmatrix} t & r \\ r' & t' \end{pmatrix} \tag{1.10}$$

This is the *S-matrix*. As we've seen, for any given problem the entries of the matrix are rather complicated functions of k.

The S-matrix has many nice properties, some of which we will describe in these lectures. One of the simplest and most important is that $\mathcal{S}$ is unitary. To see this note that

$$\mathcal{S}\mathcal{S}^\dagger = \begin{pmatrix} |t'|^2 + |r|^2 & t'r'^\star + rt^\star \\ t'^\star r' + tr^\star & |t|^2 + |r'|^2 \end{pmatrix}$$

Unitarity then follows from the conservation of probability. The off-diagonal elements vanish by virtue of the relations $t' = t$ and $r' = -r^\star t/t^\star$ that we found in (1.6). Meanwhile, the diagonal elements are equal to one by (1.4) and so $\mathcal{S}\mathcal{S}^\dagger = \mathbf{1}$. The equivalence between conservation of probability and unitarity of the S-matrix is important, and will generalise to higher dimensions. Indeed, in quantum mechanics the word "unitarity" is often used synonymously with "conservation of probability".

One further property follows from the fact that the wavefunctions $\psi_R(x)$ and $\psi_L(x)$ do not change under complex conjugation if we simultaneously flip $k \to -k$. In other words $\psi(x;k) = \psi^\star(x;-k)$. This means that the S-matrix obeys

$$\mathcal{S}^\star(k) = \mathcal{S}(-k)$$

There are a number of other, more hidden properties of the S-matrix that we will uncover below.

1.1.3 A Parity Basis for Scattering

As we've seen above, for symmetric potentials, with $V(x) = V(-x)$, scattering from the left and right is the same. Let's first make this statement more formal.

We introduce the *parity* operator P which acts on functions $f(x)$ as

$$P : f(x) \to f(-x)$$

For symmetric potentials, we have $[P, H] = 0$ which means that eigenstates of the Hamiltonian can be chosen so that they are also eigenstates of P. The parity operator is Hermitian, $P^\dagger = P$, so its eigenvalues λ are real. But we also have $P^2 f(x) = f(x)$, which means that the eigenvalues must obey $\lambda^2 = 1$. Clearly there are only two possibilities: $\lambda = +1$ and $\lambda = -1$, This means that eigenstates of the Hamiltonian can be chosen to be either even functions ($\lambda = +1$) or odd functions ($\lambda = -1$).

Above we worked with scattering eigenstates ψ_R and ψ_L. These are neither odd nor even. Instead, for a symmetric potential, they are related by $\psi_L(x) = \psi_R(-x)$. This is the reason that symmetric potentials have $r = r'$. If we want to work with the parity eigenstates, we take

$$\begin{aligned}\psi_+(x) &= \psi_R(x) + \psi_L(x) = \psi_R(x) + \psi_R(-x) \\ \psi_-(x) &= -\psi_R(x) + \psi_L(x) = -\psi_R(x) + \psi_R(-x)\end{aligned}$$

which obey $P\psi_\pm(x) = \pm\psi_\pm(x)$.

Often, working with parity eigenstates makes the algebra a little easier. This is particularly true if our problem has a parity-invariant potential, $V(x) = V(-x)$.

The Pothole Example Revisited

Let's see how the use of parity eigenstates can make our calculations simpler. We'll redo the scattering calculation in the pothole, but now we'll take the asymptotic states to be ψ_+ and ψ_-. Physically, you can think of this experiment as throwing in particles from both the left and right at the same time, with appropriate choices of signs.

We start with the even parity wavefunction ψ_+. We want to patch this onto a solution in the middle, but this too must have even parity. This mean that the solution in the pothole takes the form

$$\psi_+(x) = A(e^{iqx} + e^{-iqx}) \qquad x \in [-a/2, a/2]$$

which now has only one unknown coefficient, A. As previously, $q^2 = k^2 + 2mV_0/\hbar^2$. We still need to make sure that both the wavefunction and its derivative are continuous at $x = \pm a/2$. But, because we're working with even functions, we only need to look at one of these points. At $x = a/2$ we get

$$\begin{aligned}e^{-ika/2} + (r+t)e^{ika/2} &= A(e^{iqa/2} + e^{-iqa/2}) \\ \left(-e^{-ika/2} + (r+t)e^{ika/2}\right) &= \frac{q}{k}A(e^{iqa/2} - e^{-iqa/2})\end{aligned}$$

Notice that only the combination $(r + t)$ appears. We have two equations with two unknowns. If we divide the two equations and rearrange, we get

$$r + t = -e^{-ika}\ \frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik} \tag{1.11}$$

which is all a lot easier than the messy manipulations we had to do when working with ψ_L and ψ_R. Of course, we've only got an expression for $(r + t)$. But we can play the same game for the odd parity eigenstates to get a corresponding expression for $(r-t)$. Now, the solution in the pothole takes the form

$$\psi_-(x) = B(e^{iqx} - e^{-iqx}) \qquad x \in [-a/2, a/2]$$

Requiring continuity of the wavefunction and its derivative at $x = a/2$ we get

$$\begin{aligned} e^{-ika/2} + (r-t)e^{ika/2} &= B(e^{iqa/2} - e^{-iqa/2}) \\ \left(-e^{-ika/2} + (r-t)e^{ika/2}\right) &= \frac{q}{k} B(e^{iqa/2} + e^{-iqa/2}) \end{aligned}$$

Once again, dividing we find

$$r - t = e^{-ika} \frac{q + ik\tan(qa/2)}{q - ik\tan(qa/2)} \tag{1.12}$$

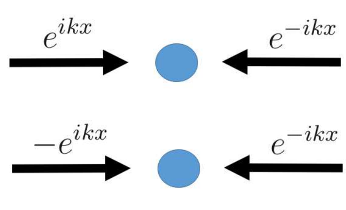
It's not immediately obvious that the expressions (1.11) and (1.12) are the same as those for r and t that we derived previously. But a little bit of algebra should convince you that they agree.

[A helping hand: this little bit of algebra is extremely fiddly if you don't go about it in the right way! Here's a reasonably a streamlined approach. First define the denominator of (1.8) as $D(k) = (q^2 + k^2)\sin(qa) + 2iqk\cos(qa)$. Using the double-angle formula from trigonometry, we can write this as $D(k) = 2\cos^2(qa/2)(q\tan(qa/2) + ik)(q - ik\tan(qa/2))$. We can then add the two expressions in (1.8), and use the double-angle formula again, to get $r + t = 2e^{-ika}\cos^2(qa/2)(q\tan(qa/2) - ik)(ik\tan(qa/2) - q)/D(k)$ This coincides with our formula (1.11). Similar games give us the formula (1.12).]

The S-Matrix in the Parity Basis

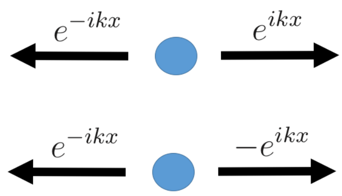
We can also think about the S-matrix using our new basis of states. The asymptotic ingoing modes are even and odd functions, given at $|x| \to \infty$ by

$$\text{Ingoing} \begin{cases} \text{parity-even:} \qquad \mathcal{I}_+(x) = e^{-ik|x|} \\ \text{parity-odd:} \qquad \mathcal{I}_-(x) = \text{sign}(x)\, e^{-ik|x|} \end{cases}$$



The two asymptotic outgoing modes are

$$\text{Outgoing} \quad \begin{cases} \text{parity-even:} \qquad \mathcal{O}_+(x) = e^{+ik|x|} \\ \\ \text{parity-odd:} \qquad \mathcal{O}_-(x) = -\text{sign}(x)\, e^{+ik|x|} \end{cases}$$



These are related to our earlier modes by a simple change of basis,

$$\begin{pmatrix} \mathcal{I}_+ \\ \mathcal{I}_- \end{pmatrix} = \mathcal{M} \begin{pmatrix} \mathcal{I}_R \\ \mathcal{I}_L \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathcal{O}_+ \\ \mathcal{O}_- \end{pmatrix} = \mathcal{M} \begin{pmatrix} \mathcal{O}_R \\ \mathcal{O}_L \end{pmatrix} \quad \text{with} \quad \mathcal{M} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

We can define an S-matrix with respect to this parity basis. In analogy with (1.9), we write asymptotic solutions as

$$\begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \begin{pmatrix} \mathcal{I}_+ \\ \mathcal{I}_- \end{pmatrix} + \mathcal{S}^P \begin{pmatrix} \mathcal{O}_+ \\ \mathcal{O}_- \end{pmatrix} \tag{1.13}$$

where we use the notation $\mathcal{S}^P$ to denote the S-matrix with respect to the parity basis. We write

$$\mathcal{S}^P = \begin{pmatrix} S_{++} & S_{+-} \\ S_{-+} & S_{--} \end{pmatrix}$$

This is related to our earlier S-matrix by a change of basis. We have

$$\mathcal{S}^P = \mathcal{M}\mathcal{S}\mathcal{M}^{-1} = \begin{pmatrix} t + (r+r')/2 & (r-r')/2 \\ (r'-r)/2 & t - (r+r')/2 \end{pmatrix}$$

As you may expect, this basis is particularly useful if the underlying potential is symmetric, so $V(x) = V(-x)$. In this case we have $r = r'$ and the S-matrix becomes diagonal. The diagonal components are simply

$$S_{++} = t + r \quad \text{and} \quad S_{--} = t - r$$

In fact, because $\mathcal{S}^p$ is unitary, each of these components must be a phase. This follows because r and t are not independent. First, they obey $|r|^2 + |t|^2 = 1$. Moreover, when $r' = r$, the relation (1.6) becomes

$$rt^\star + r^\star t = 0 \qquad \Rightarrow \qquad \text{Re}(rt\star) = 0$$

This is enough to ensure that both S_{++} and S_{--} are indeed phases. We write them as

$$S_{++} = e^{2i\delta_+(k)} \quad \text{and} \quad S_{--} = e^{2i\delta_-(k)}$$

We learn that for scattering off a symmetric potential, all the information is encoded in two momentum-dependent *phase shifts*, $\delta_\pm(k)$ which tell us how the phases of the outgoing waves $\mathcal{O}_\pm$ are changed with respect to the ingoing waves $\mathcal{I}_\pm$.

1.1.4 Bound States

So far we've focussed only on the scattering states of the problem. We now look at the bound states, which have energy $E < 0$ and are localised near inside the potential. Here, something rather magical happens. It turns out that the information about these bound states can be extracted from the S-matrix, which we constructed purely from knowledge of the scattering states.

To find the bound states, we need to do something clever. We take our scattering solutions, which depend on momentum $k \in \mathbf{R}$, and extend them to the complex momentum plane. This means that we analytically continue out solutions so that they depend on $k \in \mathbf{C}$.

First note that the solutions with $k \in \mathbf{C}$ still obey our original Schrödinger equation (1.1) since, at no point in any of our derivation did we assume that $k \in \mathbf{R}$. The only difficulty comes when we look at how the wavefunctions behave asymptotically. In particular, any putative solution will, in general, diverge exponentially as $x \to +\infty$ or $x \to -\infty$, rendering the wavefunction non-normalisable. However, as we will now show, there are certain solutions that survive.

For simplicity, let's assume that we have a symmetric potential $V(x) = V(-x)$. As we've seen above, this means that there's no mixing between the parity-even and parity-odd wavefunctions. We start by looking at the parity-even states. The general solution takes the form

$$\psi_+(x) = \mathcal{I}_+(x) + S_{++}\mathcal{O}_+(x) = \begin{cases} e^{+ikx} \; + \; S_{++}e^{-ikx} & x \to -\infty \\ e^{-ikx} \; + \; S_{++}e^{+ikx} & x \to +\infty \end{cases}$$

Suppose that we make k pure imaginary and write

$$k = i\lambda$$

with $\lambda > 0$. Then we get

$$\psi_+(x) = \begin{cases} e^{-\lambda x} \; + \; S_{++}e^{+\lambda x} & x \to -\infty \\ e^{+\lambda x} \; + \; S_{++}e^{-\lambda x} & x \to +\infty \end{cases} \tag{1.14}$$

Both terms proportional to S_{++} decay asymptotically, but the other terms diverge. This is bad. However, there's a get-out. For any fixed k (whether real or complex), S_{++} is simply a number. That means that we're quite at liberty to divide by it. Indeed, the wavefunction above isn't normalised anyway, so dividing by a constant isn't going to change anything. We get

$$\psi_+(x) = \begin{cases} S_{++}^{-1}\, e^{-\lambda x} \;+\; e^{+\lambda x} & x \to -\infty \\ S_{++}^{-1}\, e^{+\lambda x} \;+\; e^{-\lambda x} & x \to +\infty \end{cases} \tag{1.15}$$

Now we can see the loop-hole. The wavefunction above is normalisable whenever we can find a $\lambda > 0$ such that

$$S_{++}(k) \to \infty \quad \text{ as } k \to i\lambda$$

This, then, is the magic of the S-matrix. Poles in the complex momentum plane that lie on the positive imaginary axis (i.e. $k = i\lambda$ with $\lambda > 0$) correspond to bound states. This information also tells us the energy of the bound state since, as we saw in (1.2), it is given by

$$E = -\frac{\hbar^2\lambda^2}{2m}$$

We could also have set $k = -i\lambda$, with $\lambda > 0$. In this case, it is the terms proportional to S_{++} in (1.14) which diverge and the wavefunction is normalisable only if $S_{++}(k = -i\lambda) = 0$. However, since S_{++} is a phase, this is guaranteed to be true whenever $S_{++}(k = i\lambda)$ has a pole, and simply gives us back the solution above.

Finally, note that exactly the same arguments hold for parity-odd wavefunctions. There is a bound state whenever $S_{--}(k)$ has a pole at $k = i\lambda$ with $\lambda > 0$.

An Example: Stuck in the Pothole

We can illustrate this with our favourite example of the square well, of depth $-V_0$ and width a. We already computed the S-matrix in (1.11) and (1.12). We have,

$$S_{++}(k) = r + t = -e^{-ika}\,\frac{q\tan(qa/2) - ik}{q\tan(qa/2) + ik}$$

where $q^2 = 2mV_0/\hbar^2 + k^2$. Setting $k = i\lambda$, we see that this has a pole when

$$\lambda = q\tan\left(\frac{qa}{2}\right) \quad \text{ with } \quad \lambda^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

These are the usual equations that you have to solve when finding parity-even bound states in a square well. The form of the solutions is simplest to see if we plot these equations, as shown in the left-hand of Figure 4. There is always at least one bound state, with more appearing as the well gets deeper.

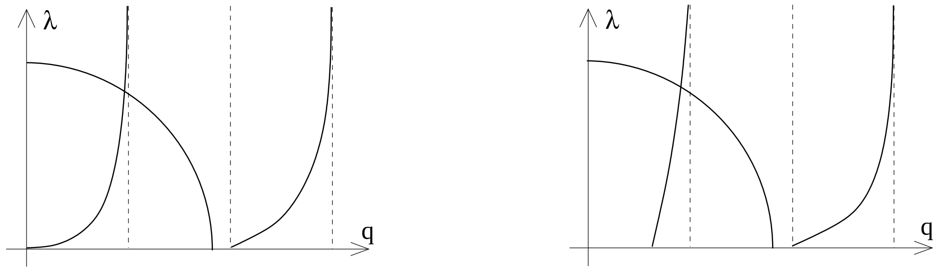


Figure 4: Bound state of even parity always exist, since the two equations shown on the left always have a solution with $\lambda, q > 0$. Bound states of odd parity, shown on the right, exist if the potential is deep enough.

Similarly, if we look at the parity-odd wavefunctions, we have

$$S_{--}(k) = t - r = e^{-ika}\frac{q + ik\tan(qa/2)}{q - ik\tan(qa/2)}$$

which has a pole at $k = i\lambda$ when

$$q = -\lambda \tan\left(\frac{qa}{2}\right) \quad \text{with} \quad \lambda^2 + q^2 = \frac{2mV_0}{\hbar^2} \tag{1.16}$$

This too reproduces the equations that we found in earlier courses in quantum mechanics when searching for bound states in a square well. Now there is no guarantee that a bound state exists; this only happens if the potential is deep enough.

1.1.5 Resonances

We might wonder if there's any other information hidden in the analytic structure of the S-matrix. In this section, we will see that there is, although its interpretation is a little more subtle.

First, the physics. Let's think back again to the example shown on the right. One the one hand, we know that there can be no bound states in such a trap because they will have $E > 0$. Any particle that we place in the trap will ultimately tunnel out. On the other hand, if the walls of the trap are very large then we might expect that the particle stays there for a long time before it eventually escapes. In this situation, we talk of a *resonance*. These are also referred to as *unstable* or *metastable* states. Our goal is to show how such resonances are encoded in the S-matrix.

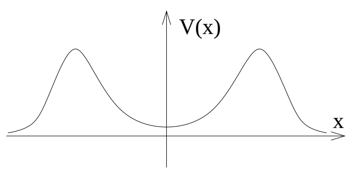


Figure 5:

Now, the maths. We'll restrict attention to parity-even functions. Suppose that the S-matrix S_{++} has a pole that lies on the complex momentum plane at position

$$k = k_0 - i\gamma$$

On general grounds, the wavefunction will have a second pole at $-k^\star = -k_0 - i\gamma$. We'd like to interpret these poles. First note that the energy is also imaginary

$$E = \frac{\hbar^2 k^2}{2m} \equiv E_0 - i\frac{\Gamma}{2} \tag{1.17}$$

with $E_0 = \hbar^2(k_0^2 - \gamma^2)/2m$ and $\Gamma = 2\hbar^2\gamma k_0/m$. An imaginary energy may sound strange, but it is has a very natural interpretation. Recall that the time dependence of the wavefunction is given by

$$e^{-iEt/\hbar} = e^{-iE_0 t/\hbar}\, e^{-\Gamma t/2\hbar} \tag{1.18}$$

This is the first clue that we need. We see that, for $\gamma > 0$, the overall form of the wavefunction decays exponentially with time. This is the characteristic behaviour of unstable states. A wavefunction that is initially supported inside the trap will be very small there at time much larger than $\tau = 1/\Gamma$. Here τ is called the *half-life* of the state, while Γ is usually referred to as the *width* of the state. (We'll see why in Section 1.2).

Where does the particle go? Including the time dependence (1.18), the same argument that led us to (1.15) now tells us that when $S_{++} \to \infty$, the solution takes the asymptotic form

$$\psi_+(x,t) = \begin{cases} e^{-iE_0 t/\hbar}\, e^{-ik_0 x}\, e^{-\gamma x - \Gamma t/2\hbar} & x \to -\infty \\ e^{-iE_0 t/\hbar}\, e^{+ik_0 x}\, e^{+\gamma x - \Gamma t/2\hbar} & x \to +\infty \end{cases} \tag{1.19}$$

The first two exponential factors oscillate. But the final factor varies as

$$e^{\pm\gamma(x \mp vt)} \quad \text{where} \quad v = \frac{\Gamma}{2\hbar\gamma} = \frac{\hbar k_0}{m}$$

This has the interpretation of a particle moving with momentum $\hbar k_0$. This, of course, is the particle which has escaped the trap.

Note that for fixed time t, these wavefunctions are not normalisable: they diverge at both $x \to \pm\infty$. This shouldn't concern us, because, although our wavefunctions are eigenstates of the Hamiltonian, they are not interpreted as stationary states. Indeed, it had to be the case. An unstable state has complex energy, but standard theorems in linear algebra tell us that a Hermitian operator like the Hamiltonian must have real eigenvalues. We have managed to evade this theorem only because these wavefunctions are non-normalisable and so do not, strictly speaking, live in the Hilbert space.

There's a lesson buried in all of this. If we were to take the standard axioms of quantum mechanics, we would simply throw away wavefunctions of the form (1.19) on the grounds that they do not lie in the Hilbert space and so are unphysical. But this would be a mistake: the wavefunctions do contain interesting physics, albeit of a slightly different variety than we are used to. Sometimes it's worth pushing our physical theories beyond our comfort zone to see what is lurking there.

The upshot of this discussion is that poles of the S-matrix in the lower-half complex plane correspond to resonances. It is often useful to write S_{++} as a function of energy rather than momentum. (They are related by (1.17)). Since S_{++} is a phase, close to a resonance it necessarily takes the form

$$S_{++} = \frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2}$$

An Example: A Pair of Delta-Functions

A pair of delta functions provide a simple and tractable example to illustrate the idea of resonances. The potential is given by

$$V(x) = V_0\Big[\delta(x-1) + \delta(x+1)\Big]$$

Recall that the effect of the delta-functions is simply to change the boundary conditions at $x = \pm 1$ when solving the Schrödinger equation. All wavefunctions should be continuous at $x = \pm 1$, but their derivatives are discontinuous. For example, at $x = +1$, solutions obey

$$\lim_{\epsilon \to 0} \Big[\psi'(1+\epsilon) - \psi'(1-\epsilon)\Big] = U_0 \psi(1) \quad \text{ with } \quad U_0 = \frac{2mV_0}{\hbar^2}$$

Working in the parity basis makes life simpler, not least because you only need to consider the matching at one of the delta-functions, with the other then guaranteed. The computation of the S-matrix is a problem on the exercise sheet. You will find

$$S_{++} = e^{-2ik}\left[\frac{(2k - iU_0)e^{ik} - iU_0 e^{-ik}}{(2k + iU_0)e^{-ik} + iU_0 e^{ik}}\right]$$

Note that the denominator is the complex conjugate of the numerator, ensuring that S_{++} is a phase, as expected. The poles of this S-matrix are given by solutions to the equation

$$e^{2ik} = -\left(1 - \frac{2ik}{U_0}\right) \tag{1.20}$$

To understand the physics behind this, let's first look at the situation where $U_0 \to \infty$, so that the weight of the delta-functions gets infinitely large. Then the poles sit at

$$e^{2ik} = -1 \quad \Rightarrow \quad k = k_n = \left(n + \frac{1}{2}\right)\pi$$

These correspond to bound states trapped between the two wavefunctions. For example, the $n = 0$ state is shown in the figure. Note that they're rather unusual because the poles sit on the real k-axis, rather than the imaginary k-axis. Correspondingly, these bound states have $E > 0$. This strange behaviour is only allowed because we have an infinitely large potential which forbids particles on one side of the barrier to cross to the other.

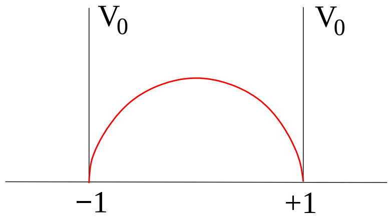


Figure 6:

As a side remark, we note that this same impenetrable behaviour is seen in scattering. When $U_0 \to \infty$, the S-matrix becomes $S_{++} \to -e^{2ik}$. This tells us that a particle coming from outside is completely reflected off the infinitely large barrier. The minus sign is the standard phase change after reflection. The factor of e^{2ik} is because the waves are forbidden from travelling through the region between the delta functions, which has width $x = 2$. As a result, the phase is shifted by e^{ikx} from what it would be if the barriers were removed.

Let's now look at what happens when U_0 is large, but finite? We'll focus on the lowest energy bound state with $n = 0$. We can expand (1.20) in $1/U_0$. (This too is left as a problem on the exercise sheet.) We find

$$k = \frac{\pi}{2} + \alpha - i\gamma$$

with

$$\alpha \approx -\frac{\pi}{2U_0} + \frac{\pi}{2U_0^2} + \mathcal{O}\left(\frac{1}{U_0^3}\right) \quad \text{and} \quad \gamma \approx \frac{\pi^2}{4U_0^2} + \mathcal{O}\left(\frac{1}{U_0^3}\right)$$

Note, in particular, that $\gamma > 0$, so the pole moves off the real axis and into the lower half-plane. This pole now has all the properties that we described at the beginning of this section. It describes a state, trapped between the two delta-functions, which decays with half-life

$$\tau = \frac{\hbar}{\Gamma} = \frac{4mU_0^2}{\hbar\pi^3}\left(1 + \mathcal{O}\left(\frac{1}{U_0}\right)\right)$$

This is the resonance.

1.2 Scattering in Three Dimensions

Our real interest in scattering is for particles moving in three spatial dimensions, with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$$

Recall that there are two distinct interpretations for such a Hamiltonian

- We could think of this as the motion of a single particle, moving in a fixed background potential $V(\mathbf{r})$. This would be appropriate, for example, in Rutherford's famous experiment where we fire an alpha particle at a gold nucleus.

- Alternatively, We could think of this as the relative motion of two particles, separated by distance $\mathbf{r}$, interacting through the force $\mathbf{F} = -\nabla V(\mathbf{r})$. We could take $V(r)$ to be the Coulomb force, to describe the scattering of electrons, or the Yukawa force to describe the scattering of neutrons.

In this section, we will use language appropriate to the first interpretation, but everything we say holds equally well in the second. Throughout this section, we will work with rotationally invariant (i.e. central) potentials, so that $V(\mathbf{r}) = V(|\mathbf{r}|)$.

1.2.1 The Cross-Section

Our first goal is to decide what we want to calculate. The simple reflection and transmission coefficients of the one-dimensional problem are no longer appropriate. We need to replace them by something a little more complicated. We start by thinking of the classical situation.

Classical Scattering

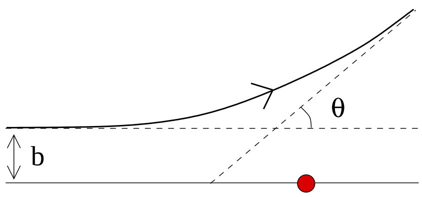


Figure 7:

Suppose that we throw in a single particle with kinetic energy E. Its initial trajectory is characterised by the *impact parameter* b, defined as the closest the particle would get to the scattering centre at $r = 0$ if there were no potential. The particle emerges with *scattering angle* θ, which is the angle between the asymptotic incoming and outgoing trajectories, as shown in the figure. By solving the classical equations of motion, we can compute $\theta(b; E)$ or, equivalently, $b(\theta; E)$.

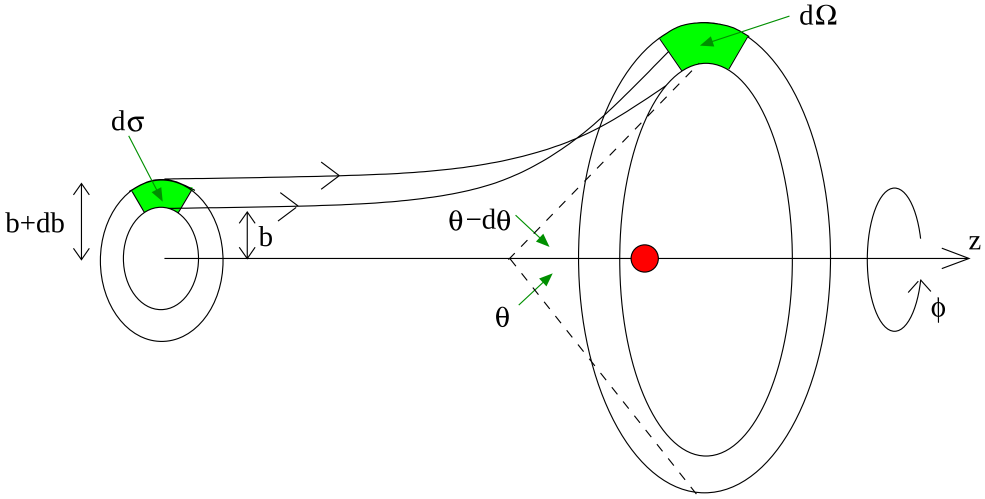


Figure 8: What becomes of an infinitesimal cross-sectional area after scattering.

Now consider a uniform beam of particles, each with kinetic energy E. We want to understand what becomes of this beam. Consider the cross-sectional area, denoted $d\sigma$ in Figure 8. We write this as

$$d\sigma = b\, d\phi\, db$$

The particles within $d\sigma$ will evolve to the lie in a cone of solid angle $d\Omega$, given by

$$d\Omega = \sin\theta\, d\phi\, d\theta$$

where, for central potentials, the infinitesimal angles $d\phi$ are the same in both these formulae. The *differential cross-section* is defined to be

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right|$$

The left-hand side should really be $|d\sigma/d\Omega|$, but we'll usually drop the modulus. The differential cross-section is a function of incoming momentum k, together with the outgoing angle θ.

More colloquially, the differential cross-section can be thought of as

$$\frac{d\sigma}{d\Omega}\, d\Omega = \frac{\text{Number of particles scattered into } d\Omega \text{ per unit time}}{\text{Number of incident particles per area } d\sigma \text{ per unit time}}$$

We write this in terms of *flux*, defined to be the number of particles per unit area per unit time. In this language, the differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{\text{Scattered flux}}{\text{Incident flux}}$$

We can also define the total cross-section

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

Both the differential cross-section and the total cross-section have units of area. The usual unit used in particle physics, nuclear physics and atomic physics is the *barn*, with 1 barn $= 10^{-28}\ m^2$. The total cross-section is a crude characterisation of the scattering power of the potential. Roughly speaking, it can be thought of as the total area of the incoming beam that is scattered. The differential cross-section contains more detailed information.

An Example: The Hard Sphere

Suppose that our particle bounces off a hard sphere, described by the potential $V(r) = \infty$ for $r \leq R$. By staring at the geometry shown in the figure, you can convince yourself that $b = R\sin\alpha$ and $\theta = \pi - 2\alpha$. So in this case

$$b = R\sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right) = R\cos\frac{\theta}{2}$$

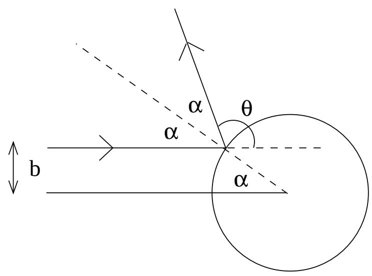


Figure 9:

If $b > R$, clearly there is no scattering. The differential cross-section is

$$\frac{d\sigma}{d\Omega} = \frac{R^2\cos(\theta/2)\sin(\theta/2)}{2\sin\theta} = \frac{R^2}{4}$$

Rather unusually, in this case $d\sigma/d\Omega$ is independent of both θ and E. The total cross-section is

$$\sigma_T = \int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos\theta)\, \frac{d\sigma}{d\Omega} = \pi R^2 \tag{1.21}$$

which, happily, coincides with the geometrical cross-section of the sphere.

This result reinforces the interpretation of the total cross-section that we mentioned above; it is the area of the beam that is scattered. In general, the area of the beam that is scattered will depend on the energy E of the incoming particles.

Another Example: Rutherford Scattering

Rutherford scattering is the name given to scattering off a repulsive Coulomb potential of the form

$$V(r) = \frac{A}{r} \qquad \text{with} \qquad A > 0$$

where, for two particles of charge q_1 and q_2, we have $A = q_1 q_2/4\pi\epsilon_0$. We studied Rutherford scattering in the lectures on Dynamics and Relativity. We found[1]

$$2bE = A\cot\frac{\theta}{2}$$

This gives the differential cross-section,

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \left(\frac{A}{4E}\right)^2 \frac{1}{\sin^4(\theta/2)} \tag{1.22}$$

This scattering amplitude played an important role in the history of physics. Rutherford, together with Geiger and Marsden, fired alpha particles (a helium nucleus) at gold foil. They discovered that the alpha particles could be deflected by a large angle, with the cross-section given by (1.22). Rutherford realised that this meant the positive charge of the atom was concentrated in a tiny, nucleus.

There is, however, a puzzle here. Rutherford did his experiment long before the discovery of quantum mechanics. While his data agreed with the classical result (1.22), there is no reason to believe that this classical result carries over to a full quantum treatment. We'll see how this pans out later in this section.

There's a surprise when we try to calculate the total cross-section σ_T. We find that it's infinite! This is because the Coulomb force is long range. The potential decays to $V(r) \to 0$ as $r \to \infty$, but it drops off very slowly. This will mean that we will have to be careful when applying our formalism to the Coulomb force.

1.2.2 The Scattering Amplitude

The language of cross-sections is also very natural when we look at scattering in quantum mechanics. As in Section 1.1, we set up the scattering problem as a solution to the time-independent Schrödinger equation, which now reads

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1.23}$$

We will send in a plane wave with energy E which we choose to propagate along the z-direction. This is just

$$\psi_{\text{incident}}(\mathbf{r}) = e^{ikz}$$

[1]See equation (4.20) of the Dynamics and Relativity lecture notes, where we denoted the scattering angle by ϕ instead of θ.

where $E = \hbar^2 k^2/2m$. However, after scattering off the potential, the wave doesn't only bounce back in the z direction. Instead, it spreads out spherically, albeit with a phase and amplitude which can vary around the sphere. It's hard to take photographs of quantum wavefunctions, but the water waves shown on the right give a good analogy for what's going on. Asymptotically, as $r \to \infty$, this scattered wave takes the form

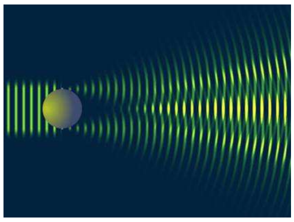


Figure 10:

$$\psi_{\text{scattered}}(\mathbf{r}) = f(\theta, \phi)\, \frac{e^{ikr}}{r} \tag{1.24}$$

The $1/r$ fall-off follows from solving the free Schrödinger equation; we'll see this explicitly below. However, there is a simple intuition for this behaviour which follows from thinking of $|\psi|^2$ as a probability, spreading over a sphere which grows as r^2 as $r \to \infty$. The $1/r$ fall-off ensures that this probability is conserved. Our final ansatz for the asymptotic wavefunction is then

$$\psi(\mathbf{r}) = \psi_{\text{incident}}(\mathbf{r}) + \psi_{\text{scattered}}(\mathbf{r}) \tag{1.25}$$

The function $f(\theta, \phi)$ is called the *scattering amplitude*. For the central potentials considered here it is independent of ϕ, so $f = f(\theta)$. It is the 3d generalisation of the reflection and transmission coefficients that we met in the previous section. Our goal is to calculate it.

The scattering amplitude is very closely related to the differential cross-section. To see this, we can look at the probability current

$$\mathbf{J} = -i\frac{\hbar}{2m}\Big(\psi^\star \nabla\psi - (\nabla\psi^\star)\psi\Big)$$

which obeys $\nabla \cdot \mathbf{J} = 0$. For the incident wave, we have

$$\mathbf{J}_{\text{incident}} = \frac{\hbar k}{m}\hat{\mathbf{z}}$$

This is interpreted as a beam of particles with velocity $v = \hbar k/m$ travelling in the z-direction. Meanwhile, the for the scattered wave we use the fact that

$$\nabla\psi_{\text{scattered}} = \frac{ikf(\theta)e^{ikr}}{r}\hat{\mathbf{r}} + \mathcal{O}\left(\frac{1}{r^2}\right)$$

to find

$$\mathbf{J}_{\text{scattered}} = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta)|^2\,\hat{\mathbf{r}} + \mathcal{O}\left(\frac{1}{r^3}\right)$$

This means that, as $r \to \infty$, the flux of outgoing particles crossing an area dA subtended by the solid angle $d\Omega$

$$\mathbf{J}_{\text{scattered}} \cdot \hat{\mathbf{r}}\, dA = \frac{\hbar k}{m} |f(\theta)|^2 \, d\Omega$$

The differential cross-section is defined to be the ratio of the scattered flux through $d\Omega$, divided by the incident flux. In other words, it is

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

This is rather nice. It means that if we can compute the scattering amplitude $f(\theta)$, it immediately tells us the differential cross-section. The total cross-section is defined, as before, as

$$\sigma_T = \int d\Omega \; |f(\theta)|^2$$

1.2.3 Partial Waves

To make progress, we need to start to look in a more detail at the solutions to the Schrödinger equation (1.23). Because we've decided to work with rotationally invariant potentials, it makes sense to label our wavefunctions by their angular momentum, l. Let's quickly review what this looks like.

A general wavefunction $\psi(r, \theta, \phi)$ can be expanded in terms of spherical harmonics. In this section, however, we only need to deal with wavefunctions of the for form $\psi(r, \theta)$, which are independent of ϕ. Such functions have an expansion in terms of *partial waves*

$$\psi(r, \theta) = \sum_{l=0} R_l(r)\, P_l(\cos\theta)$$

Here the $P_l(\cos\theta)$ are *Legendre polynomials.* They appear by virtue of being eigenstates of the angular momentum operator $\mathbf{L}^2$,

$$\mathbf{L}^2\, P_l(\cos\theta) = \hbar^2 l(l+1) P_l(\cos\theta)$$

In more concrete terms, this is the statement that the Legendre polynomials $P_l(w)$ obey the differential equation

$$\frac{d}{dw}(1 - w^2)\frac{dP_l}{dw} + l(l+1)P_l(w) = 0$$

Meanwhile, the original Schrödinger equation (1.23) becomes an ordinary differential equation for the radial functions R_l,

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} - U(r) + k^2\right) R_l(r) = 0 \tag{1.26}$$

where we've used the expression for the energy, $E = \hbar^2 k^2/2m$, and rescaled the potential

$$U(r) = \frac{2m}{\hbar^2} V(r)$$

Spherical Waves when $U(r) = 0$

We will assume that our potential drops off sufficiently quickly so that asymptotically our waves obey (1.26) with $U(r) = 0$. (We will be more precise about how fast $U(r)$ must fall off later.) We can write the equation obeyed by R_l as

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right)(rR_l(r)) = 0 \tag{1.27}$$

There are two s-wave solutions with $l = 0$, given by

$$R_0(r) = \frac{e^{\pm ikr}}{r} \tag{1.28}$$

These are ingoing (minus sign) and outgoing (plus sign) spherical waves.

The solutions for $l \neq 0$ are more known as *spherical Bessel functions* and are described below.

Plane Waves when $U(r) = 0$

Of course, when $U = 0$, the plane wave

$$\psi_{\text{incident}}(\mathbf{r}) = e^{ikz} = e^{ikr\cos\theta}$$

is also a solution to the Schrödinger equation. Although it feels rather unnatural, it must be possible to expand these solutions in terms of the spherical waves. To do this, it is convenient to briefly introduce the coordinate $\rho = kr$. We write the plane wave solution as

$$\psi_{\text{incident}}(\rho, \theta) = e^{i\rho\cos\theta} = \sum_l (2l+1) u_l(\rho) P_l(\cos\theta) \tag{1.29}$$

where the factor of $(2l+1)$ is for convenience and the function $u_l(\rho)$ are what we want to determine. The Legendre polynomials have a nice orthogonality property,

$$\int_{-1}^{+1} dw\; P_l(w) P_m(w) = \frac{2}{2l+1}\delta_{lm} \tag{1.30}$$

We can use this to write

$$u_l(\rho) = \frac{1}{2}\int_{-1}^{+1} dw\ e^{i\rho w} P_l(w) \tag{1.31}$$

Our interest is only in the behaviour of the plane wave as $\rho \to \infty$. To extract this, we start by integrating by parts

$$u_l(\rho) = \frac{1}{2}\left[\frac{e^{i\rho w}P_l(w)}{i\rho}\right]_{-1}^{+1} - \frac{1}{2i\rho}\int_{-1}^{+1} dw\ e^{i\rho w}\frac{dP_l}{dw}$$

The Legendre polynomials obey $P_l(1) = 1$ and $P_l(-1) = (-1)^l$. We then find

$$u_l(\rho) = \frac{1}{2i\rho}\left[e^{i\rho} - (-1)^l e^{-i\rho}\right] + \mathcal{O}\left(\frac{1}{\rho^2}\right) \tag{1.32}$$

where a further integration by parts will convince you that the remaining terms do indeed drop off as $1/\rho^2$. This is the result we need. As $r \to \infty$, the incident plane wave can be written as

$$\psi_{\text{incident}} = \sum_{l=0}^{\infty} \frac{2l+1}{2ik}\left[\frac{e^{ikr}}{r} - (-1)^l \frac{e^{-ikr}}{r}\right] P_l(\cos\theta) \tag{1.33}$$

We learn that the ingoing plane wave decomposes into an outgoing spherical wave (the first term) together with an ingoing spherical wave (the second term).

Phase Shifts

It's been quite a long build up, but we now know what we want to calculate, and how to do it! To recapitulate, we'd like to calculate the scattering amplitude $f(\theta)$ by finding solutions of the asymptotic form

$$\psi(\mathbf{r}) = e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \quad \text{ as } r \to \infty$$

We still have a couple more definitions to make. First, we expand the scattering amplitude in partial waves as

$$f(\theta) = \sum_{l=0}^{\infty} \frac{2l+1}{k} f_l\, P_l(\cos\theta) \tag{1.34}$$

The normalisation coefficients of $1/k$ and $(2l+1)$ mean that the coefficients f_l sit nicely with the expansion (1.33) of the plane wave in terms of spherical waves. We can then write the asymptotic form of the wavefunction as a sum of ingoing and outgoing waves

$$\psi(\mathbf{r}) \sim \sum_{l=0}^{\infty} \frac{2l+1}{2ik}\left[(-1)^{l+1}\frac{e^{-ikr}}{r} + (1+2if_l)\frac{e^{ikr}}{r}\right] P_l(\cos\theta) \tag{1.35}$$

where the first term is ingoing, and the second term is outgoing. For a given potential $V(r)$, we would like to compute the coefficients f_l which, in general, are functions of k.

Note that the problem has decomposed into decoupled angular momentum sectors, labelled by $l = 0, 1, \ldots$. This is because we're working with a rotationally symmetric potential, which scatters an incoming wave, but does not change its angular momentum. Moreover, for each l, our ansatz consists of an ingoing wave, together with an outgoing wave. This is entirely analogous to our 1d solutions (1.9) when we first introduced the S-matrix. We identify the coefficients of the outgoing terms as the elements of the S-matrix. For rotationally invariant potentials, the 3d S-matrix $\mathcal{S}$ is diagonal in the angular momentum basis, with elements given by

$$S_l = 1 + 2if_l \quad \text{ with } \; l = 0, 1, 2, \ldots$$

Now unitarity of the S-matrix — which is equivalent to conservation of particle number — requires that these diagonal elements are a pure phase. We write

$$S_l = e^{2i\delta_l} \quad \Rightarrow \quad f_l = \frac{1}{2i}(e^{2i\delta_l} - 1) = e^{i\delta_l} \sin \delta_l$$

where δ_l are the phase shifts. Comparing back to (1.34), we see that the phase shifts and scattering amplitude are related by

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

The picture that we have is entirely analogous to the 1d situation. A wave comes in, and a wave goes out. Conservation of probability ensures that the amplitudes of these waves are the same. All information about scattering is encoded in the phase shifts $\delta_l(k)$ between the ingoing and outgoing waves.

1.2.4 The Optical Theorem

The differential cross-section is $d\sigma/d\Omega = |f(\theta)|^2$. Using the partial wave decomposition (1.34), we have

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2} \sum_{l,l'} (2l+1)(2l'+1) f_l f_{l'}^\star P_l(\cos\theta) P_{l'}(\cos\theta)$$

In computing the total cross-section σ_T, we can use the orthogonality of Legendre polynomials (1.30) to write

$$\sigma_T = 2\pi \int_{-1}^{+1} d(\cos\theta)\, \frac{d\sigma}{d\Omega} = \frac{4\pi}{k^2} \sum_l (2l+1)|f_l|^2 = \frac{4\pi}{k^2} \sum_l (2l+l) \sin^2 \delta_l \qquad (1.36)$$

We can compare this to our expansion (1.34). Using the fact that $P(1) = 1$, we have

$$f(0) = \sum_l \frac{2l+1}{k} e^{i\delta_l} \sin\delta_l$$

This tells us that the total cross-section is given by

$$\sigma_T = \frac{4\pi}{k} \,\mathrm{Im} f(0)$$

This is known as the *optical theorem.*

Here's some words that will hopefully build some intuition for the optical theorem. The potential causes scattering from the forward direction ($\theta = 0$) to other directions. Because total probability is conserved, clearly the amount of particles going in the forward direction must decrease. However, this decrease in the forward direction must be equal to the total increase in other directions – and this is what the total cross-section σ_T measures. Finally, the amount of decrease in forward scattering is due to interference between the incoming wave and outgoing waves, and so is proportional to $f(0)$.

Unitarity Bounds

If we think of the total cross-section as built from the cross-sections for each partial wave then, from (1.36), we have

$$\sigma_T = \sum_{l=0}^{\infty} \sigma_l \quad \text{with} \quad \sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l \tag{1.37}$$

Clearly each contribution is bounded as $\sigma_l \leq 4\pi(2l+1)/k^2$, with the maximum arising when the phase shift is given by $\delta_l = \pm\pi/2$. This is called the *unitarity bound.*

There's a straightforward, semi-classical way to understand these unitarity bounds. If we send in a particle with momentum $\hbar k$ and impact parameter b, then it has angular momentum $L = \hbar kb$. This angular momentum is quantised. Roughly speaking, we might expect that the particle has angular momentum $\hbar l$, with $l \in \mathbf{Z}$, when the impact parameter lies in the window

$$\frac{l}{k} \leq b \leq \frac{l+1}{k} \tag{1.38}$$

If the particle gets scattered with 100% probability when it lies in this ring, then the cross-section is equal to the area of the ring. This is

$$\frac{(l+1)^2\pi}{k^2} - \frac{l^2\pi}{k^2} = \frac{(2l+1)\pi}{k^2}$$

This is *almost* the unitarity bound (1.37). It differs by a factor 4. As we will now see, that same factor of 4 difference often arises between simple classical arguments and a full quantum treatment of scattering processes.

1.2.5 An Example: A Hard Sphere and Spherical Bessel Functions

After all this formalism, let's finally do an example. Our scattering region will be a hard sphere of radius a, with potential

$$V(r) = \begin{cases} \infty & r < a \\ 0 & r > a \end{cases}$$

Since the wavefunction vanishes inside the sphere and is continuous, this potential is equivalent to imposing the boundary condition $\psi(a) = 0$.

For $r > a$, the wavefunction can be decomposed in partial waves

$$\psi(r,\theta) = \sum_{l=0} R_l(r)\, P_l(\cos\theta)$$

where the radial wavefunction obeys the free Schrödinger equation

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + 1\right)(\rho R_l(\rho)) = 0 \tag{1.39}$$

where we're again using the coordinate $\rho = kr$. Solutions $R_l(\rho)$ to this equation are known as *spherical Bessel functions* and are denoted $j_l(\rho)$ and $n_l(\rho)$. They are important enough that we take some time to describe their properties.

An Aside: Spherical Bessel Functions

The solutions to (1.39) are given by *spherical Bessel functions*, $R_l(\rho) = j_l(\rho)$ and $R_l(\rho) = n_l(\rho)$, and can be written as[2]

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\sin\rho}{\rho} \quad \text{and} \quad n_l(\rho) = -(-\rho)^l \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^l \frac{\cos\rho}{\rho}$$

Note that $j_0(\rho) = \sin\rho/\rho$ and $n_0(\rho) = -\cos\rho/\rho$, so the solutions (1.28) for free spherical waves can be written as $R_0(\rho) = n_0(\rho) \pm i n_0(\rho)$.

[2]Proofs of this statement, together with the asymptotic expansions given below, can be found in the handout http://www.damtp.cam.ac.uk/user/tong/aqm/bessel.pdf.

In what follows, it will be useful to have the asymptotic form of j_l and n_l. They are given by

$$j_l(\rho) \to \frac{\sin(\rho - \frac{1}{2}l\pi)}{\rho} \quad \text{and} \quad n_l(\rho) \to -\frac{\cos(\rho - \frac{1}{2}l\pi)}{\rho} \quad \text{as } \rho \to \infty \tag{1.40}$$

We see that at large r, the spherical Bessel functions look more or less the same for all l, differing only by a phase. In particular, the combinations $j_l \pm n_l$ look essentially the same as the $l = 0$ spherical waves that we met in (1.28). However, the spherical Bessel functions differ as we come in towards the origin. In particular, close to $\rho = 0$ we have

$$j_l(\rho) \to \frac{\rho^l}{(2l+1)!!} \quad \text{and} \quad n_l(\rho) \to -(2l-1)!!\,\rho^{-(l+1)} \quad \text{as } \rho \to 0 \tag{1.41}$$

where $(2l+1)!! = 1 \cdot 3 \cdot 5 \cdot \dots \cdot (2l+1)$ is the product of all odd numbers up to $2l+1$. Note that $j_l(\rho)$ is regular near the origin, while n_l diverges.

Before we proceed, it's worth seeing how we write the plane wave e^{ikz} in terms of spherical Bessel functions. We wrote the partial wave expansion (1.29) in terms of functions $u_l(\rho)$, whose asymptotic expansion was given in (1.32). This can be rewritten as

$$u_l(\rho) \;\to\; i^l\, \frac{\sin(\rho - \frac{1}{2}l\pi)}{\rho} \quad \text{as} \quad \rho \to \infty$$

which tells us that we can identify the functions $u_l(\rho)$ as

$$u_l(\rho) = i^l j_l(\rho)$$

Back to the Hard Sphere

Returning to our hard sphere, the general solution for $r \geq a$ can be written in the form,

$$R_l(r) = A_l\Big[\cos\alpha_l\, j_l(\rho) - \sin\alpha_l\, n_l(\rho)\Big] \tag{1.42}$$

where, as before, $\rho = kr$. Here A_l and α_l are two integration constants which we will fix by the boundary condition. Because the Schrödinger equation is linear, nothing fixes the overall coefficient A_l. In contrast, the integration constant α_l will be fixed by the boundary conditions at $r = a$. Moreover, this integration constant turns out to be precisely the phase shift δ_l that we want to compute. To see this, we use the asymptotic form of the spherical Bessel functions (1.40) to find

$$R_l(r) \sim \frac{1}{\rho}\left[\cos\alpha_l\, \sin(\rho - \frac{1}{2}l\pi) + \sin\alpha_l\, \cos(\rho - \frac{1}{2}l\pi)\right] = \frac{1}{\rho}\sin(\rho - \frac{1}{2}l\pi + \alpha_l)$$

We can compare this to the expected asymptotic form (1.35) of the wavefunction

$$R_l(r) \sim \left[(-1)^{l+1}\frac{e^{-i\rho}}{\rho} + e^{2i\delta_l}\frac{e^{i\rho}}{\rho}\right] = \frac{e^{i\delta_l}e^{i\pi l/2}}{\rho}\left[-\,e^{-i(\rho+\delta_l-\pi l/2)} + e^{i(\rho+\delta_l-\pi l/2)}\right]$$

to see that, as a function of $\rho = kr$, the two expressions agree provided

$$\alpha_l = \delta_l$$

In other words, if we can figure out the integration constant α_l then we've found our sought-after phase shift.

The boundary condition imposed by the hard sphere is simply $R_l(a) = 0$. This tells us that

$$\cos\delta_l\, j_l(ka) = \sin\delta_l\, n_l(ka) \quad \Rightarrow \quad \tan\delta_l = \frac{j_l(ka)}{n_l(ka)}$$

This is the final result for this system. Now let's try to extract some physics from it.

First note that for the $l = 0$ s-wave, the phase shift is given by exactly by

$$\delta_0 = -ka$$

For small momenta, $ka \ll 1$, we can extract the behaviour of the higher l phase shifts from $\rho \to 0$ behaviour of the spherical Bessel functions (1.41). We have

$$\delta_l \approx -\frac{(ka)^{2l+1}}{(2l+1)!!\,(2l-1)!!}$$

We see that for low momentum the phase shifts decrease as l increases. This is to be expected: the higher l modes have to penetrate the repulsive angular momentum $\sim \hbar l(l+1)/r^2$. Classically, this would prohibit the low-momentum modes from reaching the sphere. Quantum mechanically, only the exponential tails of these modes reach $r = a$ which is why their scattering is suppressed.

For low momentum $ka \ll 1$, we now have all the information we need to compute the total cross-section. The sum (1.36) is dominated by the $l = 0$ s-wave, and given by

$$\sigma_T = 4\pi a^2\Big(1 + \mathcal{O}\left((ka)^4\right)\Big)$$

This is a factor of 4 bigger than the classical, geometric result (1.21)

It's also possible to extract analytic results for the phase shifts at high momentum $ka \gg 1$. For this we need further properties of the spherical Bessel functions. Here we simply state the results. The phase shifts δ_l vary between 0 and 2π for $l \lesssim ka$. However, when $l < ka$, the phase shifts quickly drop to zero. The intuition behind this follows from the semi-classical analysis (1.38) which tells us that for $l \gg ka$, the impact parameter is $b \gg a$. This makes it unsurprising that no scattering takes place in this regime. It turns out that as $ka \to \infty$, the total cross-section becomes $\sigma_T \to 2\pi^2 a^2$.

The Scattering Length

The low-momentum behaviour $\delta_l \sim (ka)^{2l+1}$ that we saw is common to all scattering potentials. It means that low-energy scattering is always dominated by the s-wave whose phase shift scales as

$$\delta_0 \sim -ka_s + \mathcal{O}(k^3) \tag{1.43}$$

The coefficients a_s is called the *scattering length*. As we have seen, for the hard sphere $a_s = a$, the radius of the sphere. At low energies, the total cross-section is always given by

$$\sigma_T \approx \sigma_0 = 4\pi a_s^2$$

The scattering length is a useful way to characterise the low-energy behaviour of a potential. As we will see in examples below, a_s can be positive or negative and can, at times, diverge.

1.2.6 Bound States

In this section we describe the effects of bound states on scattering. Such states only occur for attractive potentials, so we again take a sphere of radius a, but this time with potential

$$V(r) = \begin{cases} -V_0 & r < a \\ 0 & r > a \end{cases} \tag{1.44}$$

It will be useful to define the following notation

$$U(r) = \frac{2mV(r)}{\hbar^2} \quad \text{and} \quad \gamma^2 = \frac{2mV_0}{\hbar^2} \tag{1.45}$$

We'll start by focussing on the $l = 0$ s-wave. Outside the sphere, the wavefunction satisfies the usual free Schrödinger equation (1.27)

$$\left(\frac{d^2}{dr^2} + k^2\right)(r\psi) = 0 \qquad r > a$$

with general solution

$$\psi(r) = \frac{A\sin(kr+\delta_0)}{r} \qquad r > a \tag{1.46}$$

The same argument that we made when discussing the hard sphere shows that the integration constant δ_0 is the phase shift that we want to calculate. We do so by matching the solution to the wavefunction inside the sphere, which satisfies

$$\left(\frac{d^2}{dr^2} + k^2 + \gamma^2\right)(r\psi) = 0 \qquad r < a$$

The requirement that the wavefunction is regular at the origin $r = 0$ picks the solution inside the sphere to be

$$\psi(r) = \frac{B\sin(\sqrt{k^2+\gamma^2}\,r)}{r} \qquad r < a \tag{1.47}$$

The solutions (1.46) and (1.47) must be patched at $r = a$ by requiring that both $\psi(a)$ and $\psi'(a)$ are continuous. We get the answer quickest if we combine these two and insist that ψ'/ψ is continuous at $r = a$, since this condition does not depend on the uninteresting integration constants A and B. A quick calculation shows that it is satisfied when

$$\frac{\tan(ka+\delta_0)}{ka} = \frac{\tan(\sqrt{k^2+\gamma^2}\,a)}{\sqrt{k^2+\gamma^2}\,a} \tag{1.48}$$

For very high momentum scattering, $k^2 \gg \gamma^2$, we have $\delta_0 \to 0$. This is to be expected: the energy of the particle is so large that it doesn't much care for the small, puny potential and there is no scattering.

Bound States and the Scattering Length

Things are more interesting at low energies, $k^2 \ll \gamma^2$ and $ka \ll 1$. We have

$$\frac{\tan(ka+\delta_0)}{ka} \approx \frac{\tan(\gamma a)}{\gamma a} \quad \Rightarrow \quad \frac{\tan(ka)+\tan(\delta_0)}{1-\tan(ka)\tan(\delta_0)} \approx \frac{k}{\gamma}\tan(\gamma a)$$

Rearranging, we get

$$\tan\delta_0 = ka\left(\frac{\tan(\gamma a)}{\gamma a} - 1\right) + \mathcal{O}(k^3) \tag{1.49}$$

If the phase shift δ_0 is small, then we can write $\tan\delta_0 \approx \delta_0$ and, from (1.43), read off the scattering length

$$a_s = a - \frac{\tan(\gamma a)}{\gamma} \tag{1.50}$$

Note that, for this approximation to hold, we need $ka_s \ll 1$, but the scattering length a_s exhibits somewhat surprising behaviour. For small γ, the scattering length is negative. This can be thought of as due to the attractive nature of the potential, which pulls the particle into the scattering region rather than repelling it. However, as γ is increased, the scattering length diverges to $-\infty$, before reappearing at $+\infty$. It continues this pattern, oscillating between $+\infty$ and $-\infty$. Our task is to understand why this striking behaviour is happening.

Before we proceed, note that all the calculations above also hold for repulsive potentials with $V_0 < 0$. In this case γ, defined in (1.45) is pure imaginary and the scattering length (1.50) becomes

$$a_s = a - \frac{\tanh(|\gamma|a)}{|\gamma|} \qquad (V_0 < 0)$$

Now the scattering length is always positive. It increases monotonically from $a_s = 0$ when $\gamma = 0$, corresponding to no scattering, through to $a_s = a$ when $|\gamma| \to \infty$, which is our previous result for the hard-sphere. We see that whatever is causing the strange oscillations in (1.50) does not occur for the repulsive potential.

The key to the divergent behaviour of the scattering length lies in the bound states of the theory. It's a simple matter to construct $l = 0$ bound states. We solve the Schrödinger equation with the form

$$r\psi(r) = \begin{cases} A\sin(\sqrt{\gamma^2 - \lambda^2}\,r) & r < a \\ Be^{-\lambda r} & r > a \end{cases}$$

The two solutions have the same energy $E = -\hbar^2\lambda^2/2m$. Matching the logarithmic derivatives across $r = a$ gives

$$\tan(\sqrt{\gamma^2 - \lambda^2}\,a) = -\frac{\sqrt{\gamma^2 - \lambda^2}}{\lambda} \tag{1.51}$$

This structure of the solutions is similar to what we saw in Section 1.1.4. Indeed, if we write $q^2 = \gamma^2 - \lambda^2$, then these equations take the same form as (1.16) that describe odd-parity states in one-dimension. In particular, this means that if the potential is too shallow then no bound states exist. As γ gets larger, and the potential gets deeper, bound states start to appear. They first arise when $\lambda = 0$ and $\tan(\gamma a) = \infty$, so that

$$\gamma = \gamma_\star = \left(n + \frac{1}{2}\right)\frac{\pi}{a} \qquad \text{with} \qquad n = 0, 1, \ldots$$

This coincides with the values for which the scattering length (1.50) diverges. For γ slightly less than $\gamma_\star$, the bound state has not yet appeared and the scattering length is very large and negative. For γ slightly greater than $\gamma_\star$, the new state exists and is weakly bound, and the scattering length is large and positive. Meanwhile, when $\gamma = \gamma_\star$, then there is a bound state which has energy $E = 0$. Such bound states are said to be "*at threshold*".

The incoming wave has energy slightly above $E = 0$ and mixes strongly with the state with bound state – or almost bound state – with energy a little below $E = 0$. This is what gives rise to the divergence in the cross-section. Specifically, when there is a bound state exactly at threshold, $\tan\delta_0 \to \infty$ and so the phase shift is $\delta_0 = (n + \frac{1}{2})\pi$. (Note that at this point, we can no longer write $\delta_0 \approx -ka_s$ because a_s this is valid only for $ka_s \ll 1$, but a_s is diverging.) The s-wave cross-section saturates the unitarity bound (1.37)

$$\sigma_0 = \frac{4\pi}{k^2}$$

To understand why the formation of bound states gives rise to a divergent scattering length, we can look at the analytic structure of the S-matrix at finite k. We know from (1.48) that the phase shift is given by

$$\tan(ka + \delta_0) = \frac{k}{\sqrt{k^2 + \gamma^2}} \tan(\sqrt{k^2 + \gamma^2}a) \equiv f(k)$$

Rearranging, we get the s-wave component of the S-matrix

$$S_0(k) = e^{2i\delta_0} = e^{-2ika}\frac{1 + if(k)}{1 - if(k)}$$

The S-matrix has a pole at $f(k) = -i$, or for values of k such that

$$\tan(\sqrt{k^2 + \gamma^2}a) = \frac{\sqrt{k^2 + \gamma^2}}{ik} \tag{1.52}$$

This has no solutions for real k. However, it does have solutions along the positive imaginary k axis. If we set $k = i\lambda$, the equation (1.52) coincides with the condition for bound states (1.51).

Close to the pole, the S-matrix takes the form

$$S_0(k) = e^{2i\delta_0} = \frac{i\lambda + k}{i\lambda - k}$$

When the bound state approaches threshold, λ is small and this form is valid in the region $k = 0$. For $k \ll \lambda$, we can expand in k/λ to find $\delta_0 \approx -k/\lambda$, which tells us that we should indeed expect to see a divergent scattering length $a_s = 1/\lambda$.

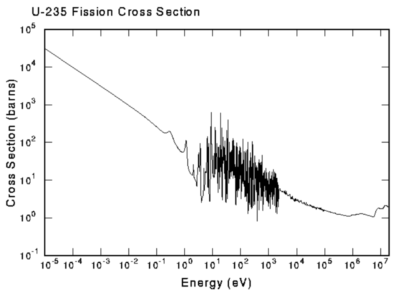


Figure 11: The cross-section for neutron scattering off U-235.

When neutrons scatter off large nuclei at low-energies they are very close to forming a threshold bound state. The total cross-section for neutron scattering off uranium 235 is shown in the figure[3]. You can see the large enhancement of the cross-section. This is partly due to the bound state, although it is complicated by the presence of a large number of resonances whose effects we'll discuss in the next section.

1.2.7 Resonances

We already met the idea of resonances in Section 1.1.5. These are unstable bound states, which appear as poles of the S-matrix in the lower-half complex plane. Here we see how these resonances affect scattering in 3d.

It's not hard to construct examples which exhibit resonances. Indeed, the attractive, spherical potential (1.44) which has bound states also exhibits resonances. These don't occur for s-waves, but only for higher l, where the effective potential includes an effective, repulsive angular momentum barrier. The algebra is not conceptually any more difficult than what we did above, but in practice rapidly becomes a blur of spherical Bessel functions.

Alternatively, we could look at the somewhat simpler example of a delta-function cage of the form $V(r) = V_0\delta(r-a)$, which is the obvious 3d generalisation of the example we looked at in Section 1.1.5 and has s-wave resonances.

Rather than getting bogged down in any of these details, here we focus on the features that are common to all these examples. In each case, the S-matrix has a pole. Thinking in terms of energy $E = \hbar^2k^2/2m$, these poles occur at

$$E = E_0 - \frac{i\Gamma}{2}$$

[3]The data is taken from the Los Alamos on-line nuclear information tour.

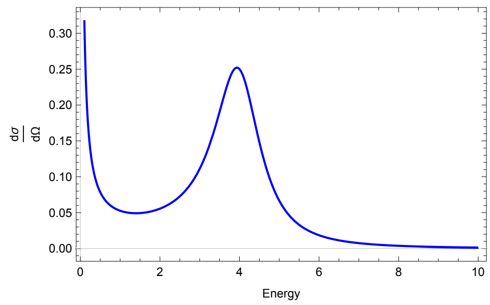


Figure 12: Distribution with $\Gamma^2 = 2$...

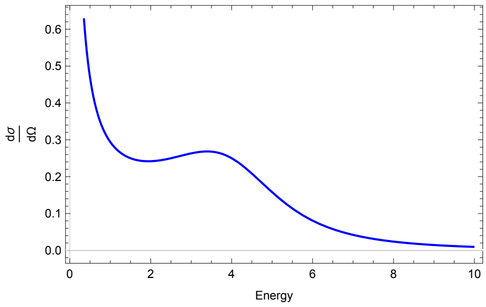


Figure 13: ...and with $\Gamma^2 = 15$

This is the same result (1.17) that we saw in our 1d example. Close to the pole, the S-matrix — which, by unitarity, is simply a phase — must take the form

$$S(E) = e^{2i\delta(E)} = e^{2i\theta(E)} \frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2} \tag{1.53}$$

Here $e^{2i\theta(E)}$ is the so-called continuum contribution; it is due to the usual, run-of-the-mill phase shift that arises from scattering off the potential. Here our interest is in the contributions that come specifically from the resonance, so we'll set $\theta = 0$. From (1.53), we have

$$\cos 2\delta = \frac{(E-E_0)^2 - \Gamma^2/4}{(E-E_0)^2 + \Gamma^2/4} \quad \Rightarrow \quad \sin^2\delta = \frac{\Gamma^2}{4(E-E_0)^2 + \Gamma^2}$$

From this we can read off the contribution to the total cross-section using (1.36). If the pole occurs for a partial wave with angular momentum l, we have

$$\sigma_T \approx \frac{4\pi}{k^2}(2l+1)\frac{\Gamma^2}{4(E-E_0)^2 + \Gamma^2}$$

This distribution is plotted in the figure, with $E_0 = 4$ and $\Gamma^2 = 2$ and 15. (Remember that there is an extra factor of E sitting in the k^2 in the formula above). It is called the *Breit-Wigner distribution*, or sometimes the *Lorentzian distribution* (although, strictly speaking, neither of these has the extra factor of $1/k^2$). It exhibits a clear peak at $E = E_0$, whose width is given by $\Gamma/2$. Comparing to our discussion in Section 1.1.5, we see that the lifetime of the resonance can be read off from the width of the peak: the narrower the peak, the longer lived the resonance.

The Breit-Wigner distribution is something of an iconic image in particle physics because this is the way that we discover new particles. To explain this fully would require us to move to the framework of quantum field theory, but we can get a sense

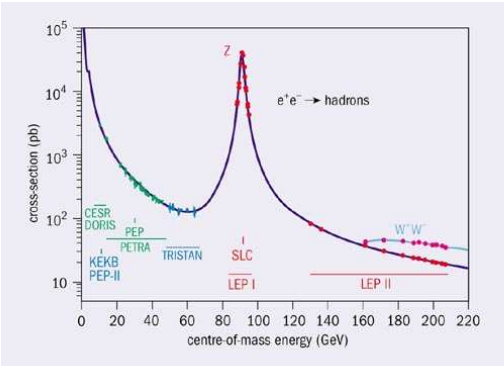


Figure 14: The cross-section for the Z-boson.

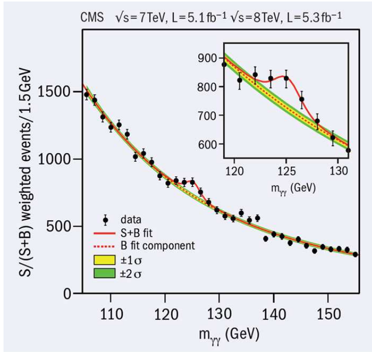


Figure 15: And for the Higgs boson.

for what's going on from what we've seen above. The key fact is that most particles in Nature are not stable. The exceptions are the electron, the proton, neutrinos and photons. All other decay with some lifetime τ. When we collide known particles — typically electrons or protons — we can create new particles which, since they are unstable, show up as resonances. The energy E_0 corresponds to the mass of the new particle through $E_0 = mc^2$, while the lifetime is seen in the width, $\tau = 1/\Gamma$.

Two examples are shown in the figures. The left-hand figure shows the cross-section, now measured in pico-barns $= 10^{-40}\ m^2$, for high-energy electron-positron scattering. We see a large resonance peak which sits at a centre of mass energy $E_0 \approx 91\ GeV$ with width $\Gamma \approx 2.5\ GeV$. Since we're measuring the width in unit of energy, we need a factor of $\hbar$ to convert to the lifetime

$$\tau = \frac{\hbar}{\Gamma}$$

Using $\hbar \approx 6.6 \times 10^{-16}\ eV$, we find the lifetime of the Z-boson to be $\tau \approx 3 \times 10^{-25}\ s$.

The right-hand figure shows the 2012 data from the discovery of the Higgs boson, with mass $E_0 \approx 125\ GeV$. I should confess that the experiment doesn't have the resolution to show the Breit-Wigner shape in this case. The best that can be extracted from this plot is a bound on the width of $\Gamma < 17\ MeV$ or so, while the true width is predicted by theory to be $\Gamma \sim 4\ MeV$.

1.3 The Lippmann-Schwinger Equation

So far, we've developed the machinery necessary to compute cross-sections, but our examples have been rather artificial. The interactions between particles do not look like spherical potential wells or shells of delta-functions. Instead, they are smooth potentials $V(r)$, such as the Coulomb or Yukawa potentials. We would like to understand scattering in these more realistic settings .

In principle, this is straightforward: you simply need to solve the relevant Schrödinger equation, impose regularity at the origin, and then read off the appropriate phase shifts asymptotically. In practice, the solution to the Schrödinger equation is rarely known analytically. (A counterexample to this is the Coulomb potential which will be discussed in Section 1.4.) In this section, we present a different approach to scattering that makes use of Green's functions. This provides a platform to develop a perturbative approach to understanding scattering for potentials that we actually care about. Moreover, these Green's functions methods also have applications in other areas of physics.

Our starting point is the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1.54}$$

We'll briefly use a more formal description of this equation, in order to write the Lippmann-Schwinger equation in its most general form. We'll then revert back to the form (1.54) which, for the purposes of these lectures, is all we really care about. With this in mind, we write the Schrödinger equation as

$$(H_0 + V)|\psi\rangle = E|\psi\rangle$$

The idea here is that we've split the Hamiltonian up into a piece that is simple to solve – in this case $H_0 = -\hbar^2\nabla^2/2m$ – and a more complicated piece, V. Trivially re-arranging this equation gives

$$(E - H_0)|\psi\rangle = V|\psi\rangle \tag{1.55}$$

We can then formally re-arrange this equation once more to become

$$|\psi\rangle = |\phi\rangle + \frac{1}{E - H_0}V|\psi\rangle \tag{1.56}$$

Here $|\phi\rangle$ is a zero mode which obeys $H_0|\phi\rangle = E|\phi\rangle$. If (1.56) is multiplied by $E - H_0$ then the state $|\phi\rangle$ is annihilated and we get back to (1.55). However, the inverse quantum operator $(E - H_0)^{-1}$ is somewhat subtle and, as we will see below, there is very often an ambiguity in its definition. This ambiguity is resolved by writing this inverse operator as $(E - H_0 + i\epsilon)^{-1}$, and subsequently taking the limit $\epsilon \to 0^+$. We then write

$$|\psi\rangle = |\phi\rangle + \frac{1}{E - H_0 + i\epsilon}V|\psi\rangle \tag{1.57}$$

This is the *Lippmann-Schwinger equation*. It is not really a solution to the Schrödinger equation (1.54) since $|\psi\rangle$ appears on both sides. It is more a rewriting of the Schrödinger equation, but one which gives us a new way to move forward.

The Green's Function

Let's now write down the Lippmann-Schwinger equation for our Schrödinger equation (1.54). We want the inverse operator $(E - H_0)^{-1}$. But this is precisely what we call the Green's function G_0. It obeys

$$\left(E + \frac{\hbar^2}{2m}\nabla^2\right) G_0(E;\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$$

The formulae will be somewhat simpler if we scale out the factor $\hbar^2/2m$. We write

$$E = \frac{\hbar^2 k^2}{2m}$$

so that

$$\left(\nabla^2 + k^2\right) G_0(k;\mathbf{r},\mathbf{r}') = \frac{2m}{\hbar^2}\delta(\mathbf{r}-\mathbf{r}') \tag{1.58}$$

We can solve for this Green's function using the Fourier transform. First, we note that translational invariance ensures that $G_0(k;\mathbf{r},\mathbf{r}') = G_0(k;\mathbf{r}-\mathbf{r}')$. Then we define the Fourier transform

$$\tilde{G}_0(k;\mathbf{q}) = \int d^3x\; e^{-i\mathbf{q}\cdot\mathbf{x}}\, G_0(k;\mathbf{x}) \quad \Rightarrow \quad G_0(k;\mathbf{x}) = \int \frac{d^3q}{(2\pi)^3}\; e^{i\mathbf{q}\cdot\mathbf{x}}\, \tilde{G}_0(k;\mathbf{q})$$

Plugging this into our formula (1.58), we have

$$(-q^2 + k^2)\tilde{G}(k;\mathbf{q}) = \frac{2m}{\hbar^2} \quad \Rightarrow \quad \tilde{G}_0(k;\mathbf{q}) = -\frac{2m}{\hbar^2}\frac{1}{q^2 - k^2}$$

So it's simple to get the Green's function in momentum space. Now we must invert it. We have

$$G_0(k;\mathbf{x}) = -\frac{2m}{\hbar^2}\int \frac{d^3q}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{q^2 - k^2}$$

Here we run into the ambiguity that we promised above. When we do the integral over $\mathbf{q}$, we run into a singularity whenever $q^2 = k^2$. To define the integral, when we integrate over $q = |\mathbf{q}|$, we should define a contour in the complex q plane which skips around the pole. We do this through the so-called "$i\epsilon$ prescription" which, as the name suggests, replaces the integral with

$$G_0^+(k;\mathbf{x}) = -\frac{2m}{\hbar^2}\int \frac{d^3q}{(2\pi)^3}\frac{e^{i\mathbf{q}\cdot\mathbf{x}}}{q^2 - k^2 - i\epsilon}$$

Where we subsequently take $\epsilon \to 0^+$. This shifts the pole slightly off the real q axis.

The simplest way to do this integral is to go to polar coordinates for the q variable. We have

$$\begin{aligned}
G_0^+(k;\mathbf{x}) &= -\frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos\theta)\int_0^\infty dq\ \frac{q^2\, e^{iqx\cos\theta}}{q^2-k^2-i\epsilon} \\
&= -\frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\int_0^\infty dq\ \frac{q}{ix}\frac{e^{iqx}-e^{-iqx}}{q^2-k^2-i\epsilon} \\
&= -\frac{2m}{\hbar^2}\frac{1}{(2\pi)^2}\frac{1}{ix}\int_{-\infty}^{\infty} dq\ \frac{qe^{iqx}}{(q-k-i\epsilon)(q+k+i\epsilon)}
\end{aligned}$$

where we're allowed to factorise the denominator in this way, with $k > 0$, only because we're ultimately taking $\epsilon \to 0^+$. We can now complete the derivation by contour integral. Since $x > 0$, we can complete the contour in the upper half-plane, picking up the residue from the pole at $q = k + i\epsilon$. This gives our final answer,

$$G_0^+(k;\mathbf{r}-\mathbf{r}') = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{+ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \qquad (1.59)$$

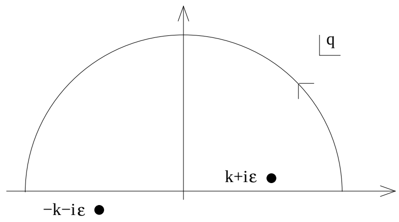


Figure 16:

Note that had we chosen to add $+i\epsilon$ rather than $-i\epsilon$ to the denominator, we would find the alternative Green's function $G_0^-(k;\mathbf{x}) \sim e^{-ikx}/4\pi x$. We will justify the choice of G_0^+ below.

Our Lippmann-Schwinger Equation

To finally write down the Lippmann-Schwinger equation, we need to determine the state $|\phi\rangle$ which is annihilated by $E - H_0$. But, for us, this is simply the plane wave solution

$$\phi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$$

We can now write the formal Lippmann-Schwinger equation (1.57) in more concrete form. It becomes

$$\psi(k;\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{\hbar^2}\int d^3r'\ \frac{e^{+ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\,V(\mathbf{r}')\psi(k;\mathbf{r}') \qquad (1.60)$$

It is simple to check that acting on this equation with the operator $(\nabla^2 + k^2)$ indeed brings us back to the original Schrödinger equation (1.54). The Lippmann-Schwinger equation is an integral equation, a reformulation of the more familiar Schrödinger differential equation. It is not solution to the Schrödinger equation because we still have to figure out what ψ is. We'll offer a strategy for doing this in Section 1.3.1.

The equation (1.60) has a very natural interpretation. The first term is simply the ingoing wave with momentum $\hbar\mathbf{k}$. The second term is the scattered wave. Note that the factor $e^{ik|\mathbf{r}-\mathbf{r}'|}$ tells us that this wave is moving outwards from the point $\mathbf{r}'$. Had we instead chosen the Green's function G_0^-, we would have found a wave moving inwards from infinity of the form $e^{-ik|\mathbf{r}-\mathbf{r}'|}$. This is unphysical. This is the reason that we pick the $-i\epsilon$ prescription rather than $+i\epsilon$.

To make contact with our earlier discussion of scattering, we look at the asymptotic form of this outgoing wave at $r \to \infty$. For this to work, we'll assume that $V(r')$ has support only in some finite region. We can then take the limit $r \gg r'$ and expand

$$|\mathbf{r}-\mathbf{r}'| = \sqrt{r^2 - 2\mathbf{r}\cdot\mathbf{r}' + r'^2} \approx r - \frac{\mathbf{r}\cdot\mathbf{r}'}{r}$$

With $V(\mathbf{r}')$ localised within some region, it makes sense to perform this expansion inside the integral. In this approximation the Green's function (1.59) can be written as

$$G_0^+(k;\mathbf{r}-\mathbf{r}') \approx -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{+ikr}}{r}e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}$$

and the Lippmann-Schwinger equation then becomes

$$\psi(k;\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\left[\int d^3r'\; e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(\mathbf{r}')\psi(k;\mathbf{r}')\right]\frac{e^{ikr}}{r}$$

Although we derived this by assuming that $V(\mathbf{r})$ has compact support, we can actually be a little more relaxed about this. The same result holds if we require that $V(r') \to 0$ suitably quickly as $r' \to \infty$. Any potential which falls off exponentially, or as a power-law $V(r) \sim 1/r^n$ with $n \geq 2$, can be treated in this way. Note, however, that this excludes the Coulomb potential. We will deal with this separately in Section 1.4.

If we set the ingoing wave to be along the z-axis, $\mathbf{k} = k\hat{\mathbf{z}}$, then this takes the asymptotic form (1.25) that we discussed previously

$$\psi(\mathbf{r}) \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r} \tag{1.61}$$

The upshot of this analysis is that we identify the scattering amplitude as

$$f(\theta,\phi) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\int d^3r'\; e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'}V(\mathbf{r}')\psi(k;\mathbf{r}')$$

where θ and ϕ are the usual polar angles such that $\hat{\mathbf{r}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. This gives a simple way to compute the scattering amplitude, but only if we already know the form of the wavefunction $\psi(\mathbf{r}')$ in the scattering region where $V(\mathbf{r}') \neq 0$. Our next task is to figure out how to compute $\psi(\mathbf{r}')$.

An Equation for Bound States

Above we've focussed on scattering states with energy $E = \hbar^2 k^2/2m > 0$. However, it is not difficult to repeat everything for bound states with energy $E = -\hbar^2\lambda^2/2m$. Indeed, in this case there is no ambiguity in the definition of the Green's function. We find that bound states must obey the integral equation

$$\psi(\mathbf{r}) = \frac{2m}{\hbar^2}\int d^3r' \frac{e^{-\lambda|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\,V(\mathbf{r}')\psi(\mathbf{r}')$$

We won't attempt to solve this equation; instead our interest will focus on the Lippmann-Schwinger equation for scattering states (1.60).

1.3.1 The Born Approximation

In this section we describe a perturbative solution to the Lippmann-Schwinger equation,

$$\psi(k;\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \int d^3r'\; G_0^+(k;\mathbf{r}-\mathbf{r}')\,V(\mathbf{r}')\psi(k;\mathbf{r}') \tag{1.62}$$

This solution is known as the *Born series*.

We write ψ as a series expansion

$$\psi(\mathbf{r}) = \sum_{n=0}^{\infty}\phi_n(\mathbf{r}) \tag{1.63}$$

where we take the leading term to be the plane wave

$$\phi_0(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}$$

This series solves (1.62) if the ϕ_n obey the recursion relation

$$\phi_{n+1}(\mathbf{r}) = \int d^3r'\; G_0^+(k;\mathbf{r}-\mathbf{r}')\,V(\mathbf{r}')\phi_n(\mathbf{r}')$$

We will not be very precise here about the convergent properties of this series. Roughly speaking, things will work nicely if the potential V is small, so each successive term is smaller than those preceding it.

The *Born approximation* consists of taking just the leading order term ϕ_1 in this expansion. (Strictly speaking this is the first Born approximation; the n^{th} Born approximation consists of truncating the series at the n^{th} term.) This is

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{\hbar^2}\frac{1}{4\pi}\left[\int d^3r'\; e^{i\mathbf{q}\cdot\mathbf{r}'}\,V(\mathbf{r}')\right]\frac{e^{ikr}}{r} \tag{1.64}$$

where

$$\mathbf{q} = \mathbf{k} - k\hat{\mathbf{r}}$$

can be thought of as the momentum transferred from the incoming wave to the outgoing wave. With this in mind, it's traditional to define the momentum of the outgoing wave to be

$$\mathbf{k}' = k\hat{\mathbf{r}}$$

so that $\mathbf{q} = \mathbf{k} - \mathbf{k}'$. Comparing the Born approximation (1.64) to the asymptotic form (1.61), we see that the scattering amplitude is simply the Fourier transform of the potential,

$$f(\theta, \phi) \approx f_0(\theta, \phi) = -\frac{2m}{\hbar^2}\frac{1}{4\pi}\left[\int d^3r' \; e^{i\mathbf{q}\cdot\mathbf{r}'}\; V(\mathbf{r}')\right] \equiv -\frac{m}{2\pi\hbar^2}\tilde{V}(\mathbf{q})$$

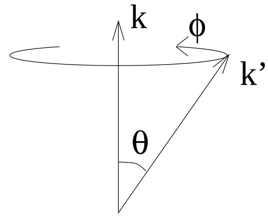


Figure 17:

Note that the scattering amplitude is a function of θ and ϕ, but these variables are somewhat hidden on the notation of the right-hand side. They're sitting in the definition of $\mathbf{q}$, with $\mathbf{k}\cdot\mathbf{k}' = k^2\cos\theta$, and the variable ϕ determining the relative orientation as shown in the figure. As we've seen before, for a central potential $V(\mathbf{r}) = V(r)$, the resulting scattering amplitude will be independent of ϕ. Because the angular variables are somewhat disguised, the scattering amplitude is sometimes written as $f(\mathbf{k}, \mathbf{k}')$ instead of $f(\theta, \phi)$. Indeed, we'll adopt this notation in Section 3.4.

Finally, the cross-section in the Born approximation is simply

$$\frac{d\sigma}{d\Omega} \approx |f_0|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 |\tilde{V}(\mathbf{q})|^2 \tag{1.65}$$

There's some physics in this simple formula. Suppose that your potential has some short-distance structure on scales $\sim L$. Then the Fourier transform $\tilde{V}(\mathbf{q})$ is only sensitive to this when the momentum transfer is of order $q \sim 1/L$. This is a manifestation of the uncertainty principle: if you want to probe short distance physics, you need high momentum transfer.

1.3.2 The Yukawa Potential and the Coulomb Potential

At long distances, the strong nuclear force between, say, a proton and a neutron is well modelled by the Yukawa potential

$$V(r) = \frac{Ae^{-\mu r}}{r}$$

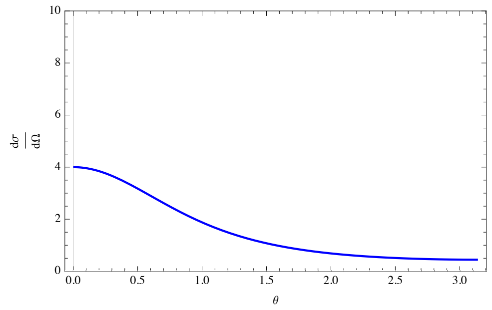


Figure 18: The cross-section for the Yukawa potential...

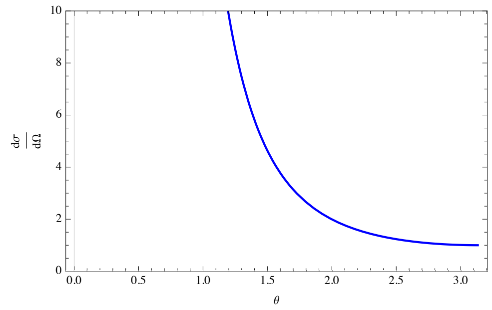


Figure 19: ...and for the Coulomb potential.

where $1/\mu$ is said to be the *range of the force*. We can compute the Fourier transform using the same kind of contour methods that we used in the previous section. We have

$$\tilde{V}(\mathbf{q}) = \frac{4\pi A}{q^2 + \mu^2}$$

Writing this in terms of the scattering angle θ, we recall that $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ with $\mathbf{k}' = k\hat{\mathbf{r}}$, so that

$$q^2 = 2k^2 - 2\mathbf{k}\cdot\mathbf{k}' = 2k^2(1-\cos\theta) = 4k^2\sin^2(\theta/2)$$

If we translate from momentum k to energy $E = \hbar^2 k^2/2m$, then from (1.65), we have the leading order contribution to the cross-section for the Yukawa potential given by

$$\frac{d\sigma}{d\Omega} = \left(\frac{2Am}{\hbar^2\mu^2 + 8mE\sin^2(\theta/2)}\right)^2 \tag{1.66}$$

This is shown in the left-hand figure (for values $A = m = \hbar\mu = 1$ and $E = 1/4$).

An Attempt at Rutherford Scattering

It's tempting to look at what happens when $\mu \to 0$, so that the Yukawa force becomes the Coulomb force. For example, for electron-electron or proton-proton scattering, the strength of the Coulomb force is $A = e^2/4\pi\epsilon_0$. In this case, the cross-section (1.66) becomes,

$$\frac{d\sigma}{d\Omega} = \left(\frac{A}{4E}\right)^2 \frac{1}{\sin^4(\theta/2)} \tag{1.67}$$

This is shown in the right-hand figure (with the same values). Note that there is an enhancement of the cross-section at all scattering angles, but a divergence at forward scattering.

Rather remarkably, the quantum result (1.67) agrees with the classical cross-section that we found in (1.22)! This is a surprise and is special to the Coulomb potential. Rutherford was certainly a great scientist but, like many other great scientists before him, he had his fair share of luck.

In fact, Rutherford's luck ran deeper than you might think. It turns out that the Born approximation is valid for the Yukawa potential in certain regimes, but is never valid for the Coulomb potential! The difficulty stems from the long range nature of the Coulomb force which means that the plane wave solutions $\phi_0 \sim e^{i\mathbf{k}\cdot\mathbf{r}}$ are never really good approximations to the asymptotic states. We will describe the correct treatment of the Coulomb potential in Section 1.4 where we will see that, although our approximation wasn't valid, the result (1.67) is correct after all.

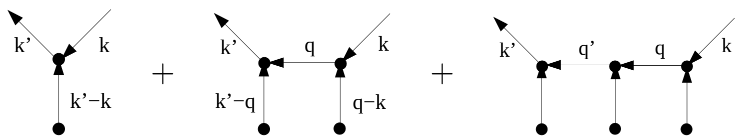
1.3.3 The Born Expansion

One can continue the Born expansion to higher orders. In compressed notation, the solution (1.63) takes the form

$$\psi = \phi_0 + \int G_0^+ V\phi_0 + \int\int G_0^+ V G_0^+ V\phi_0 + \int\int\int G_0^+ V G_0^+ V G_0^+ V\phi_0 + \ldots$$

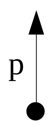
This has a natural interpretation. The first term describes the incident plane wave which doesn't scatter at all. The second term describes the wave scattering once of the potential, before propagating by G_0^+ to the asymptotic regime. The third term describes the wave scattering off the potential, propagating some distance by G_0^+ and then scattering for a second time before leaving the region with the potential. In general, the term with n copies of V should be thought of as the wave scattering n times from the potential region.

There's a useful diagrammatic way to write the resulting scattering amplitude. It is given by

$f(\mathbf{k},\mathbf{k}') =$ 

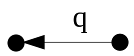
$+ \ldots$

Each diagram is shorthand for an integral. Every black dot describes an insertion



$= \tilde{U}(\mathbf{p})$

while each line describes an insertion of



$$= \frac{-1}{q^2 - k^2 + i\epsilon}$$

Meanwhile, for each internal line we include the integral

$$-\frac{1}{4\pi}\int \frac{d^3q}{(2\pi)^3}$$

Although we're dealing with wave scattering, it's tempting to think of the lines as describing the trajectory of a particle. Indeed, this diagrammatic picture is a precursor to Feynman diagrams that occur in quantum field theory, where there's a much closer connection to the underlying particles.

1.4 Rutherford Scattering

Historically, some of the most important scattering problems in particle physics involved the Coulomb potential. This is the problem of Rutherford scattering. Yet, as we mentioned above, none of the techniques that we've mentioned so far are valid for the Coulomb potential. This is mitigated somewhat by the fact that we get the right answer whether we work classically (1.22) or using the Born approximation (1.67). Nonetheless, this is a little unsatisfactory. After all, how do we know that this is the right answer!

Here we show how to do Rutherford scattering properly. We want to solve the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{A}{r}\right)\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

where $A > 0$ for repulsive interactions and $A < 0$ for attractive interactions. It will prove useful to rewrite this as

$$\left(\nabla^2 + k^2 - \frac{2\gamma k}{r}\right)\psi(\mathbf{r}) = 0 \tag{1.68}$$

where, as usual, $E = \hbar^2k^2/2m$ while $\gamma = mA/\hbar^2 k$ is a dimensional parameter which characterises the strength of the Coulomb force.

The Asymptotic Form of the Wavefunction

Let's start by understanding what the wavefunctions look like asymptotically. Repeating the analysis of Section 1.2.3, the radial wavefunction $R_l(r)$ satisfies

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + k^2 - \frac{l(l+1)}{r^2} - \frac{2\gamma k}{r}\right)R_l(r) = 0$$

Already here we can see what the issue is. At large distances, $r \to \infty$, the Coulomb force is more important than the angular momentum barrier. We saw in previous sections that when $\gamma = 0$, the asymptotic form of the wavefunction is given by $R_l(r) = e^{\pm ikr}/r$ regardless of the value of l. However, when $\gamma \neq 0$ we have to revisit this conclusion.

With the previous solution in mind, we will look for solutions which asymptotically take the form

$$R_l(r) \sim \frac{e^{\pm ikr + g(r)}}{r}$$

for some function $g(r)$. Inserting this ansatz, we find that $g(r)$ must satisfy

$$\frac{d^2 g}{dr^2} + \left(\frac{dg}{dr}\right)^2 \pm 2ik\frac{dg}{dr} = \frac{2\gamma k}{r}$$

But, for now, we care only about the asymptotic expression where the left-hand side is dominated by the last term. We then have

$$\pm i\frac{dg}{dr} = \frac{\gamma}{r} \quad \text{as} \quad r \to \infty$$

which is solved, up to some constant, by $g = \mp i\gamma \log(kr)$. Clearly this diverges as $r \to \infty$ and so should be included in te asymptotic form. We learn that asymptotically the radial wavefunctions take the form

$$R_l(r) \sim \frac{e^{\pm i(kr - \gamma \log(kr))}}{r}$$

This extra logarithm in the phase of the wavefunction means that the whole framework we described previously needs adjusting.

Note that this same analysis tells us that our previous formalism for scattering works fine for any potential $V(r) \sim 1/r^n$ with $n \geq 2$. It is just the long-range Coulomb potential that needs special treatment.

1.4.1 The Scattering Amplitude

To compute the amplitude for Rutherford scattering, we don't need any new conceptual ideas. But we do need to invoke some technical results about special functions. This is because the solution to the Schrödinger equation (1.68) can be written as

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} e^{-\pi\gamma/2}\Gamma(1 + i\gamma)\, {}_1F_1\big(-i\gamma;\, 1;\, i(kr - \mathbf{k}\cdot\mathbf{r})\big)$$

where ${}_1F_1\big(a;b;w\big)$ is the confluent hypergeometric function, defined by the series expansion

$$
{}_1F_1\big(a;b;w\big) = 1 + \frac{a}{b}w + \frac{a(a+1)}{b(b+1)}\frac{w^2}{2!} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{w^3}{3!} + \ldots
$$

We won't prove that this is a solution to the Schrödinger equation. Moreover, the only fact we'll need about the hypergeometric function is its expansion for large $|w|$. For our solution, this is an expansion in $1/(kr - \mathbf{k}\cdot\mathbf{r})$ and so is valid at large distance, but not along the direction of the incident beam $\mathbf{k}$. If we take $\mathbf{k} = k\hat{\mathbf{z}}$, we have

$$
\psi(\mathbf{r}) \sim e^{ikz+i\gamma\log(k(r-z))} - \frac{\gamma}{k(r-z)}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}e^{ikr-i\gamma\log(k(r-z))} + \ldots
$$

where the $+\ldots$ are corrections to both terms which are suppressed by $1/k(r-z)$. This is now very similar to our usual asymptotic form (1.61), but with the corrected phases. The first term describes the ingoing wave, the second term the scattered outgoing wave. We can therefore write

$$
\psi(\mathbf{r}) \sim e^{ikz+i\gamma\log(k(r-z))} + f(\theta)\,\frac{e^{ikz-i\gamma\log(k(r-z))}}{r}
$$

where the scattering amplitude is given by

$$
f(\theta) = -\frac{\gamma}{k}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\frac{r}{r-z} = -\frac{\gamma}{2k}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\frac{1}{\sin^2(\theta/2)} \tag{1.69}
$$

We learn that the cross-section is

$$
\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \left(\frac{mA}{2\hbar^2k^2}\right)^2\frac{1}{\sin^4(\theta/2)}
$$

This is the same result as we saw using the invalid Born approximation (1.67) and the same result that we saw from a classical analysis (1.22). This shouldn't give you the wrong idea. In most situations if you use the wrong method you will get the wrong answer! The Coulomb potential is an exception.

Recovering the Hydrogen Atom

There's a rather nice exercise we can do with the scattering amplitude (1.69). When $\gamma < 0$, the Coulomb potential is attractive and has bound states. Moreover, these bound states are simply those of the hydrogen atom that we met in our first course on quantum mechanics. From our earlier analysis, we should be able to recover this from the poles in the scattering amplitude.

These arise from the gamma function $\Gamma(z)$ which has no zeros, but has poles at $z = 0, -1, -2, \ldots$. The scattering amplitude therefore has poles when

$$1 + i\gamma = -(n-1) \quad \Rightarrow \quad k = -i\,\frac{mA}{\hbar^2}\frac{1}{n} \qquad \text{with } \ n = 1, 2, 3, \ldots$$

For an attractive potential with $A < 0$, these poles lie along the positive imaginary k-axis, as they should. We see that they correspond to bound states with energy

$$E_n = \frac{\hbar^2 k^2}{2m} = -\frac{mA^2}{2\hbar^2}\frac{1}{n^2}$$

This, of course, is the familiar spectrum of the hydrogen atom.