Chapter 11

One Dimensional Scattering

We have spent most of our time in this course discussing normalisable stationary states, their properties, and the methods used to calculate them. In the application of quantum theory to the real world, there is another large and important subject that has something of a different flavour: the theory of *scattering*.

The basic formulation of the problem is as follows: we imagine that there is some "stuff" that is localised in space, and we want to predict what will happen if we throw some probe particle at the stuff. (Alternatively, one might be interested in observing the result of such throwing-a-particle-at-stuff experiments and reconstructing a microscopic model of the stuff. This is referred to as an *inverse scattering problem*.) The scattering problem arises in both classical dynamics and in quantum mechanics, but of course here we consider the quantum version. In this case one wants to assess the *probability amplitude* for various configurations of outgoing scattered particles.

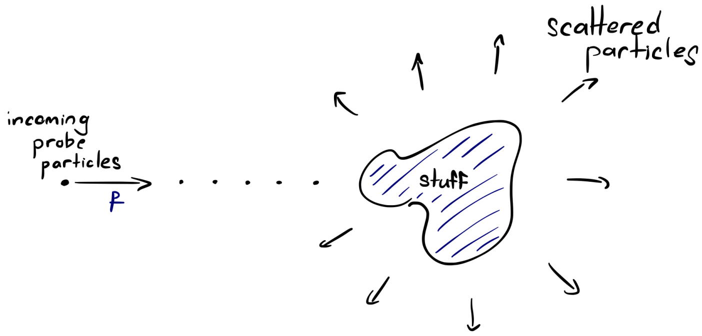

Figure 6. Cartoon representation of a scattering problem.

In the classical setting, we would specify the asymptotic trajectory (say, momentum and impact parameter) of the incoming probe particle in the far past (as you will recall from your study of hyperbolic orbits in the Kepler problem in prelims Dynamics) and predict the subsequent trajectory and, in particular, the late-time trajectory when the particle escapes back to infinity.

In the quantum mechanical setting, there is some subtlety in how we realise this intuitive scattering question within our mathematical formalism. The general treatment is quite technical. In this chapter we consider a simplified version of the story, where space is one-dimensional.

11.1 Left-right asymmetric scattering

We consider a situation as depicted in Figure 7, where the potential takes constant values outside of a bounded *interaction region*. The idea is then that particles will propagate freely in the L and R regions, so we can consider particles incident from (say) the left and ask for the amplitude for them to be either reflected back to the left or transmitted through the interaction region out to the right.

To really model the process described above, we would need to perform a time-dependent analysis in which our initial state is a kind of a wave packet localised in the L region and moving to the right, and then we would ask for the late time behaviour of that state. This would require a more involved investigation than we want to pursue for now. Fortunately, it turns out that we can treat this as a time *independent* problem. We consider (generalised) energy eigenstates with

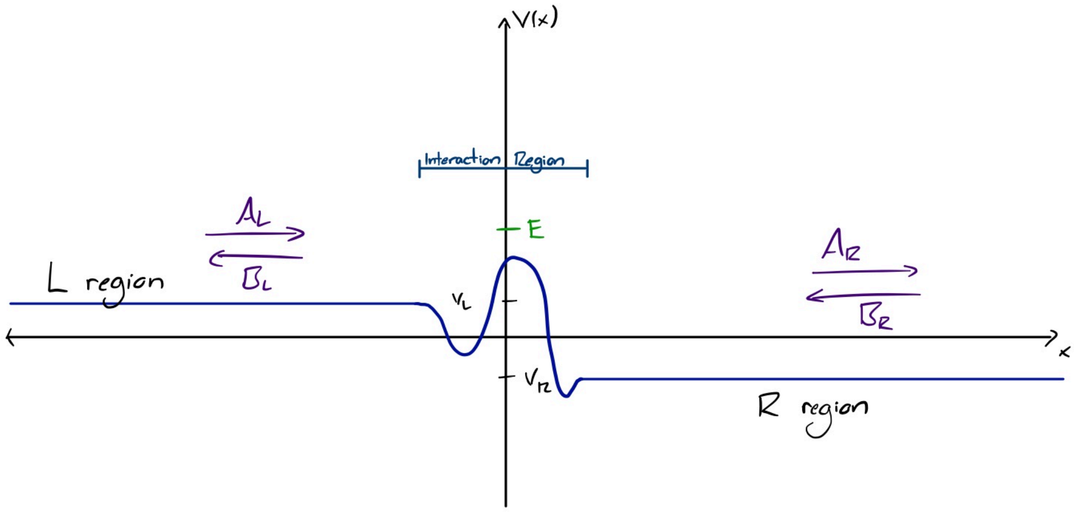

Figure 7. One-dimensional scattering with a localised interaction region.

energy $E > V_{L,R}$, which will necessarily look like plane waves in the L and R regions,

$$\begin{aligned} &\text{for } x \in L\,, \quad \psi(x) = \psi_L(x) = A_L e^{ik_L x} + B_L e^{-ik_L x}\,, \qquad \hbar k_L = p_L\,, \qquad \frac{p_L^2}{2m} = E - V_L\,, \\ &\text{for } x \in R\,, \quad \psi(x) = \psi_R(x) = A_R e^{ik_R x} + B_R e^{-ik_R x}\,, \qquad \hbar k_R = p_R\,, \qquad \frac{p_R^2}{2m} = E - V_R\,. \end{aligned} \tag{11.1}$$

The $A_{L,R}$ terms correspond to the particle having positive momentum, while the $B_{L,R}$ terms describe negative momentum. In the "interaction region" the potential is nontrivial, and it may be difficult to produce an exact expression for the stationary state wave functions there, but on general grounds as the solutions to the time-independent Schrödinger equation we know there will be a two-dimensional space of such wave functions at fixed energy that will interpolate between the plane wave behaviour to the left and the right. Matching onto the solutions in the L and R regions, the detailed form of these solutions will give rise to a linear relationship between the coefficients (A_L, B_L) and (A_R, B_R), which we encode in a (energy-dependent) matrix M,

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = M \begin{pmatrix} A_R \\ B_R \end{pmatrix}\,. \tag{11.2}$$

Here we will focus on the case of *scattering from the left*, which we encode by setting $B_R = 0$, as a nonzero value for B_R would be interpreted as indicating some nonzero probability for the particle to be *arriving* from the right. In this case, we define the following physically important quantities.

Definition 11.1.1. The *reflection coefficient* R and the *transmission coefficient* T are defined (as functions of energy) for one-dimensional scattering according to

$$R = \frac{|B_L|^2}{|A_L|^2}\,, \qquad T = \frac{k_R|A_R|^2}{k_L|A_L|^2}\,. \tag{11.3}$$

These coefficients obey an important conservation condition related to their probabilistic interpretation.

Proposition 11.1.2. The reflection and transmission coefficients are related according to

$$R + T = 1\,. \tag{11.4}$$

We interpret R as the probability that a particle incident from the left with energy E will be reflected off of the potential, and T to be the probability that the particle is transmitted through the potential.

Proof. The simple relation follows from the probability conservation condition for stationary states, which in one dimension reads as§

$$\partial_x j(x) = 0 \,, \qquad j(x) = \frac{\hbar}{2mi}\left(\overline{\psi(x)}\partial_x\psi(x) - \psi(x)\partial_x\overline{\psi}(x)\right) \,. \tag{11.5}$$

You have encountered this conservation rule in your **A11 Quantum Theory**, and it follows as an immediate consequence of the time-independent Schrödinger equation. Applying this condition to stationary *scattering states* as above, we have

$$j(x) = \begin{cases} \frac{p_L}{m}|A_L|^2 - \frac{p_L}{m}|B_L|^2 \,, & x \in L \,, \\ \frac{p_R}{m}|A_R|^2 - \frac{p_R}{m}|B_R|^2 \,, & x \in R \,. \end{cases} \tag{11.6}$$

Conservation of the probability current then equates the value of $j(x)$ on either side of the interaction region and gives

$$\frac{p_L}{m}|A_L|^2 + \frac{p_R}{m}|B_R|^2 = \frac{p_L}{m}|B_L|^2 + \frac{p_R}{m}|A_R|^2 \,. \tag{11.7}$$

setting $B_R = 0$ and dividing through by the left hand side gives $R + T = 1$. ■

Remark 11.1.3. Equation (11.7) is often understood in slightly different terms by making a somewhat different (and non-canonical) interpretation of these generalised energy eigenstates. If we say that a wave function of the form

$$\psi(x) = Ae^{\frac{ipx}{\hbar}} \,, \tag{11.8}$$

describes an *ensemble of particles* (sometimes people say a *beam of particles*) travelling with momentum p and density $|A|^2$, then the flow rate of these particles will be given by $\frac{p}{m}|A|^2$. In these terms, our probability current j is reinterpreted as an actual flow rate of particles, and the conservation rule becomes a conservation condition for the number of particles in a given region in a steady state: the rate of particles entering into the interaction region (left hand side) is equal to the rate of particles exiting (right hand side).

Remark 11.1.4. It is a remarkable (and not all that obvious) fact that the time-independent analysis given here is sufficient to make predictions about what happens in a more physical scattering setup when one starts with a wave packet approaching the interaction region from the left. The idea is that one can decompose a wave packet in, say, the L region in terms of the scattering states (rather than the usual plane waves of Fourier analysis), and then the time evolution of the wave packet will proceed analogously to what we saw in our discussion of the propagator in Chapter 2. Because the scattering states know about the structure of the interaction region, as the wave packet evolves the it will arrive from the left at the interaction region, do something in the interaction region, and ultimately there will be a reflected and a transmitted wave packet emitted to the left and right, respectively. Importantly, the relative amplitudes will be controlled by R and T (up to the issue of there being a spread of energies in the wave packet, but if the experiment is repeated many times then the law of large numbers dictates that R and T will control the average behaviour, which justifies the "ensemble of particles" interpretation to some extent). A careful analysis of this story goes well beyond our treatment here, but the important conclusion is that this time-independent analysis captures the real physics of the situation!

11.2 Local potential scattering and the S matrix

To have a one-dimensional analogue of higher-dimensional scattering off of a localised potential, it is natural to impose that $V_L = V_R$. (In higher dimensions, if the potential is localised in one region then you can go *around* the potential and so the asymptotic value of the potential should be the same in every direction.) In this case, the conservation condition takes the even nicer form

$$|A_L|^2 + |B_R|^2 = |B_L|^2 + |A_R|^2 \,. \tag{11.9}$$

From a physical point of view (rather than that of solving ODEs), we should be inclined to think of the problem as being that of determining B_R and A_L (the amplitudes of the outgoing parts of the wave function) given A_L and B_R (the amplitudes of the incident parts of the wave function). As long as the upper left-hand component M_{11} of the matrix M, we can find such a relation,

$$\begin{pmatrix} A_R \\ B_L \end{pmatrix} = S\begin{pmatrix} A_L \\ B_R \end{pmatrix} \,, \qquad S = \begin{pmatrix} \frac{1}{M_{11}} & -\frac{M_{12}}{M_{11}} \\ \frac{M_{21}}{M_{11}} & \frac{\det M}{M_{11}} \end{pmatrix} \,. \tag{11.10}$$

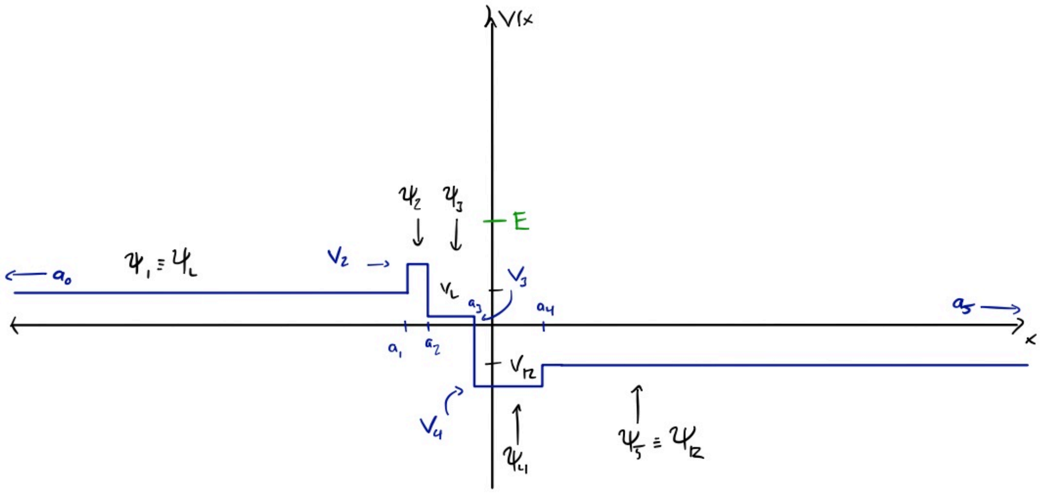

Figure 8. Scattering off of a piecewise constant potential.

By virtue of (11.9), the matrix S is a norm-preserving endomorphism of $\mathbb{C}^2$ and so a *unitary* 2×2 matrix. Indeed, this is a baby version an important object, the *unitary S-matrix*, which encodes the relationship between incoming and outgoing scattering wavefunctions. (This is an object of significant importance in relativistic quantum field theory and high energy particle physics, where scattering experiments are the main tool of the trade.)

We can then recognise the R and T coefficients in terms of the S matrix coefficients,

$$T = |S_{11}|^2 , \qquad R = |S_{21}|^2 , \tag{11.11}$$

and the condition $R + T = 1$ is a simple consequence of unitarity of S.

Remark 11.2.1. We specialised to scattering from the left, but we could also consider scattering from the right, in which case $A_L = 0$. Then the corresponding reflection and transmission coefficients would be given by $T_{\text{right}} = |S_{22}|^2$ and $R_{\text{right}} = |S_{12}|^2$, which obey an analogous conservation condition.

11.3 Piecewise constant potentials

A (somewhat contrived) class of examples that can be solved exactly, and consequently form a nice test environment for our methods, are the *piecewise constant* potentials (see Figure 8). For these we have a set of junction points $-\infty = a_0 < a_1 < \cdots < a_{n-1} < a_n = \infty$ and set

$$V(x) = V_i , \quad x \in (a_{i-1}, a_i) , \tag{11.12}$$

where in these conventions we have $V_L = V_0$ and $V_R = V_n$. Then our wave function will be piecewise a linear combination of plane waves or exponentials,

$$\psi(x) = \psi_i(x) = A_j e^{ik_j x} + B_j e^{-ik_j x} , \qquad x \in [a_{j-1}, a_j] . \tag{11.13}$$

(If in some region we have $E < V_j$, then we will define $k_j = i\mu_j$ with $\mu_j > 0$. Then the plane wave $e^{ik_j x}$ becomes a decaying exponential $e^{-\mu_j x}$ while $e^{-ik_j x}$ becomes a growing exponential $e^{\mu_j x}$.)

The boundary conditions (continuity of ψ and ψ') at $x = a_i$ require

$$\begin{aligned} \psi_j(a_j) = \psi_{j+1}(a_j) \;&\Rightarrow \qquad A_j \mathrm{e}^{ik_j a_j} + B_j \mathrm{e}^{-ik_j a_j} = A_{j+1} \mathrm{e}^{ik_{j+1} a_j} + B_{j+1} \mathrm{e}^{-ik_{j+1} a_j} , \\ \psi'_j(a_j) = \psi'_{j+1}(a_j) \;&\Rightarrow \; k_j \left(A_j \mathrm{e}^{ik_j a_j} - B_j \mathrm{e}^{-ik_j a_j} \right) = k_{j+1} \left(A_{j+1} \mathrm{e}^{ik_{j+1} a_j} - B_{j+1} \mathrm{e}^{-ik_{j+1} a_j} \right) , \end{aligned} \tag{11.14}$$

and this condition can be solved to express the coefficients (A_j, B_j) in terms of (A_{j+1}, B_{j+1}). We encode the relation in a matrix M_j:

$$M_j = \frac{1}{2k_j}\begin{pmatrix} s_j e^{-id_j a_j} & d_j e^{-is_j a_j} \\ d_j e^{is_j a_j} & s_j e^{id_j a_j} \end{pmatrix} , \qquad s_j = k_j + k_{j+1} , \quad d_j = k_j - k_{j+1} . \tag{11.15}$$

We then have for our total scattering process, $M = M_1 M_2 \cdots M_{n-1}$

Example 11.3.1 (Single barrier scattering and tunnelling)**.** The simplest case of a piecewise constant scattering problem is that of scattering off of a rectangular barrier. In this case there are just two junction points, and as in Figure 9, for ease of notation we will set $a_1 = 0$, $a_2 = a$, $V_L = V_R = 0$, $V_1 = V$. For scattering from the left (in which case $B_R = 0$) we can write

$$\begin{pmatrix} A_L \\ B_L \end{pmatrix} = M_1 M_2 \begin{pmatrix} A_R \\ 0 \end{pmatrix} , \tag{11.16}$$

So ultimately we are interested in the left-hand column of the M matrix. Now specialising our general expression for the matrices M_j to our case, we have

$$M_1 = \frac{1}{2k}\begin{pmatrix} s & d \\ d & s \end{pmatrix} , \quad M_i = \frac{1}{2k'}\begin{pmatrix} se^{ida} & -de^{-isa} \\ -de^{isa} & se^{-ida} \end{pmatrix} , \quad s = k + k' , \quad d = k - k' , \tag{11.17}$$

which when composed gives us

$$M = \frac{1}{s^2 - d^2}\begin{pmatrix} s^2 e^{ida} - d^2 e^{isa} & sd(e^{-ida} - e^{-isa}) \\ sd(e^{ida} - e^{isa}) & s^2 e^{-ida} - d^2 e^{-isa} \end{pmatrix} . \tag{11.18}$$

With some massaging we compute the full S matrix, which is given by

$$\begin{aligned} S &= \frac{1}{d^2 e^{ias} - s^2 e^{iad}}\begin{pmatrix} d^2 - s^2 & ds(e^{-iad} - e^{-ias}) \\ ds(e^{iad} - e^{-ias}) & d^2 - s^2 \end{pmatrix} , \\ &= \frac{1}{2ikk'\cos(k'a) + (k^2 + k'^2)\sin(k'a)}\begin{pmatrix} 2ikk' e^{-ika} & (k^2 - k'^2)\sin(ak')e^{-2ika} \\ (k^2 - k'^2)\sin(ak') & 2ikk' e^{-ika} \end{pmatrix} . \end{aligned} \tag{11.19}$$

From this we extract the reflection and transmission coefficients,

$$\begin{aligned} T &= \frac{4k^2 k'^2}{(k^2 + k'^2)^2 \sin^2(k'a) + 4k^2 k'^2 \cos^2(k'a)} , \\ R &= \frac{(k^2 - k'^2)^2 \sin^2(k'a)}{(k^2 + k'^2)^2 \sin^2(k'a) + 4k^2 k'^2 \cos^2(k'a)} . \end{aligned} \tag{11.20}$$

As sanity checks, we can observe that as $k' \to k$ (so no barrier), $(T, R) \to (1, 0)$, and as $k' \to \infty$ (infinite barrier), $(T, R) \to (0, 1)$, and also that the unitarity condition $T + R = 1$ does indeed hold here.

To treat the case where $E < V$ transparently, we make the replacement $k' = i\mu'$ with $\mu' > 0$. Being careful with signs coming from imaginary arguments in trigonometric functions, we have

$$\begin{aligned} T &= \frac{4k^2 \mu'^2}{(k^2 - \mu'^2)^2 \sinh^2(\mu'a) + 4k^2 \mu'^2 \cosh^2(\mu'a)} , \\ R &= \frac{(k^2 + \mu'^2)^2 \sinh^2(\mu'a)}{(k^2 - \mu'^2)^2 \sinh^2(\mu'a) + 4k^2 \mu'^2 \cosh^2(\mu'a)} . \end{aligned} \tag{11.21}$$

The most striking result here (though it was clear from the setting up of our problem that this would be the case) is that $T \neq 0$ when $E < V$. This is the phenomenon of *quantum tunnelling*, wherein a particle can transmit through a barrier that would classically block it completely; this behaviour have important technological applications, such as in scanning tunnelling microscopes.

Example 11.3.2 (Bound states and poles)**.** A close relative of our previous example is scattering from a rectangular potential *well*, as in Figure 10. In the first instance, we can simply repurpose our S matrix from the previous example, where now we will have $k' > k$, but otherwise everything will be the same as in (11.19).

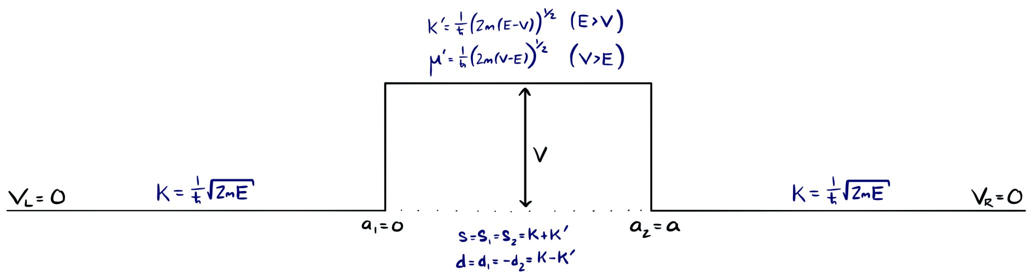

Figure 9. Scattering from a rectangular barrier.

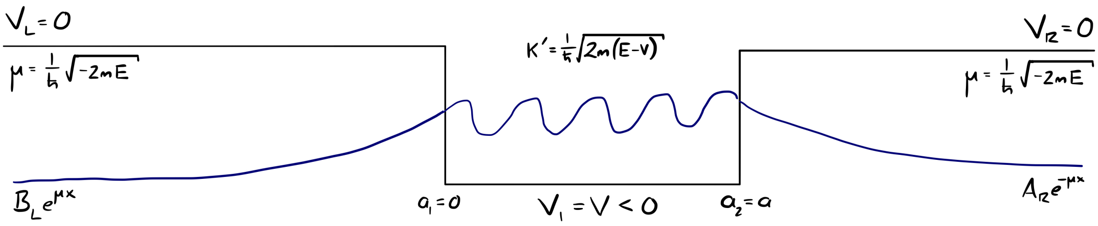

Figure 10. Bound state in a rectangular well.

The novel feature of this example is that in addition to the scattering states we've been studying, there are also bound states with $V < E < 0$; the bound state wave functions will be of the form

$$\psi_{\text{bound}}(x) = \begin{cases} B_L e^{\mu x} \,, & x < 0 \,, \\ A_1 e^{ik'x} + B_1 e^{-ik'x} \,, & 0 < x < a \,, \\ A_R e^{-\mu x} \,, & x > a \,, \end{cases} \tag{11.22}$$

We observe that this is a wave function of precisely the type we considered for scattering states but with the replacement $k = i\mu$, $\mu = \sqrt{-2mE}$ just as in the previous example but now for the wavefunctions in the left and right regions.

Now the bound states correspond to solutions with $A_L = B_R = 0$, which by (11.10) requires that the S matrix become singular. Indeed, upon making the replacement $k \to i\mu$ the (now somewhat formal, as there is no scattering) S matrix takes the form

$$S = \frac{1}{2\mu k' \cos(k'a) + (\mu^2 - k'^2)\sin(k'a)} \begin{pmatrix} 2\mu k' e^{\mu a} & (\mu^2 + k'^2)\sin(ak')e^{2\mu a} \\ (\mu^2 + k'^2)\sin(ak') & 2\mu k' e^{\mu a} \end{pmatrix} , \tag{11.23}$$

and each term becomes singular precisely when

$$2\mu k' \cos(k'a) + (\mu^2 - k'^2)\sin(k'a) = 0 \,. \tag{11.24}$$

Looking back to (11.2), the condition to be able to find a solution with $A_L = B_R = 0$ requires precisely that $M_{11} = 0$, and it is the M_{11} denominator in each entry of the S-matrix that is being set to zero by the condition above. For your own entertainment, you may wish to observe that if instead we take $k \to -i\mu$, then the *same bound states* are responsible for the S matrix developing a kernel.

Remark 11.3.3. What we've observed here is a shadow of a much more general phenomenon in quantum mechanical scattering, where information about bound states can be extracted from the analytic structure (zeroes and poles) of the continuation of scattering data to complex kinematical variables (in this case the asymptotic momentum).