5 Tunnelling and Scattering

Let us reconsider the bound state solutions for the finite square well potential:

$$\psi(x) \sim \begin{cases} e^{-kx} & x > a\,, \\ e^{kx} & x < -a\,, \\ \cos(lx) \text{ or } \sin(lx) & |x| < a. \end{cases} \tag{5.1}$$

Although ψ tends to zero rapidly outside the well, it *is* non-zero there. In particular

$$\int_{|x|>a} |\psi(x)|^2 dx > 0 \tag{5.2}$$

for a bound state solution, although the energy $E = -\frac{\hbar^2 k^2}{2m} < 0$.

The Born rule (3.13) thus tells us that the probability of finding the particle outside the well is *non-zero*, even though the particle's energy is less than the potential height in this region ($V = 0$ in $|x| > a$ by our convention).

Clearly, a classical particle with $E < 0$ would never make its way outside the well. We have here a suggestive argument for the existence of an intrinsically quantum phenomenon – the possibility of *tunnelling* through a potential barrier into a classically forbidden state.

However, the physical interpretation of this calculation is complicated by the fact that we can only assign meaning in quantum mechanics to things we can detect, and we do not have any way to detect negative energy particles. So, we cannot actually observe a bound state particle outside the region $|x| < a$ unless we alter the potential.

What we can and do observe are quantum particles tunnelling through *finite* width potential barriers through which a classical particle of the same energy could not pass.

5.1 Scattering states

To understand tunnelling we need a general treatment of *scattering*: the transmission or reflection of particles by potential barriers (or potential wells).

In principle, we could take as initial state an incoming wavepacket (e.g. an approximately Gaussian packet) far from the potential barrier, solve the time-dependent Schrödinger equation, and obtain a solution that at asymptotic late times takes the form of a superposition of two wavepackets, one reflected by the barrier and one transmitted through it:

$$\psi \sim \psi_r + \psi_t\,. \tag{5.3}$$

We could then calculate the *reflection probability*

$$|\psi_r|^2 \approx \int_{\infty}^{0} |\psi(x,t)|^2 dx \text{ for large } t \tag{5.4}$$

and *transmission probability*

$$|\psi_t|^2 \approx \int_{0}^{\infty} |\psi(x,t)|^2 dx \text{ for large } t\,. \tag{5.5}$$

Some pictures of this process can be found in Schiff (3rd edition, pp 106-9), and in Brandt and Dahmen, "Picture Book of Quantum Mechanics".

However, studying wavepacket scattering directly is mathematically **complicated**. We can model it computationally, and this is often helpful and illuminating, but it is not so easy to prove simple analytic results.

A simpler way to obtain scattering probabilities is to consider unnormalised stationary state solutions that asymptotically take the form of superpositions of plane waves as $x \to \pm\infty$. Thus:

$$\psi = \exp(ikx) + R\exp(-ikx) \text{ as } x \to -\infty$$
$$\psi = T\exp(ik'x) \text{ as } x \to \infty\,.$$

If $V = 0$ as $x \to \pm\infty$ then $k = k'$. We are also interested in examples where V has different limits as $x \to \pm\infty$, so allow $k' \neq k$.

Here we follow the convention that incoming plane waves arrive from $-\infty$ but not ∞. Now $\exp(ikx - \omega t)$ is rightward travelling, and $\exp(-ikx - \omega t)$ is leftward travelling. We consider a stationary solution at (for simplicity) $t = 0$. We thus allow a component of the rightward travelling incoming wave $\exp(ikx)$ as $x \to -\infty$ but do not allow any component of a leftward travelling wave $\exp(-ik'x)$ as $x \to \infty$, which would represent a wave incoming from ∞.

We expect in general a *reflected plane wave* of form

$$R\exp(-ikx) \text{ as } x \to -\infty\,,$$

, and a *transmitted plane wave* of form

$$T\exp(ik'x) \text{ as } x \to \infty\,.$$

5.2 Interpretation of plane wave scattering solutions

We can justify taking these unnormalised stationary state solutions as representing:

(i) an approximation to the behaviour of a 1-particle incoming wavepacket with wave vector sharply peaked about k.

(ii) an approximation to the behaviour of a **beam** of particles (whose interactions with one another are negligible) with approximate wave vector k.

(iii) a mathematical calculation of the behaviour of the wave vector k Fourier component of (i) or (ii).

The beam picture is perhaps the most intuitive, and we will use it, considering beam scattering from various potentials. We can interpret $|R|^2$ as the density of particles in the reflected beam, $|T|^2$ as the density in the transmitted beam. Recall that we have $p = \hbar k$ and so the speed $v = \frac{p}{m} = \frac{\hbar k}{m}$. The particles in the incoming, reflected and transmitted beams thus have speeds

$$\frac{\hbar k}{m}, -\frac{\hbar k}{m}, \frac{\hbar k'}{m} \tag{5.6}$$

respectively.

We define the *particle flux* in the beams to be the number of particles per second in the beam passing a fixed point. We have

$$\text{flux} = \text{velocity} \times \text{density} = \begin{cases} \frac{\hbar k}{m} & \text{incoming}\,, \\ \frac{\hbar k}{m}|R|^2 & \text{reflected}\,, \\ \frac{\hbar k'}{m}|T|^2 & \text{transmitted.} \end{cases} \tag{5.7}$$

Particle conservation – no particles are destroyed or created in the scattering process – thus implies that

$$\frac{\hbar k}{m} = \frac{\hbar k}{m}|R|^2 + \frac{\hbar k'}{m}|T|^2\,. \tag{5.8}$$

We will verify this in particular examples.

5.3 Example I: The potential step

Consider the potential

$$V(x) = \begin{cases} 0 & x < 0\,, \\ U & x > 0\,. \end{cases} \tag{5.9}$$

A solution of energy E obeys

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \begin{cases} (E-U)\psi(x) & x > 0\,, \\ E\psi(x) & x < 0\,. \end{cases} \tag{5.10}$$

For the moment we consider $U > 0$ (a step rather than a drop).

We want solutions of the form $\exp(ikx) + R\exp(-ikx)$ for $x < 0$; these have $E = \frac{\hbar^2 k^2}{2m} > 0$.
Case 1: $E < U$ Define

$$k = \frac{\sqrt{2mE}}{\hbar}\,, \qquad l = \frac{\sqrt{2m(U-E)}}{\hbar}\,. \tag{5.11}$$

We have

$$\frac{d^2}{dx^2}\psi(x) = \begin{cases} l^2\psi(x) & x > 0\,, \\ -k^2\psi(x) & x < 0\,. \end{cases} \tag{5.12}$$

So

$$\psi(x) = \begin{cases} A\exp(-lx) & x > 0\,, \\ \exp(ikx) + R\exp(-ikx) & x < 0\,. \end{cases} \tag{5.13}$$

We see there is no transmitted plane wave in this case.

Continuity of ψ and ψ' at $x = 0$ gives

$$1 + R = A \tag{5.14}$$
$$ik(1 - R) = -lA \tag{5.15}$$

Hence

$$A = \frac{2k}{k + il} \tag{5.16}$$
$$R = \frac{k - il}{k + il} \,. \tag{5.17}$$

In particular $|R|^2 = 1$: the reflected flux equals the incoming flux, and thus the reflection probability for any given incoming particle is one.

Case 2: $E > U$ Now we have

$$l = \frac{\sqrt{2m(E - U)}}{\hbar} \tag{5.18}$$

and

$$\psi(x) = \begin{cases} T \exp(ilx) & x > 0 \,, \\ \exp(ikx) + R \exp(-ikx) & x < 0 \,. \end{cases} \tag{5.19}$$

Continuity of ψ, ψ' at $x = 0$ gives

$$T = 1 + R \tag{5.20}$$
$$\frac{l}{k} T = 1 - R \,. \tag{5.21}$$

Hence

$$T = \frac{2k}{k + l} \,, \tag{5.22}$$
$$R = \frac{k - l}{k + l} \,. \tag{5.23}$$

The incoming, reflected and transmitted fluxes are respectively

$$F_I = \frac{\hbar k}{m} \tag{5.24}$$
$$F_R = \frac{\hbar k}{m} |R|^2 = \frac{\hbar k}{m} (\frac{k - l}{k + l})^2 \tag{5.25}$$
$$F_T = \frac{\hbar l}{m} |T|^2 = \frac{\hbar l}{m} (\frac{4k^2}{(k + l)^2}) \,. \tag{5.26}$$

We see that

$$F_R + F_T = \frac{\hbar}{m}\frac{k(k-l)^2 + 4k^2 l}{(k+l)^2}$$
$$= \frac{\hbar}{m}\frac{k(k+l)^2}{(k+l)^2}$$
$$= \frac{\hbar k}{m}$$
$$= F_I \tag{5.27}$$

as particle conservation requires.

Comments 1. Case 1 ($E < U$) accords at least roughly with classical intuition: a particle with insufficient energy to climb the step is (eventually) reflected back.

2. The calculations for case 2 ($E > U$) apply for $U < 0$ – a downward step – as well as for $U > 0$. In the classical limit in which the step is negligible compared to the particle energy, $E \gg |U|$, we have

$$k \approx l\,,\, F_R \approx 0\,,\, F_T \approx 1\,.$$

This implies near-perfect transmission, again as classical intuition would suggest.

3. But the results in general do *not* accord with classical intuition. Consider for example the case $U < 0$ and $E \ll |U|$. Here we have

$$l \gg k\,,\, |R|^2 \approx 1\,,\, |T|^2 \approx 0\,.$$

In other words, we find near perfect **reflection** from a **downward** step, precisely the opposite result to that indicated by classical intuition.

5.4 Example II: The square potential barrier

Consider an incoming beam of particles with $E < U$ scattering from the potential

$$V(x) = \begin{cases} 0 & \text{for } x < 0\,, \\ U & \text{for } 0 < x < a \\ 0 & \text{for } x > a\,. \end{cases} \tag{5.28}$$

We have

$$\psi(x) = \begin{cases} T\exp(ikx) & \text{for } x > a\,, \\ A\exp(-lx) + B\exp(lx) & \text{for } 0 < x < a\,, \\ \exp(ikx) + R\exp(-ikx) & \text{for } x < 0\,, \end{cases} \tag{5.29}$$

where

$$E = \frac{\hbar^2 k^2}{2m}, \qquad U - E = \frac{\hbar^2 l^2}{2m}. \tag{5.30}$$

Continuity of ψ and ψ' at $x = 0$ gives

$$1 + R = A + B, \tag{5.31}$$

$$ik(1 - R) = l(B - A), \tag{5.32}$$

Continuity of ψ and ψ' at $x = a$ gives

$$A\exp(-la) + B\exp(la) = T\exp(ika), \tag{5.33}$$

$$-lA\exp(-la) + lB\exp(la) = ikT\exp(ika). \tag{5.34}$$

Exercise Solve the algebra, to obtain

$$T = \frac{4ikle^{-ika}}{(2ikl + l^2 - k^2)e^{-la} + (2ikl - l^2 + k^2)e^{la}}. \tag{5.35}$$

This gives

$$|T|^2 = \frac{16k^2l^2}{4k^2l^2(e^{la} + e^{-la})^2 + (l^2 - k^2)^2(e^{la} - e^{-la})^2}. \tag{5.36}$$

In the case $la \gg 1$ we can neglect the $\exp(-la)$ terms, obtaining

$$|T|^2 \approx \frac{16k^2l^2}{4k^2l^2\exp(2la) + (l^2 - k^2)^2\exp(2la)}. \tag{5.37}$$

$$\approx \frac{16k^2l^2}{(k^2 + l^2)^2}\exp(-2la). \tag{5.38}$$

Since $l = \frac{\sqrt{2m(U-E)}}{\hbar}$, we find

$$|T|^2 \approx \exp(-\frac{2a}{\hbar}\sqrt{2m(U - E)}). \tag{5.39}$$

<u>Comments</u> 1. The most immediately striking result is the fact that T is *nonzero*: quantum particles *can* tunnel through classically impenetrable potentials.

2. If $la \gg 1$ the tunnelling probability is small; we approach the classical limit as $la \to \infty$. The tunnelling probability in this regime depends inverse exponentially on the barrier width a and on $\sqrt{U - E} \approx \sqrt{U}$ (if $E \ll U$). This is a general feature of tunnelling, true for a wide class of barrier potentials.

5.4.1 *Important examples

- Nuclear fission.
- Nuclear fusion.
- Muon-catalysed nuclear fusion.
- Scanning tunnelling electron microscopy. *