Chapter 2

WKB Approximation

Quantum tunnelling is a very important application of wave-function quantum mechanics. Classical physics would tell us that the particle cannot penetrate a region where its energy E is less than the potential $V(x)$, nevertheless, a quantum mechanical treatment shows that the particle is able to "tunnel through" the forbidden region, and then propagate freely on the other side of the barrier. In your previous quantum mechanics courses, you are likely to have studied tunnelling in an idealised setting, where the potential is modelled by a step function (see figure 2.1). In this case, the time-independent Schrödinger equation (TISE)

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\psi(x) \tag{2.1}$$

can be separately integrated for each distinct region of constant potential. When $V(x)$ is a constant $V(x) = V_0$, it is straightforward to integrate the TISE exactly to obtain the solutions,

$$\psi(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar} \tag{2.2}$$

for the "classically allowed" region where $E > V_0$, where $p = \sqrt{2m(E - V_0)}$, and

$$\psi(x) = Ce^{+qx/\hbar} + De^{-qx/\hbar} \tag{2.3}$$

for the "classically forbidden" region where $E < V_0$, where $q = \sqrt{2m(V_0 - E)}$. To find a full wavefunction solution for the TISE across all regions, we apply boundary conditions *connecting* these solutions at the boundaries between forbidden and allowed regions. The boundary conditions are derived from the necessity that both the wave function and its first derivative are continuous across the boundary.

Identifying the eigenfunctions of the Hamiltonian provides a full solution to the problem as one can then calculate the dynamics for any initial quantum state, and derive tunnelling rates, etc. We call points at which $E = V(x)$ classical turning points, since they correspond to points at which the speed of a classical particle would slow to zero, and where the direction of its momentum reverses. Note that the classical turning point depends upon the energy of the particle being considered.

While the above treatment provides a qualitative study of quantum tunnelling, and similar treatments can be applied to quantum wells, the step-function potentials are poor approximations for the potentials found in nature, which tend to be smooth and without discontinuities. Unfortunately, solving the TISE exactly for an arbitrary smooth $V(x)$ can be very hard and often impossible with known techniques. While one can utilise numerical techniques to perform an ap-

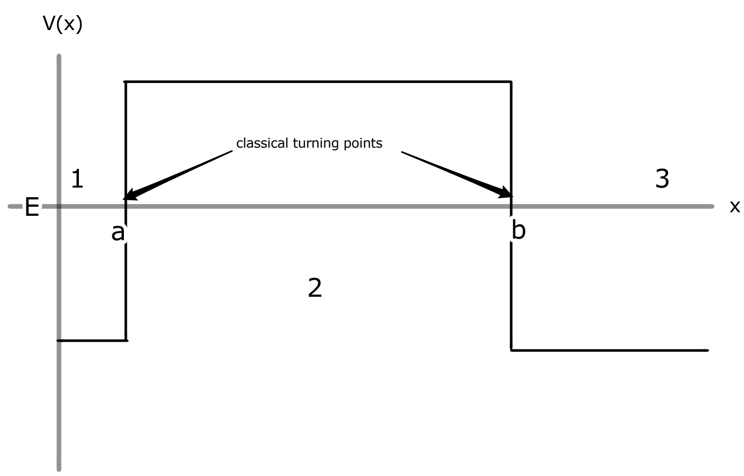

Figure 2.1: An idealised potential illustrating quantum tunnelling. The potential is constant everywhere except at the boundaries between regions, where it is discontinuous.

proximate integration on a computer, it often gives more physical insight to find an approximate analytical solution. In this chapter, we shall study the Wentzel-

Kramers-Brillouin or WKB approximation, which allows us to solve the TISE approximately under the condition that the potential $V(x)$ is varying sufficiently slowly.

Recall that, in a constant potential in a classically allowed region, the eigenfunctions of the TISE are plane-waves, eigenstates of momentum with momentum $p = \sqrt{2m(E-V)}$ and which have a de Broglie wave-length $\lambda = \frac{h}{p}$.

If $V(x)$ is varying slowly, in particular, slowly with respect to λ, it can still be meaningful to define a local momentum

$$p(x) = \sqrt{2m(E - V(x))} \tag{2.4}$$

and corresponding local wavelength $\lambda(x) = \frac{h}{p(x)}$.

We will see that these quantities play an important role in the WKB approximation, which provides an approximate solution to the TISE valid for non-flat potentials $V(x)$ which are sufficiently slowly varying.

2.1 WKB Wave-function

Our starting point is to assume that, if $V(x)$ is varying sufficiently slowly, the wave-function ought to have a form similar to the idealised case where $V(x)$ is constant, such as in equation (2.2), we therefore start with a trial solution (Ansatz) of the form:

$$\psi(x) = Ae^{\frac{i}{\hbar}S(x)} \tag{2.5}$$

We then substitute this expression into the TISE to derive an expression for $S(x)$ for eigenstates of energy. Using

$$\begin{aligned}\frac{\partial^2\psi(x)}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{i}{\hbar}S'(x)Ae^{\frac{i}{\hbar}S(x)}\right)\\ &= \left(\frac{i}{\hbar}S''(x) - \frac{S'(x)^2}{\hbar^2}\right)Ae^{\frac{i}{\hbar}S(x)}\end{aligned} \tag{2.6}$$

where $S'(x) = \partial S(x)/\partial x$ and $S''(x) = \partial^2 S(x)/\partial x^2$, we obtain,

$$\frac{-i\hbar}{2m}S''(x) + \frac{1}{2m}\left(S'(x)\right)^2 + V(x) - E = 0. \tag{2.7}$$

At this point we have not yet made any approximation. Equation (2.7) is fully equivalent to the original TISE, and, in fact, looks harder to solve, being a non-linear second order differential equation. We notice, however that if the first term of equation (2.7) is neglected, the solution is $S(x) = \int p(x)dx + c$, recovering the form of the plane-wave solution. This first term is the only term proportional to $\hbar$, and would vanish in the limit $\hbar \to 0$. Even though $\hbar$ is a fundamental constant, it can sometimes be mathematically convenient to treat it as a small variable. Since taking the limit $\hbar \to 0$ often (but not always!) allows us to derive classical equations of motion from quantum expressions, this technique is sometimes called a "semi-classical" approach. Here, since equation (2.7) tends to the plane-wave solution in the $\hbar \to 0$ limit, it is mathematically convenient to pretend $\hbar$ is a variable and expand $S(x)$ as a power series in $\hbar$.

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \cdots = \sum_{j=0}^{\infty} \hbar^j S_j(x) \tag{2.8}$$

We substitute this power series into equation (2.7) to obtain

$$\frac{-i\hbar}{2m} \sum_j h^j S_j''(x) + \frac{1}{2m} \left(\sum_j h^j S_j'(x) \right)^2 + V(x) - E = 0. \tag{2.9}$$

We now identify terms in this expression which correspond to matching powers of $\hbar$. Continuing to treat $\hbar$ as a variable, we demand that each of these terms must independently sum to zero, (in linear algebraic terms, we are utilising the linear independence of $\hbar^j$). We therefore obtain a set of simultaneous equations which we can sequentially solve to find $S_0(x)$, $S_1(x)$, etc.

0th order ($\hbar^0$)

$$\frac{1}{2m} \left(S_0'(x)\right)^2 + V(x) - E = 0, \tag{2.10}$$

1st order ($\hbar^1$)

$$\frac{-i}{2m} S_0''(x) + \frac{2}{2m} S_1'(x) S_0'(x) = 0, \tag{2.11}$$

and so on. We now integrate these expressions one-by-one.

0th order ($\hbar^0$)

We rewrite equation (2.10) as

$$\frac{\partial S_0(x)}{\partial x} = \pm\sqrt{2m(E - V(x))} \tag{2.12}$$

and integrate to obtain

$$S_0(x) = \pm \int^x dx' p(x') + c. \tag{2.13}$$

For the moment, we shall not specify limits for the integral, but will return to this issue below.

1st order ($\hbar^1$)

We rewrite equation (2.11) as

$$-iS_0''(x) = -2S_1'(x)S_0'(x) \tag{2.14}$$

or

$$\frac{S_0''(x)}{S_0'(x)} = -i2S_1'(x) \tag{2.15}$$

Recalling that $\int f'(x)/f(x)dx = \ln(f(x)) + c$ we integrate to achieve

$$\ln(S_0'(x)) = -2iS_1(x) + c \tag{2.16}$$

By integrating the second order equation (see Bransden and Joachain for details) one can similarly achieve the following expression for $S_2(x)$

$$S_2(x) = \frac{1}{2}\frac{m}{p(x)^3}\frac{\partial V(x)}{\partial x} - \frac{1}{4}m^2 \int \frac{1}{p(x')^5}\left(\frac{\partial V(x')}{\partial x'}\right)^2 dx \tag{2.17}$$

We shall not undertake a detailed analysis of this term here, but notice that it vanishes provided $\frac{\partial V(x)}{\partial x}$ is sufficiently small, as long as $p(x)$ does not get too close to zero. This justifies taking only the first two terms in the expansion provided these conditions hold and we thus approximate $S(x)$ to first order in $\hbar$

$$S(x) \approx S_0(x) + \hbar S_1(x) \tag{2.18}$$

Substituting back into equation (2.5) we obtain

$$
\begin{aligned}
\psi(x) &= Ae^{\frac{i}{\hbar}S(x)} \\
&= Ae^{\frac{i}{\hbar}S_0(x)}e^{iS_1(x)} \\
&= Ae^{\pm\frac{i}{\hbar}\int^x dx' p(x')}e^{-\ln\sqrt{\pm p(x)}+ic} \\
&= \frac{Ae^{iC}}{\sqrt{\pm 1}}\frac{1}{\sqrt{p(x)}}e^{\pm\frac{i}{\hbar}\int^x dx' p(x')}
\end{aligned}
\tag{2.19}
$$

Note that since the constant of integration c can be absorbed into the normalising factor, we are free to choose whatever lower limit for the integral is most convenient. Also, the $\pm$ factor means that we can, if convenient reverse the lower and upper limits of the integral. We shall use this freedom below, where we will choose a standard set of choices for the limits of this integral.

We can take a superposition of positive and negative solutions to write a general wavefunction for a state of energy E under the WKB approximation.

$$
\psi(x) = \frac{A}{\sqrt{p(x)}}e^{i\int^x p(x')dx'/\hbar} + \frac{B}{\sqrt{p(x)}}e^{-i\int^x p(x')dx'/\hbar} \tag{2.20}
$$

where A and B are constants to be determined.

The form of this state has an intuitive explanation which can make it easier to remember. If this were a classical particle distributed at random, you'd expect the probability of finding the particle at a given point to be inversely proportional to its velocity, i.e. proportional to how long the particle spent at that position. The WKB wave-function has precisely that property. If we loosely interpret $p(x)$ as the momentum of the particle, the probability density of finding a particle at position x, $|\psi(x)|^2$ is proportional to $1/p(x)$ and hence inversely proportional to velocity. The phase integral $e^{i\int^x p(x')dx'/\hbar}$ is a natural generalisation of the plane-wave behaviour, but for a momentum which varies with x.

Classically forbidden region

So far we have not considered whether the particle is situated in a classically allowed region $E > V(x)$ or a forbidden region $E < V(x)$. In fact the above analysis is valid for both regions, with $p(x) = \sqrt{2m(E - V(x))}$ becoming imaginary in the forbidden case. It is convenient and illustrative to work with real numbers, so we define $q(x) = \sqrt{2m(V(x) - E)}$ and write the wave-function in the forbidden region as follows:

$$\psi(x) = \frac{C}{\sqrt{q(x)}} e^{+\int^x q(x')dx'/\hbar} + \frac{D}{\sqrt{q(x)}} e^{-\int^x q(x')dx'/\hbar} \tag{2.21}$$

where C and D are constants to be determined. We see, similar to the idealised constant potential analysis, exponential growth and decay in the forbidden region.

Classical Turning Point

To fully solve the TISE for the idealised potential, we apply boundary conditions at the classical turning points (CTPs), which mark the transition between allowed and forbidden regions. At the CTP, $E = V(x)$ and hence $p(x) = 0$, the WKB solutions $\propto 1/\sqrt{p(x)}$ diverge to infinity. Wave-functions must remain finite at all times, hence the WKB solutions in equations (2.20) and (2.21) cannot be valid close to the CTP. Therefore in order to connect the solutions and calculate coefficients A, B, etc. a different approach is needed. We need to find an additional family of wave-functions which while valid at the CTP, converge to the WKB solutions away from the CTP. This is what we will introduce in the next section.

2.2 Connection Formulae

To find such a wave-function, we use the observation that very close the classical turning point, which we will label $x = a$, $V(x)$ is approximately linear. This can be seen by expanding $V(x)$ as a Taylor expansion around $V(a)$, to first order the expansion is linear. We therefore shall solve the TISE with the linear potential $V(x) - E = A(x-a)$ where $A = \partial V(x)/\partial x|_{x=a}$. Substituting this into the TISE, we obtain:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + A(x-a)\psi(x) = 0. \tag{2.22}$$

If A is positive this represents a right hand barrier, with allowed region for negative x, etc.

We then perform a change of variables, to simplify the form of the equation, using $z = (2mA/\hbar^2)^{1/3}(x-a)$. After the change of variables, the TISE takes the simple form

$$\frac{\partial^2\psi(z)}{\partial z^2} - z\psi(z) = 0 \tag{2.23}$$

This equation is called the Airy equation. It has been studied since the 19th century, and we label its solutions $Ai(z)$ and $Bi(z)$. A general solution will be a linear combination of these functions. $Ai(z)$ and $Bi(z)$ are illustrated in figure 2.2. Notice that they have precisely the behaviour we want, interpolating between oscillatory behaviour for negative z (corresponding to the classical allowed region) and exponentially growing or decaying for positive z.

These solutions do not have a closed forms, but away from $z = 0$ converge quickly to the following expressions.

Large positive z

$$Ai(z) \approx \frac{1}{2\sqrt{\pi}} \frac{\exp[-\frac{2}{3}|z|^{3/2}]}{|z|^{1/4}} \tag{2.24}$$

$$Bi(z) \approx \frac{1}{\sqrt{\pi}} \frac{\exp[+\frac{2}{3}|z|^{3/2}]}{|z|^{1/4}} \tag{2.25}$$

These are symmetric under flipping the sign of the exponent up to an additional factor of 2 in the expression for $Ai(z)$.

Large negative z

$$Ai(z) \approx \frac{1}{\sqrt{\pi}} \frac{\cos[\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}]}{|z|^{1/4}} \tag{2.26}$$

$$Bi(z) \approx \frac{-1}{\sqrt{\pi}} \frac{\sin[\frac{2}{3}|z|^{3/2} - \frac{\pi}{4}]}{|z|^{1/4}} \tag{2.27}$$

These are symmetric under flipping cos and sin, apart from the additional -1 factor in the expression for $Bi(z)$.

These solutions have most of the behaviour we need, they are continuous across the CTP, and they converge to exponential growth and decay, and oscillatory behaviour on the appropriate sides of the CTP. However, the Airy function alone cannot be our full solution. It was derived for a linear potential, not a smooth curve $V(x)$ so one would not expect it too. However, it gives us an idea of what the full solution might look like. The final step is to manipulate the expressions for the Airy functions by hand so that they converge to WKB solution formulae. This will essentially be a guess, but one can confirm (See Bransden and Joachain for details) that such solutions are approximate solutions to the full TISE.

To transform the Airy functions appropriately, we make two changes. First, we replace $z(x)$ with $\int_x^a p(x')dx'/\hbar$ when $z < 0$ (allowed region) and with $\int_a^x q(x')dx'/\hbar$

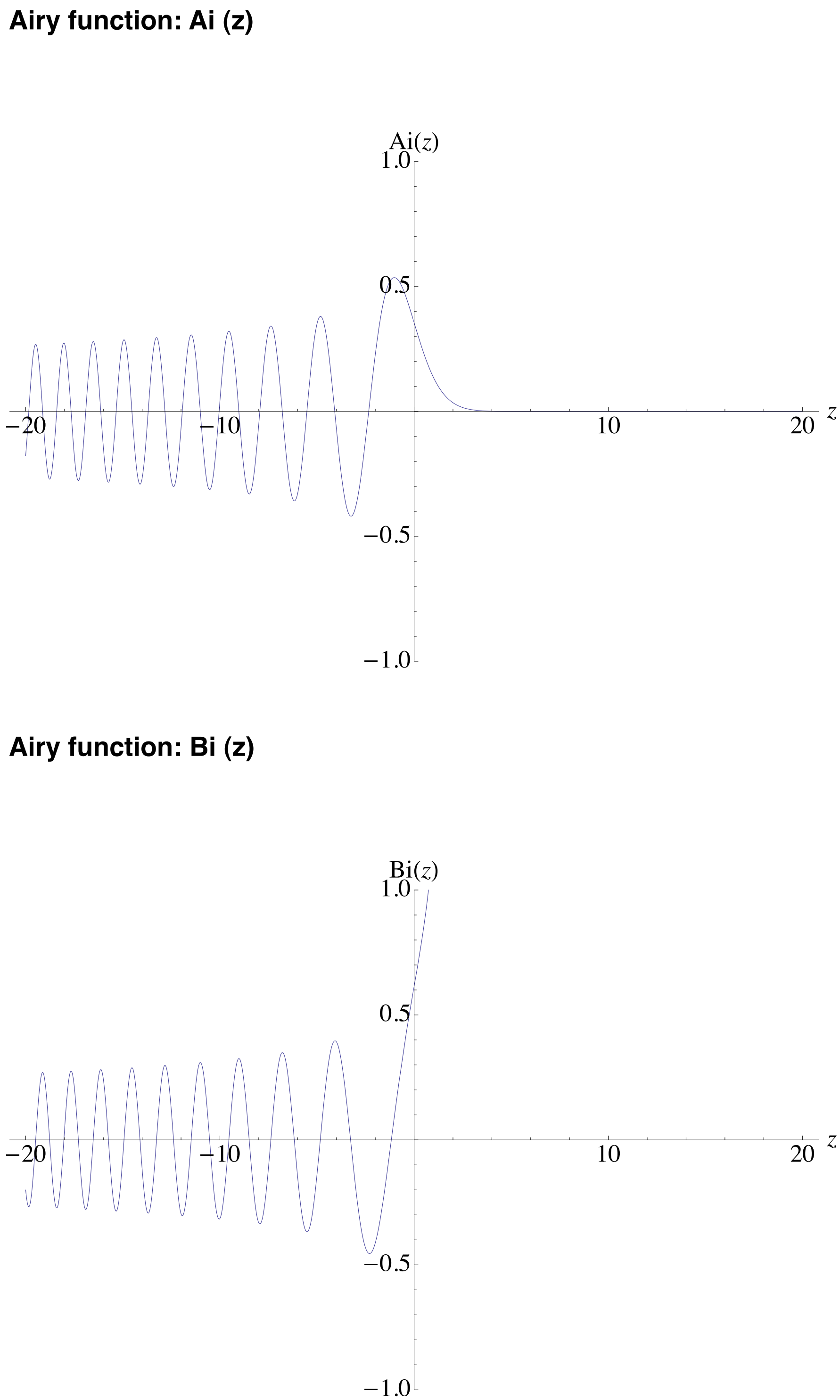

Figure 2.2: Airy functions $Ai(z)$ and $Bi(z)$.

in the forbidden region. Furthermore we alter the normalisation to obtain the correct $1/\sqrt{p(x)}$ behaviour, to obtain:

$$\psi_A(x) = \frac{|z(x)|^{1/4}}{|p(x)|^{1/2}} Ai(\int_x^a p(x')dx'/\hbar) \tag{2.28}$$

for the allowed region and

$$\psi_A(x) = \frac{|z(x)|^{1/4}}{|q(x)|^{1/2}} Ai(\int_a^x q(x')dx'/\hbar) \tag{2.29}$$

for the forbidden region. Similarly,

$$\psi_B(x) = \frac{|z(x)|^{1/4}}{|p(x)|^{1/2}} Bi(\int_x^a p(x')dx'/\hbar) \tag{2.30}$$

for the allowed region and

$$\psi_B(x) = \frac{|z(x)|^{1/4}}{|q(x)|^{1/2}} Bi(\int_a^x q(x')dx'/\hbar) \tag{2.31}$$

Note that the limits of the integrals have been chosen so that $z(x) = 0$ at the CTP as required, and with an order ensuring that the integral is always non-negative. We shall alway use limits following that convention in the following, since it aids our interpretation, and in particular helps us to prevent confusing exponential growth and exponential decay.

We shall not use the above expressions directly. Instead we shall consider their limits either side of the CTP to recover the standard WKB form. The benefit of this is that it tells us how WKB wave-functions connect across the CTP, since a general state will have the form $\psi(x) = \alpha\psi_A(x) + \beta\psi_B(x)$ and thus the part of wavefunction $\psi_A(x)$ which describes behaviour in the forbidden region must have the same coefficient, α as the corresponding limit in the allowed region.

The limits are as follows, up to an arbitrary normalisation factor, in the allowed region, left of the barrier

$$\psi_A(x) = \frac{1}{2\sqrt{\pi}} \frac{1}{\sqrt{p(x)}} \cos\left(\int_x^c p(x')dx'/\hbar - \frac{\pi}{4}\right) \tag{2.32}$$

which is a linear combination of oscillatory terms of the form (2.20). In the forbidden region, $\psi_A(x)$ takes the form

$$\psi_A(x) = \frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{q(x)}}\exp\left(-\int_a^x q(x')dx'/\hbar\right) \tag{2.33}$$

Similarly, we find

$$\psi_B(x) = \frac{-1}{\sqrt{\pi}}\frac{1}{\sqrt{p(x)}}\sin\left(\int_x^c p(x')dx'/\hbar - \frac{\pi}{4}\right) \tag{2.34}$$

in the allowed region and

$$\psi_B(x) = \frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{q(x)}}\exp\left(+\int_a^x q(x')dx'/\hbar\right) \tag{2.35}$$

in the forbidden region.

These limits allow us to construct connection formulae - which are simply rules which tell us what form of wavefunction in the forbidden region has the same coefficient as which form of wavefunction in the allowed region, "connecting" the wave-functions across the CTP.

These connection formulae are usually expressed as a table. Here follow the connection rules for both left-hand and right-handed barriers. The derivation for the left-handed barrier is similar to above.

Connection Formulae

Right-hand barrier

$$\begin{aligned}&\frac{2}{\sqrt{p(x)}}\cos\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right)\\ &\qquad\qquad \leftarrow \quad \frac{1}{\sqrt{q(x)}}\exp\left[-\int_a^x q(x')dx'/\hbar\right]\end{aligned} \tag{2.36}$$

$$\begin{aligned}&-\frac{1}{\sqrt{p(x)}}\sin\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right)\\ &\qquad\qquad \rightarrow \quad \frac{1}{\sqrt{q(x)}}\exp\left[+\int_a^x q(x')dx'/\hbar\right]\end{aligned} \tag{2.37}$$

Left-hand barrier

$$\begin{aligned}\frac{1}{\sqrt{q(x)}}\exp\left[-\int_x^a q(x')dx'/\hbar\right]\\ \rightarrow \quad \frac{2}{\sqrt{p(x)}}\cos\left(\int_a^x p(x')dx'/\hbar-\frac{\pi}{4}\right)\end{aligned} \tag{2.38}$$

$$\begin{aligned}\frac{1}{\sqrt{q(x)}}\exp\left[+\int_x^a q(x')dx'/\hbar\right]\\ \leftarrow \quad -\frac{1}{\sqrt{p(x)}}\sin\left(\int_a^x p(x')dx'/\hbar-\frac{\pi}{4}\right)\end{aligned} \tag{2.39}$$

Arrows in WKB connection formula

You will notice that in the above connection formulae, there are arrows $\rightarrow$ and $\leftarrow$. These arrows show you the direction with which it is "safe" to utilise the connection formula. The reason for their presence is the presence of exponentially growing wave-functions in the forbidden regions. If the wave-function is a superposition of exponential growth and decay, the decaying term might be neglected in calculations. This has little effect on the wave-function in the forbidden region, but can lead to a dramatic error in the accessible region. E.g. if the wavefunction is $\psi(x) = 10000\psi_A(x) + 0.01\psi_B(x)$, the $\psi_B(x)$ term will still dominate quickly, and thus ψ_A might be neglected in an approximate or numerical calculation. This would lead to a widely incorrect wave-function in the allowed region.

The arrows are important if your calculation uses numerical methods or is far from the region of validity for the WKB approximation. If you have an exact analytic solution for one region, it is safe to ignore the arrows and connect both wave-functions across the CTP, as we shall see in the following examples.

2.3 WKB Example 1: Bound states in a quantum well

In your previous quantum physics courses, you studied the energy eigenstates of the infinite square well, which has a sharp boundary between allowed ($V = 0$)

and forbidden ($V = \infty$) regions. The WKB approximation allows us to study the bound states of smooth potential wells, where $V(x)$ is constantly varying and where there is no sharp discontinuity in $V(x)$.

In this section, we shall consider a quantum well of the form illustrated in figure 2.3. We will consider a particle of energy E less than the highest potential on both sides of the well, which therefore has classical turning points (where $V(x) = E$) at points $x = a$ and $x = b$. The classical turning points divide the space into three regions, indicated as 1, 2 and 3 in figure 2.3. We shall derive the wave-functions of bound quantum states of this well - i.e. the allowed energy eigenstates for particles with energies in this range - under the WKB approximation by considering the regions one-by-one and applying the connection formulae across the turning points.

Region 1 is a classically forbidden region, and hence the WKB wave-function will take the form of equation (2.21). Let us assume that there are no more classical turning points between $x = a$ and $x = -\infty$. In this case, we need to neglect the term in (2.21) which will "blow up" at minus infinity, and thus obtain

$$\psi_1(x) = \frac{A_1}{\sqrt{q(x)}} \exp\left[-\int_x^a q(x')dx'/\hbar\right] \tag{2.40}$$

where $q(x) = \sqrt{2m(V(x) - E)}$.

For the same reasons, in classically forbidden region 3, the WKB wave-function must take the form:

$$\psi_3(x) = \frac{A_3}{\sqrt{q(x)}} \exp\left[-\int_b^x q(x')dx'/\hbar\right]. \tag{2.41}$$

We use the connection formulae to derive expressions for the wave-function in the classically allowed region 2. Using the connection formula equation (2.38) from region 1 into 2 we obtain

$$\psi_2(x) = \frac{2A_1}{\sqrt{p(x)}} \cos\left(\int_a^x p(x')dx'/\hbar - \frac{\pi}{4}\right) \tag{2.42}$$

Using connection formula (2.36) from region 3 into 2 we can derive a second form for the wave-function in this region,

$$\psi_2(x) = \frac{2A_3}{\sqrt{p(x)}} \cos\left(\int_x^b p(x')dx'/\hbar - \frac{\pi}{4}\right) \tag{2.43}$$

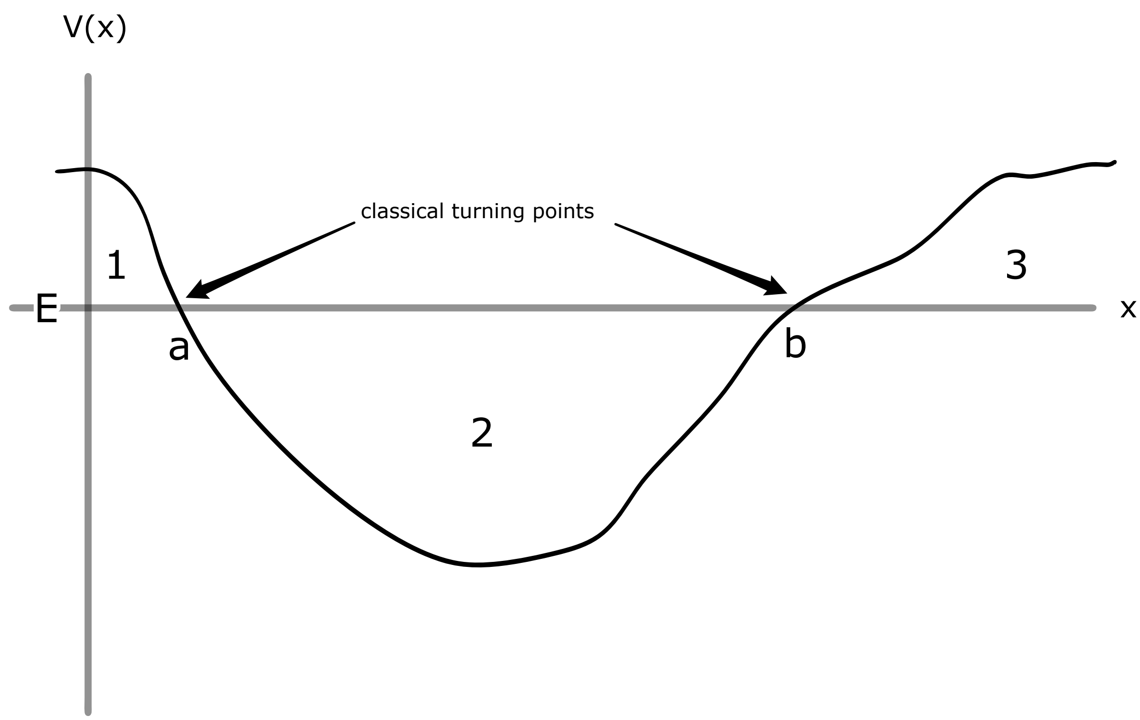

Figure 2.3: A sketch of the potential for a one-dimensional smooth well. Classical turning points for a particle of energy E are marked (where $V(x) = E$), which divides the space into three regions, labelled 1, 2 and 3.

The wavefunctions in equations (2.42) and (2.43) must be equal (they are both representing the same region of space). Equating them will place certain conditions on $p(x)$, A_1 and A_3.

Since $\int_x^b dx = \int_a^b dx - \int_a^x dx$ we can rewrite equation (2.43)

$$\psi_2(x) = \frac{2A_3}{\sqrt{p(x)}} \cos\left(\underbrace{\int_a^b p(x')dx'/\hbar}_{P} - \underbrace{\int_a^x p(x')dx'/\hbar}_{Q} - \frac{\pi}{4} \right) \tag{2.44}$$

where we have labelled the integrals within the cosine P and Q for easier manipulation. We then use standard trigonometric identities to rewrite this:

$$\begin{aligned} \cos(P - (Q + \pi/4)) &= \sin(P - (Q - \pi/4)) \\ &= \sin(P)\cos(Q - \pi/4) - \cos(P)\sin(Q - \pi/4) \end{aligned} \tag{2.45}$$

If we note that the expression for $\psi_2(x)$ in equation (2.42) is proportional to $\cos(Q - \pi/4)$, this implies that the term $\cos(P)\sin(Q - \pi/4)$ in equation (2.45) must be zero. Since $\sin(Q - \pi/4)$ cannot be always equal to zero unless $\cos(Q - \pi/4)$ is always equal to 1, which, we know is not the case, this implies that $\cos(P) = 0$. This requirement implies that $P = (n + 1/2)\pi$ for some integer n, and gives us the WKB quantum well *quantisation condition*:

$$P = \int_a^b p(x')dx'/\hbar = \left(n + \frac{1}{2}\right)\pi \tag{2.46}$$

where $n = 0, 1, 2, \ldots$.

This condition implies that the bound particle can only have energies, which leave equation (2.46) satisfied. (Recall, energy is linked to momentum via $p(x) = \sqrt{2m(E - V(x))}$). Hence the bound states are *quantised*.

Note that equation (2.46) implies that $\sin(P) = (-1)^n$ and hence equation (2.43) transforms to

$$\psi_2(x) = \frac{2A_3(-1)^n}{\sqrt{p(x)}} \cos\left(\int_a^x p(x')dx'/\hbar - \frac{\pi}{4} \right) \tag{2.47}$$

and by comparison with equation (2.42) we see that $A_1 = A_3(-1)^n$.

2.4 WKB Example 2: Tunnelling

Previously you have studied the tunnelling of particles through a square barrier (e.g. see figure 2.4) of height V. For a particle of energy $E < V$ you will have derived, by solving the TISE, wavefunctions for regions 1, 2 and 3 of the following forms .

$$\psi_1(x) = e^{ipx/\hbar} + Re^{-ipx/\hbar} \tag{2.48}$$

$$\psi_2(x) = Ce^{qx/\hbar} + De^{-qx/\hbar} \tag{2.49}$$

$$\psi_3(x) = Te^{ipx/\hbar} \tag{2.50}$$

where $p = \sqrt{2m(E)}$, and $q = \sqrt{2m(V-E)}$ and R, C, D and T are constants to be determined by imposing boundary conditions – continuity of $\psi(x)$ and $\psi(x)'$ at the classical turning points.

You may have studied the probability flux for the tunnelling particles given, in 1-D, by the following expression

$$J = \frac{\hbar}{2im}\left(\psi(x)^*\frac{\partial\psi(x)}{\partial x} - \psi(x)\frac{\partial\psi(x)^*}{\partial x}\right). \tag{2.51}$$

Using (2.48) to (2.50) we obtain expressions for the probability currents – incident current $J_I = p/m$, reflected current $J_R = |R|^2 p/m$ and transmitted $J_T = |T|^2 p/m$. The tunnelling rate is the ratio $J_I/J_T = |T|^2$.

The WKB approximation allows us to calculate approximate wave-functions, and hence tunnelling rates, for non-square potential barriers, such as the potential depicted in figure 2.5. We shall proceed, by first identifying the form of the wave-function in one of the regions, and then employing the connection formulae to derive the wave-function in the other regions.

We shall assume that the particle is incident from the left with energy less than the height of the barrier. There are thus two classical turning points at $x = a$ and $x = b$, and as above, we shall label the regions 1, 2 and 3 accordingly. The direction of the incident particle implies that region 3 will consist solely of a WKB wave-function travelling in the "from-the-left" direction, i.e. of the form

$$\psi(x)_3 = \frac{A'}{\sqrt{p(x)}}\exp\left[i\int_b^x p(x')dx'/\hbar\right] \tag{2.52}$$

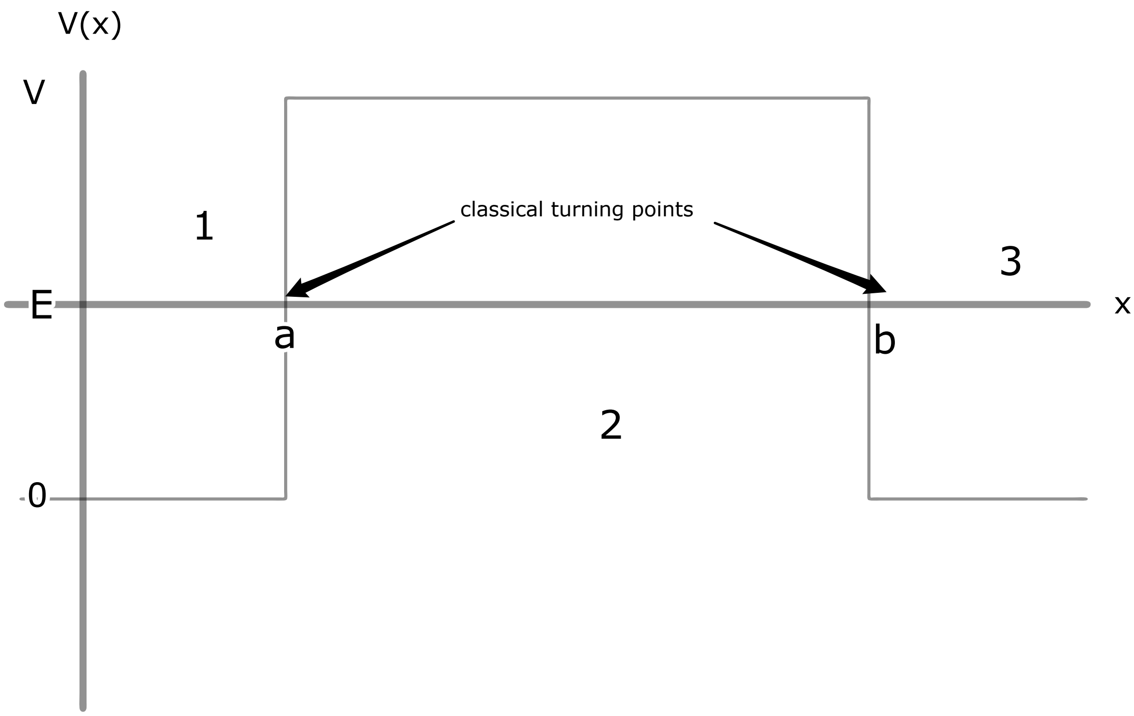

Figure 2.4: A sketch of the potential for a one-dimensional square barrier. Classical turning points for a particle of energy E are marked ($V(a) = V(b) = E$), which divides the space into three regions, labelled 1, 2 and 3.

To make it easier to apply the connection formulae, it is convenient to introduce the new constant $A = A'e^{i\pi/4}$ and write

$$\psi(x)_3 = \frac{A}{\sqrt{p(x)}} \exp\left[i \int_b^x p(x')dx'/\hbar - i\frac{\pi}{4}\right] \tag{2.53}$$

We then expand the exponential in its real and imaginary parts, to obtain

$$\psi(x)_3 = \frac{A}{\sqrt{p(x)}} \left(\cos\left[\int_b^x p(x')dx'/\hbar - \frac{\pi}{4}\right] + i\sin\left[\int_b^x p(x')dx'/\hbar - \frac{\pi}{4}\right]\right) \tag{2.54}$$

We can now directly apply the connection formulae for a left-hand barrier to get the WKB wave-function for region 2

$$\psi(x)_2 = \frac{A}{\sqrt{q(x)}} \left(\frac{1}{2}\exp\left[-\int_x^b q(x')dx'/\hbar\right] - i\exp\left[\int_x^b q(x')dx'/\hbar\right]\right) \tag{2.55}$$

Note that we have used one of the connection formulae *against* the direction of its arrow. The reasons we are allowed to do this are rather subtle. The arrows in the connection formulae are there to prevent small errors in the wave-function on one side of the classical turning point, being amplified by the exponential terms on the other side of the turning point. In this case, however, since we know that the form of the wave-function in region 3 has to be a travelling wave of WKB form, we know precisely that the cosine and sine components of equation (2.54) have to have exactly equal amplitudes. Since there can be no error here, we may safely apply connection formulae in the opposite direction to its arrow.

To derive the form of the wave-function in region 1, we need to rewrite equation (2.55) such that the limits in the integrals are in the correct form for application of connection formulae across the classical turning point at $x = a$. We do this, via the identity

$$\begin{aligned} \exp\left[\int_x^b q(x')dx'/\hbar\right] &= \exp\left[\int_a^b q(x')dx'/\hbar\right]\exp\left[-\int_a^x q(x')dx'/\hbar\right] \\ &= r\exp\left[-\int_a^x q(x')dx'/\hbar\right] \end{aligned} \tag{2.56}$$

where we define $r = \exp\left[\int_a^b q(x')dx'/\hbar\right]$. We can now write

$$\psi(x)_2 = \frac{A}{\sqrt{q(x)}} \left(\frac{1}{2r}\exp\left[\int_a^x q(x')dx'/\hbar\right] - ir\exp\left[-\int_a^x q(x')dx'/\hbar\right]\right) \tag{2.57}$$

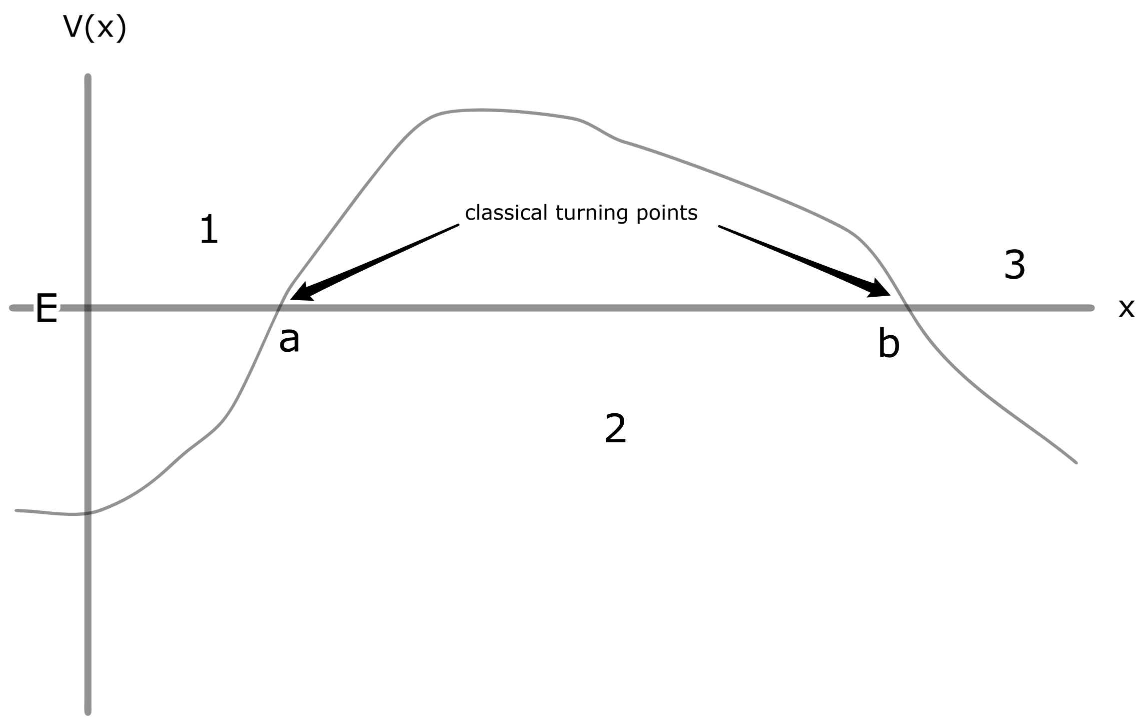

Figure 2.5: A sketch of the potential for a one-dimensional smooth barrier. Classical turning points for a particle of energy E are marked ($V(a) = V(b) = E$), which divides the space into three regions, labelled 1, 2 and 3.

and apply connection formulae across a right-hand barrier to obtain a wave-function for region 1.

$$\psi(x)_1 = \frac{A}{\sqrt{p(x)}}\left(-\frac{1}{2r}\sin\left[\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right] - 2ir\cos\left[\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right]\right) \tag{2.58}$$

To tidy up this expression a little, let's define $\phi(x) = \left[\int_x^a p(x')dx'/\hbar - \frac{\pi}{4}\right]$ and write

$$\begin{aligned}\psi(x)_1 &= \frac{A}{\sqrt{p(x)}}\left(-\frac{1}{2r}\sin\phi(x) - 2ir\cos\phi(x)\right)\\ &= \frac{iA}{\sqrt{p(x)}}\left[\left(\frac{1}{4r}-r\right)e^{i\phi(x)} - \left(\frac{1}{4r}+r\right)e^{-i\phi(x)}\right]\end{aligned} \tag{2.59}$$

The wave-function in this region is now expressed in WKB travelling waves. Somewhat counterintuitively, $e^{-i\phi(x)}$ is the incident wave and $e^{i\phi(x)}$ is the reflected wave. To see why consider the limit of $e^{i\phi(x)}$ as $x \to -\infty$. We shall assume that the potential $V(x)$ tends to a constant V_0 in this limit, and that there is a value of $x = x_0$ beyond which $V(x) \approx V_0$. In this region $p(x)$ is also approximately constant with value $p_0 = \sqrt{2m(E - V_0)}$. We can thus write, for $x < x_0$

$$\begin{aligned}e^{i\phi(x)} &= e^{-i\pi/4}\exp\left[i\int_x^a p(x')dx'/\hbar\right]\\ &= e^{-i\pi/4}\exp\left[i\int_x^{x_0} p(x')dx'/\hbar\right]\exp\left[i\int_{x_0}^a p(x')dx'/\hbar\right]\\ &\approx e^{-i\pi/4}\exp\left[i\int_{x_0}^a p(x')dx'/\hbar\right]\exp\left[i(p_0(x_0-x)/\hbar)\right]\\ &\propto \exp[-ip_0x/\hbar]\end{aligned} \tag{2.60}$$

We can write the wave-function for region 1 as

$$\psi(x)_1 = \psi_I(x) + \psi_R(x) \tag{2.61}$$

where $\psi_I(x)$ represents incident flux, travelling towards the barrier, and $\psi_R(x)$ is associated with reflected flux. In the region $x \ll x_0$ far away from the barrier, $\psi_I(x)$ takes the form

$$\psi_I(x) \approx \frac{-iA}{\sqrt{p_0}}e^{i\alpha}\left(\frac{1}{4r}+r\right)e^{ip_0x/\hbar} \tag{2.62}$$

where $e^{i\alpha} = e^{i\pi/4} \exp\left[-i\int_{x_0}^{a} p(x')dx'/\hbar\right] \exp[-ip_0x_0/\hbar]$ is a constant phase.

If we assume that on the right-hand side of the barrier, the potential also converges to the constant value $V(x) \to V_0$ as $x \to \infty$, then we can write the wave function in region 3

$$\psi_3(x) \approx \frac{A}{\sqrt{p_0}} e^{i\alpha'} e^{p_0 x/\hbar} \tag{2.63}$$

where $e^{i\alpha'}$ similarly represents constant phases which are unimportant for the following calculation.

Using equation (2.51) we find that the probability currents for the incident and transmitted (region 3) waves are

$$J_I = \frac{|A|^2}{m}\left|\frac{1}{4r} + r\right|^2 \tag{2.64}$$

and

$$J_T = \frac{|A|^2}{m} \tag{2.65}$$

and the transmission coefficient is therefore

$$\frac{J_T}{J_I} = \frac{1}{\left|\frac{1}{4r} + r\right|^2} \tag{2.66}$$

For the WKB approximation to be valid, we require that the turning points are well-separated and the barrier is significantly higher than the particle's energy. In such a domain,

$$r = \exp\left[\int_a^b q(x')dx'/\hbar\right] \gg 1 \tag{2.67}$$

In this limit, for $r \gg 1$, the transmission coefficient simplifies to

$$\frac{J_T}{J_I} \approx \frac{1}{r^2} = e^{-2\int_a^b q(x')dx'/\hbar} = e^{-2\lambda} \tag{2.68}$$

where $\lambda = \int_a^b q(x')dx'/\hbar$.

Thus we see that in the WKB approximation, the tunnelling coefficient, representing the probability of tunnelling for a single incident particle, has a simple expression, related to the integral over $q(x)$ across the barrier.