Chapter 3

Semiclassical approximation

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3.1 The classical limit

The WKB approximation provides approximate solutions for linear differential equations with coefficients that have slow spatial variation. The acronym WKB stands for Wentzel, Kramers, Brillouin, who independently discovered it in 1926. It was in fact discovered earlier, in 1923 by the mathematician Jeffreys. When applied to quantum mechanics, it is called the *semi-classical* approximation, since classical physics then illuminates the main features of the *quantum* wavefunction.

The de Broglie wavelength λ of a particle can help us assess if classical physics is relevant to the physical situation. For a particle with momentum p we have

$$\lambda = \frac{h}{p}\,. \tag{3.1.1}$$

Classical physics provides useful physical insight when λ is much smaller than the relevant length scale in the problem we are investigating. Alternatively if we take $h \to 0$ this will formally make $\lambda \to 0$, or λ smaller than the length scale of the problem. Being a constant of nature, we cannot really make $\hbar \to 0$, so taking this limit is a thought experiment in which we imagine worlds in which h takes smaller and smaller values making classical physics more and more applicable. The semi-classical approximation studied here will be applicable if a suitable generalization of the de Broglie wavelength discussed below is small and slowly varying. The semi-classical approximation will be set up mathematically by thinking of $\hbar$ as a parameter that can be taken to be as small as desired.

Our discussion in this chapter will focus on one-dimensional problems. Consider therefore a particle of mass m and total energy E moving in a potential $V(x)$. In classical physics $E - V(x)$ is the kinetic energy of the particle at x. This kinetic energy depends on position.

Since kinetic energy is $\frac{p^2}{2m}$ this suggests the definition of the **local momentum** $p(x)$:

$$p^2(x) \equiv 2m(E - V(x)).\tag{3.1.2}$$

The local momentum $p(x)$ is the momentum of the classical particle when it is located at x. With a notion of local momentum, we can define a **local de Broglie wavelength** $\lambda(x)$ by the familiar relation:

$$\boxed{\lambda(x) \equiv \frac{h}{p(x)} = \frac{2\pi\hbar}{p(x)}.}\tag{3.1.3}$$

The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = (E - V(x))\psi(x).\tag{3.1.4}$$

can be written nicely in terms of the local momentum squared :

$$-\hbar^2\frac{\partial^2}{\partial x^2}\psi = p^2(x)\,\psi.\tag{3.1.5}$$

Using the momentum operator, this equation takes the suggestive form

$$\boxed{\hat{p}^2\,\psi(x) = p^2(x)\,\psi(x).}\tag{3.1.6}$$

This has the flavor of an eigenvalue equation but it is not one: the action of the momentum operator squared on the wavefunction is not really proportional to the wavefunction, it is the wavefunction multiplied by the 'classical' position-dependent momentum-squared.

A bit of extra notation is useful. If we are in the classically allowed region, $E > V(x)$ and $p^2(x)$ is positive. We then write

$$p^2(x) = 2m(E - V(x)) = \hbar^2 k^2(x),\tag{3.1.7}$$

introducing the local, real wavenumber $k(x)$. If we are in the classically forbidden region, $V(x) > E$ and $p^2(x)$ is negative. We then write

$$-p^2(x) = 2m(V(x) - E) = \hbar^2\kappa^2(x),\tag{3.1.8}$$

introducing the local, real $\kappa(x)$.

The wavefunctions we use in the WKB approximation are often expressed in polar form. Just like any complex number z can be written as $re^{i\theta}$, where r and θ are the magnitude and phase of z, respectively, we can write the wavefunction in a similar way:

$$\Psi(\mathbf{x}, t) = \sqrt{\rho(\mathbf{x}, t)}\,\exp\left(\frac{i}{\hbar}\mathcal{S}(\mathbf{x}, t)\right).\tag{3.1.9}$$

We are using here three-dimensional notation for generality. By definition, the functions $\rho(\mathbf{x}, t)$ and $\mathcal{S}(\mathbf{x}, t)$ are real. The function ρ is non-negative and the function $\mathcal{S}(\mathbf{x}, t)$ as written, has units of $\hbar$. The name $\rho(\mathbf{x}, t)$ is well motivated, for it is in fact the probability density:

$$\rho(\mathbf{x}, t) = |\Psi(\mathbf{x}, t)|^2. \tag{3.1.10}$$

Let's compute the probability current. For this we begin by taking the gradient of the wavefunction

$$\nabla \Psi = \frac{1}{2} \frac{\nabla \rho}{\sqrt{\rho}} e^{\frac{i\mathcal{S}}{\hbar}} + \frac{i}{\hbar} \nabla \mathcal{S} \, \Psi \tag{3.1.11}$$

We then form:

$$\Psi^* \nabla \Psi = \frac{1}{2} \nabla \rho + \frac{i}{\hbar} \rho \nabla \mathcal{S} \tag{3.1.12}$$

The current is given by

$$\mathbf{J} = \frac{\hbar}{m} \, \text{Im} \left(\Psi^* \nabla \Psi \right). \tag{3.1.13}$$

It follows that

$$\boxed{\mathbf{J} = \rho \frac{\nabla \mathcal{S}}{m}.} \tag{3.1.14}$$

This formula implies that the probability current $\mathbf{J}$ is perpendicular to the surfaces of constant $\mathcal{S}$, the surfaces of constant phase in the wavefunction.

In classical physics a fluid with density $\rho(\mathbf{x})$ moving with velocity $\mathbf{v}(\mathbf{x})$ has a current density $\rho \mathbf{v} = \rho \frac{\mathbf{p}}{m}$. Comparing with the above expression for the quantum probability current, we deduce that

$$\mathbf{p}(\mathbf{x}) \simeq \nabla \mathcal{S}. \tag{3.1.15}$$

We use the $\simeq$ because this is an association that is not of general validity. Nevertheless, for 'basic' WKB solutions we will see that the gradient of $\mathcal{S}$ is indeed the classical local momentum! This association also holds for a free particle:

Example. Consider a free particle with momentum $\mathbf{p}$ and energy E. Its wavefunction is

$$\Psi(\mathbf{x}, t) = \exp \left[\frac{i\mathbf{p} \cdot \mathbf{x}}{\hbar} - \frac{iEt}{\hbar} \right]. \tag{3.1.16}$$

Here we identify the function $\mathcal{S}$ as $\mathcal{S} = \mathbf{p} \cdot \mathbf{x} - Et$ and therefore $\nabla \mathcal{S} = \mathbf{p}$. In this case $\nabla \mathcal{S}$ is equal to the momentum eigenvalue, a constant.

3.2 WKB approximation scheme

Our aim here is to find approximate solutions for the wavefunction $\psi(x)$ that solves the time independent Schrödinger equation in one dimension. We wrote before the polar decomposition (3.1.9) of the wavefunction. It will be easier to set the approximation scheme by

using a single complex function $S(x)$ to represent the time-independent wavefunction $\psi(x)$. For this we use a *pure* exponential without any prefactor:

$$\psi(x) = \exp\left(\frac{i}{\hbar}S(x)\right), \quad S(x) \in \mathbb{C}. \tag{3.2.1}$$

As before S must have units of $\hbar$. This $S(x)$ here is a *complex* number, because wavefunctions are not in general pure phases. The real part of S, divided by $\hbar$, is the phase of the wavefunction. The imaginary part of $S(x)$ determines the magnitude of the wavefunction.

Let us plug this into the Schrödinger equation (3.1.5):

$$-\hbar^2 \frac{d^2}{dx^2}\left(e^{\frac{i}{\hbar}S(x)}\right) = p^2(x)e^{\frac{i}{\hbar}S(x)}. \tag{3.2.2}$$

Let us examine the left-hand side and take the two derivatives

$$-\hbar^2 \frac{d^2}{dx^2}\left(e^{\frac{i}{\hbar}S(x)}\right) = -\hbar^2\frac{d}{dx}\left(\frac{i}{\hbar}S'(x)e^{\frac{i}{\hbar}S(x)}\right) = -\hbar^2\left(\frac{iS''}{\hbar} - \frac{(S')^2}{\hbar^2}\right)e^{\frac{i}{\hbar}S(x)}. \tag{3.2.3}$$

Back into the differential equation and canceling the common exponential

$$-\hbar^2\left(\frac{iS''}{\hbar} - \frac{(S')^2}{\hbar^2}\right) = p^2(x). \tag{3.2.4}$$

With minor rearrangements we get our final form:

$$\boxed{(S'(x))^2 - i\hbar S''(x) = p^2(x).} \tag{3.2.5}$$

The presence of an explicit i in the equation tells us that the solution for S, as expected, cannot be real. At first sight one may be baffled: we started with the linear Schrödinger equation for ψ and obtained a *nonlinear* equation for S! This is actually unavoidable when the variable ψ is parameterized as an exponential and reminds us that sometimes a change of variables can turn a linear equation into a nonlinear one and viceversa. The nonlinear equation (3.2.5) allows us set up an approximation scheme in which $\hbar$ is considered small and thus the term involving $S''(x)$ is small. We will argue that this is in fact true for slowly varying potentials.

Claim: $i\hbar S''$ small if $V(x)$ is slowly varying.

Indeed, if $V(x) = V_0$ is a constant, then the local momentum $p(x)$ is equal to a constant p_0. Equation (3.2.5) is then solved by taking $S' = p_0$. For this choice $S'' = 0$ and the term $i\hbar S''$ vanishes identically for constant V. It should therefore be small for slowly varying $V(x)$.

Alternatively the term $i\hbar S''$ in the differential equation is small as $\hbar \to 0$, which makes the local de Broglie wavelength go to zero. In that case, the potential looks constant to the quantum particle.

We will thus take $\hbar$ to be the small parameter in a systematic expansion of $S(x)$:

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + \mathcal{O}(\hbar^3) \,. \tag{3.2.6}$$

Here S_0, just like S, has units of $\hbar$. The next correction S_1 has no units, and the following, S_2 has units of one over $\hbar$. Now plug this expansion into our nonlinear equation (3.2.5)

$$\left(S_0' + \hbar S_1' + \hbar^2 S_2' + \ldots\right)^2 - i\hbar \left(S_0'' + \hbar S_1'' + \hbar^2 S_2'' + \ldots\right) - p^2(x) = 0 \,. \tag{3.2.7}$$

The left-hand side is a power series expansion in $\hbar$. Just as we argued for the parameter λ in perturbation theory, here we want the left-hand side to vanish for all values of $\hbar$ and this requires that the coefficient of each power of $\hbar$ vanishes. We thus sort the left-hand side terms neglecting terms of order $\hbar^2$ or higher. We find

$$(S_0')^2 - p^2 + \hbar\left(2S_0'S_1' - iS_0''\right) + \mathcal{O}\left(\hbar^2\right) = 0 \tag{3.2.8}$$

This gives two equations, one for the coefficient of $(\hbar)^0$ and another for the coefficient of $\hbar$:

$$\begin{aligned} (S_0')^2 - p^2(x) &= 0 \,, \\ 2S_0'S_1' - iS_0'' &= 0 \,. \end{aligned} \tag{3.2.9}$$

The first equation is easily solved:

$$S_0' = \pm p(x) \quad \rightarrow \quad S_0(x) = \pm \int_{x_0}^{x} p(x')dx' \tag{3.2.10}$$

where x_0 is a constant of integration to be adjusted. The next equation allows us to find S_1 which is in fact imaginary:

$$S_1' = \frac{i}{2}\frac{S_0''}{S_0'} = \frac{i}{2}\frac{(\pm p'(x))}{(\pm p(x))} = \frac{i}{2}\frac{p'}{p} \,. \tag{3.2.11}$$

This is readily solved to give

$$i\,S_1(x) = -\tfrac{1}{2}\ln p(x) + C' \,. \tag{3.2.12}$$

Let us now reconstruct the wavefunction to this order of approximation:

$$\psi(x) = \exp\left[\frac{i}{\hbar}(S_0 + \hbar S_1 + \mathcal{O}(\hbar^2))\right] \simeq \exp\left[\frac{i}{\hbar}S_0\right]\exp\left[iS_1\right] \tag{3.2.13}$$

Using our results for S_0 and S_1 we have that the approximate solution is

$$\psi(x) = \exp\left[\pm\frac{i}{\hbar}\int_{x_0}^{x} p(x')dx'\right]\exp\left[-\tfrac{1}{2}\log p(x) + C'\right] \,. \tag{3.2.14}$$

We thus have

$$\psi(x) = \frac{A}{\sqrt{p(x)}} \exp\left[\pm\frac{i}{\hbar}\int_{x_0}^{x} p(x')dx'\right] . \tag{3.2.15}$$

This is the basic solution in the WKB approximation. We do not attempt to normalize this wavefunction because, in fact, the region of validity of this approximation is still unclear.

Observables for the basic solution:

i) Probability density:

$$\rho = \psi^*\psi = \frac{|A|^2}{p(x)} = \frac{|A|^2}{mv(x)}, \tag{3.2.16}$$

where $v(x)$ is the local classical velocity. Note that ρ is higher where v is small as the particle lingers in those regions and is more likely to be found there. This is an intuition we developed long ago and is justified by this result.

ii) Probability current: In the language of the polar decomposition (3.1.9) of the wavefunction the basic solution corresponds to

$$S(x) = \int_{x_0}^{x} p(x')dx' \tag{3.2.17}$$

Note that, as anticipated below equation (3.1.15) the gradient of S in the basic solution is the local momentum. Recalling the result (3.1.14) for the current,

$$J = \rho\frac{1}{m}\frac{\partial S}{\partial x}, \tag{3.2.18}$$

and therefore,

$$J(x) = \frac{|A|^2}{p(x)}\frac{p(x)}{m} = \frac{|A|^2}{m}. \tag{3.2.19}$$

The fact that the current is a constant should not have taken us by surprise. A position-dependent current for an energy eigenstate is not possible, as it would violate the current conservation equation $\partial_x J(x) + \partial_t \rho = 0$, given that ρ is time independent.

We con now write the general solutions that can be built from the basic solution and apply to classically allowed and classically forbidden regions.

On the allowed region $E - V(x) > 0$ we write $p^2(x) = \hbar^2 k^2(x)$, with $k(x) > 0$ and hence the general solution is a superposition of two basic solutions with waves propagating in opposite directions:

$$\psi(x) = \frac{A}{\sqrt{k(x)}} \exp\left[i\int_{x_0}^{x} k(x')dx'\right] + \frac{B}{\sqrt{k(x)}} \exp\left[-i\int_{x_0}^{x} k(x')dx'\right] . \tag{3.2.20}$$

Note that the first wave, with coefficient A moves to the right while the second wave, with coefficient B moves to the left. This can be seen by recalling that the above energy eigenstate $\psi(x)$ is accompanied by the time factor $e^{-iEt/\hbar}$ when forming a full solution of the Schrödinger equation. Moreover, the first phase (accompanying A) grows as x grows, while the second phase becomes more negative as x grows.

On the forbidden region $p^2 = -\hbar^2\kappa^2(x)$ so we can take $p(x) = i\kappa(x)$ in the solution, with $\kappa > 0$, to find

$$\psi(x) \;=\; \frac{C}{\sqrt{\kappa(x)}} \exp\left[\int_{x_0}^{x} \kappa(x')dx'\right] + \frac{D}{\sqrt{\kappa(x)}} \exp\left[-\int_{x_0}^{x} \kappa(x')dx'\right] \tag{3.2.21}$$

The argument of the first exponential becomes more positive as x grows. Thus the first term, with coefficient C, is an increasing function as x grows. The argument of the second exponential becomes more negative x grows. Thus the second term, with coefficient D, is a decreasing function as x grows.

3.2.1 Validity of the approximation

To understand more concretely the validity of our approximations, we reconsider the expansion (3.2.8) of the differential equation:

$$(S_0')^2 - p^2 \;+\; \hbar\left(2S_0'S_1' - iS_0''\right) + \mathcal{O}\left(\hbar^2\right) = 0 \tag{3.2.22}$$

We must have that the $\mathcal{O}(\hbar)$ terms in the differential equation are much smaller, in magnitude, than the $\mathcal{O}(1)$ terms. At each of these orders we have two terms that are set equal to each other by the differential equations. It therefore suffices to check that one of the $\mathcal{O}(\hbar)$ terms is much smaller than one of the $\mathcal{O}(1)$ terms. Thus, for example, we must have

$$|\hbar S_0'S_1'| \;\ll\; |S_0'|^2. \tag{3.2.23}$$

Canceling one factor of $|S_0'|$ and recalling that $|S_0'| = |p|$ we have

$$|\hbar S_1'| \;\ll\; |p|. \tag{3.2.24}$$

From (3.2.11) we note that $|S_1'| \sim |p'/p|$ and therefore we get

$$\left|\hbar\frac{p'}{p}\right| \;\ll\; |p|. \tag{3.2.25}$$

There are two useful ways to think about this relation. First we write it as

$$\left|\frac{\hbar}{p}\right|\left|\frac{dp}{dx}\right| \;\ll\; |p| \quad \to \quad \lambda\left|\frac{dp}{dx}\right| \ll |p| \tag{3.2.26}$$

which tells us that the changes in the local momentum over a distance equal to the de Broglie wavelength are small compared to the momentum. Alternatively we write (3.2.25) as follows:

$$\left|\hbar\frac{p'}{p^2}\right| \;\ll\; 1 \quad \to \quad \left|\hbar\frac{d}{dx}\frac{1}{p}\right| \;\ll\; 1. \tag{3.2.27}$$

This now means

$$\boxed{\left|\frac{d\lambda}{dx}\right| \ll 1\,.}$$

(3.2.28)

The de Broglie wavelength must vary slowly. Note the consistency with units, the left-hand side of the inequality being unit free. More intuitive, perhaps, is the version obtained by multiplying the above by λ

$$\left|\lambda\frac{d\lambda}{dx}\right| \ll \lambda\,.$$

(3.2.29)

This tells us that the variation of the de Broglie wavelength λ over a distance λ must be much smaller that λ.

It is not hard to figure out what the above constraints tell us about the rate of change of the potential. Finally connect to the potential. Taking one spatial derivative of the equation $p^2 = 2m(E - V(x))$ we get

$$|pp'| \;=\; m\left|\frac{dV}{dx}\right| \quad \rightarrow \quad \left|\frac{dV}{dx}\right| = \frac{1}{m}|pp'|\,.$$

(3.2.30)

Multiplying by the absolute value of $\lambda = h/p$

$$\lambda(x)\left|\frac{dV}{dx}\right| = \frac{2\pi\hbar}{m}|p'| \ll \frac{p^2}{m}\,,$$

(3.2.31)

where the last inequality follows from (3.2.25). Hence, we find that

$$\boxed{\lambda(x)\left|\frac{dV}{dx}\right| \;\ll\; \frac{p^2}{2m}\,.}$$

(3.2.32)

The change in the potential over a distance equal to the de Broglie wavelength must be much smaller than the kinetic energy. This is the precise meaning of a slowly changing potential in the WKB approximation.

The slow variation conditions needed for the basic WKB solutions to be accurate fail near turning points. This could be anticipated since at turning points the local momentum becomes zero and the de Broglie wavelength becomes infinite. Under general conditions, sufficiently near a turning point the potential $V(x)$ is approximately linear, as shown in Figure 3.1. We then have

$$V(x) - E \;=\; g(x - a)\,, \quad g > 0\,.$$

(3.2.33)

In the allowed region $x < a$ the local momentum is
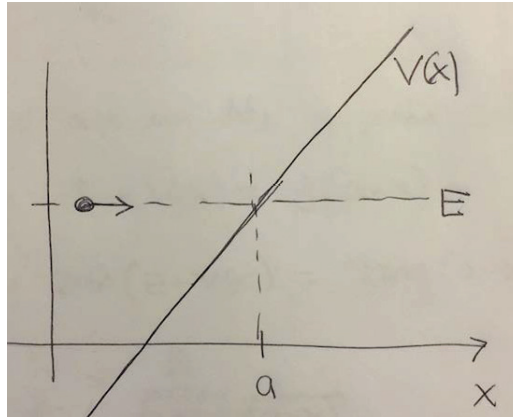
$$p^2 \;=\; 2m((E - V(x)) \;=\; 2mg(a - x)\,.$$

(3.2.34)

Figure 3.1: The slow-varying conditions in WKB are violated at turning points.

As a result, the de Broglie wavelength is given by

$$\lambda(x) \;=\; \frac{2\pi\hbar}{p} \;=\; \frac{2\pi\hbar}{\sqrt{2mg}\sqrt{a-x}}\,. \tag{3.2.35}$$

Taking a derivative, we find

$$\left|\frac{d\lambda}{dx}\right| \;=\; \frac{\pi\hbar}{\sqrt{2mg}}\frac{1}{(a-x)^{3/2}}\,. \tag{3.2.36}$$

The right-hand side goes to infinity as $x \to a$ and therefore the key condition (3.2.28) is violated as we approach turning points. Our basic WKB solutions can be valid only as long as we remain away from turning points. If we have a turning point, such as $x = a$ in the figure, we need a 'connection formula' that tells us how a solution far to the left and a solution far to the right of the turning point are related when they together form a single solution. We will consider a connection formula right below.

3.3   Connection formula

Let us first explain and then use a set of connection formulae, leaving their derivation for next section. The connection formulae refer to solutions away from a turning point $x = a$ separating a classically allowed region to the left and a classically forbidden region to the right. This is the situation illustrated in Figure 3.2.

For such turning point at $x = a$ the WKB solutions to the right are exponentials that grow or decay and the WKB solutions to the left are oscillatory functions. They connect
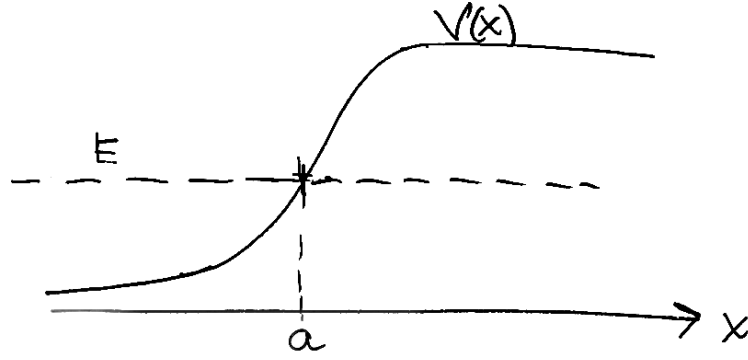
Figure 3.2:

consistent with the following relations

$$\frac{2}{\sqrt{k(x)}} \cos \left(\int_x^a k(x')dx' - \frac{\pi}{4} \right) \;\Longleftarrow\; \frac{1}{\sqrt{\kappa(x)}} \exp \left(- \int_a^x \kappa(x')dx' \right) \tag{3.3.1}$$

$$-\frac{1}{\sqrt{k(x)}} \sin \left(\int_x^a k(x')dx' - \frac{\pi}{4} \right) \;\Longrightarrow\; \frac{1}{\sqrt{\kappa(x)}} \exp \left(\int_a^x \kappa(x')dx' \right) \tag{3.3.2}$$

In the first relation the arrow tells us that if the solution is a pure decaying exponential to the right of $x = a$ the solution to the left of $x = a$ is accurately determined and given by the phase-shifted cosine function the arrow points to. The second relation says that if the solution to the left of $x = a$ is of an oscillatory type, the *growing part* of the solution to the right of $x = a$ is accurately determined and given by the exponential the arrow points to. The decaying part cannot be reliably determined. As we will elaborate upon later, any connection formula is not to be used in the direction that goes against the arrow.

Example: Find a quantization condition for the energies of bound states in a monotonically increasing potential $V(x)$ that has a hard wall at $x = 0$. Assume $V(x)$ increases without bound, as illustrated in Figure 3.3.

Let E denote the energy of our searched-for eigenstate. Clearly, the energy and the potential $V(x)$ determine the turning point $x = a$. The solution for $x > a$ must only have a decaying exponential since the forbidden region extends forever to the right of $x = a$. The wavefunction for $x > a$ is therefore of the type on the right-side of the connection formula (3.3.1). This means that we have an accurate representation of the wavefunction to the left of $x = a$. Adjusting the arbitrary normalization, we have

$$\psi(x) = \frac{1}{\sqrt{k(x)}} \cos \left(\int_x^a k(x')dx' - \tfrac{\pi}{4} \right), \quad 0 \le x \ll a. \tag{3.3.3}$$
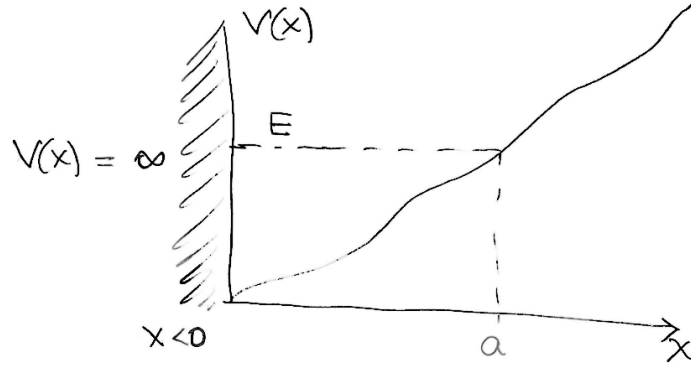
Figure 3.3: A monotonically increasing potential with a hard wall at $x = 0$. For an energy eigenstate of energy E the turning point is at $x = a$.

Since we have a hard wall, the wavefunction must vanish for $x = 0$. The condition $\psi(0) = 0$ requires that

$$\cos \Delta = 0, \quad \text{with} \quad \Delta = \int_0^a k(x')dx' - \tfrac{\pi}{4}. \tag{3.3.4}$$

This is satisfied when

$$\Delta = \int_0^a k(x')dx' - \tfrac{\pi}{4} = \tfrac{\pi}{2} + n\pi, \quad n \in \mathbb{Z}. \tag{3.3.5}$$

The quantization condition is therefore

$$\int_0^a k(x')dx' = \left(n + \tfrac{3}{4}\right)\pi, \quad n = 0, 1, 2, \dots . \tag{3.3.6}$$

Negative integers are not allowed because the left-hand side is manifestly positive. The above is easy to use in practice. Using the expression for $k(x)$ in terms of E and $V(x)$ we have

$$\int_0^a \sqrt{\frac{2m}{\hbar^2}(E - V(x'))}\, dx' = \left(n + \tfrac{3}{4}\right)\pi, \quad n = 0, 1, 2, \dots \tag{3.3.7}$$

In some special cases a can be calculated in terms of E and the integral can be done analytically. More generally, this is done numerically, exploring the value of the integral on the left hand side as a function of E and selecting the energies for which it takes the quantized values on the right-hand side.

Let us rewrite the wavefunction using $\int_x^a = \int_0^a - \int_0^x$:

$$\psi(x) = \frac{1}{\sqrt{k(x)}} \cos\left(\int_0^a k(x')dx' - \tfrac{\pi}{4} - \int_0^x k(x')dx'\right)$$

$$= \frac{1}{\sqrt{k(x)}} \cos\left(\Delta - \int_0^x k(x')dx'\right) \tag{3.3.8}$$

$$= \frac{\sin\Delta}{\sqrt{k(x)}} \sin\left(\int_0^x k(x')dx'\right),$$

where we expanded the cosine of a sum of angles and recalled that $\cos\Delta = 0$. In this form it is manifest that the wavefunction vanishes at $x = 0$. More interestingly, the quantization condition (3.3.6) indicates that the excursion of the phase in the solution from 0 to a is a bit higher than $n\pi$ (but less than $(n+1)\pi$). Thus the WKB wavefuntion produces the n nodes the n-th excited state must have, even though this wavefunction is not reliable all to way to $x = a$.

3.4 Airy functions and connection formulae

$$(3.4.9)$$
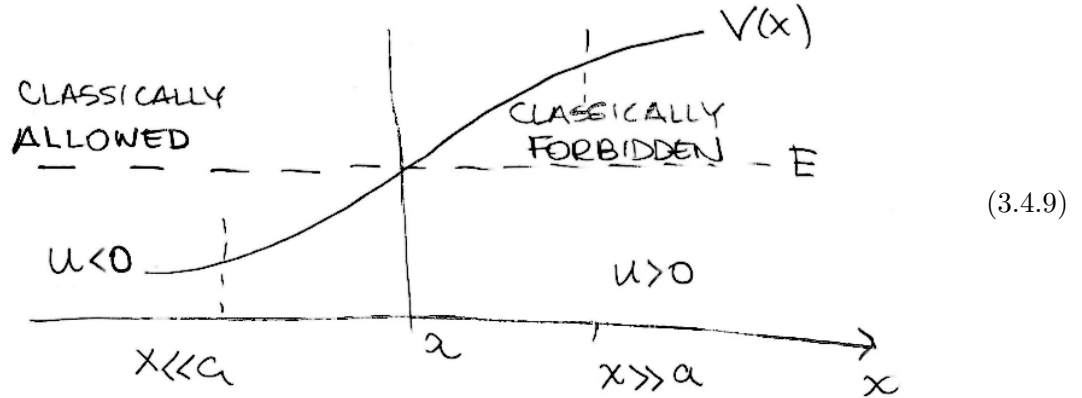
$$V(x) - E \simeq g(x - a) \qquad\qquad \text{with } g > 0 \text{ for } x \sim a \tag{3.4.10}$$

Solutions

$$\psi(x) = \frac{A}{\sqrt{\kappa(x)}} \exp\left(-\int_a^x \kappa(x')dx'\right) + \frac{B}{\sqrt{\kappa(x)}} \exp\left(\int_a^x \kappa(x')dx'\right) \qquad x \gg a \tag{3.4.11}$$

$$\psi(x) = \frac{C}{\sqrt{k(x)}} \exp\left(i\int_x^a k(x')dx'\right) + \frac{D}{\sqrt{k(x)}} \exp\left(-i\int_x^a k(x')dx'\right) \qquad x \ll a \tag{3.4.12}$$

where

$$k^2 \equiv \frac{2m}{\hbar^2}(E - V(x)) \simeq \frac{2mg}{\hbar^2}(a - x) \quad x \le a \tag{3.4.13}$$

$$\kappa^2 \equiv \frac{2m}{\hbar^2}(V(x) - E) \simeq \frac{2mg}{\hbar^2}(x - a) \quad x \ge a \tag{3.4.14}$$

Idea: Solve Schrodinger equation

$$-\frac{\hbar^2}{2m}\psi'' + (V(x) - E)\psi = 0 \tag{3.4.15}$$

with the exact linear potential, i.e.

$$-\frac{\hbar^2}{2m}\psi'' + g(x - a)\psi = 0 \tag{3.4.16}$$

- Solve (3.4.16) exactly.

- Match it to the $x \gg a$ version of (3.4.11) or $x \ll a$ version of (3.4.12).

- Find the required relations between coefficients!

Solve (3.4.16). Remove units, find length scale.

$$\frac{\hbar^2}{mL^2} = gL \implies L = \left(\frac{\hbar^2}{mg}\right)^{\frac{1}{3}} \tag{3.4.17}$$

so define

$$u = \left(\frac{2mg}{\hbar^2}\right)^{\frac{1}{3}}(x - a) \equiv \eta(x - a) \tag{3.4.18}$$

thus (3.4.16) becomes

$$\boxed{\frac{d^2\psi}{du^2} - u\psi = 0} \tag{3.4.19}$$

with solution

$$\psi = \alpha A_i(u) + \beta B_i(u) \tag{3.4.20}$$

where α and β are constants and $A_i(u)$, $B_i(u)$ are Airy functions:

$$A_i(u) \simeq \begin{cases} \frac{1}{2}\frac{1}{\sqrt{\pi}}|u|^{-\frac{1}{4}}e^{-\xi} & u \gg 1, \\ \frac{1}{\sqrt{\pi}}|u|^{-\frac{1}{4}}\cos\left(\xi - \frac{\pi}{4}\right) & u \ll -1. \end{cases} \tag{3.4.21}$$

$$B_i(u) \simeq \begin{cases} \frac{1}{\sqrt{\pi}}|u|^{-\frac{1}{4}}e^{\xi} & u \gg 1, \\ -\frac{1}{\sqrt{\pi}}|u|^{-\frac{1}{4}}\sin\left(\xi - \frac{\pi}{4}\right) & u \ll -1. \end{cases} \tag{3.4.22}$$

with

$$\xi \equiv \frac{2}{3}|u|^{\frac{3}{2}}. \tag{3.4.23}$$

These are in fact WKB solutions and special cases of connection conditions! (Explain)

3.4.1   How bad are the errors?

Take a WKB solution and find the DE it satisfies

$$\psi(u) = \frac{1}{u^{\frac{1}{4}}} e^{-\frac{2}{3}|u|^{\frac{3}{2}}} \tag{3.4.24}$$

solves

$$\frac{d^2\psi}{du^2} - \left(u + \frac{5}{16}\frac{1}{u^2}\right)\psi = 0 \tag{3.4.25}$$

so clearly for $u \gg 1$ the extra term is negligible.

To evaluate (3.4.11) and (3.4.12), determine $\kappa(x)$ and $k(x)$. Using (3.4.13) and (3.4.14):

$$k^2 = \eta^3(a - x) = -\eta^2 u = \eta^2|u| \qquad\qquad u < 0 \tag{3.4.26}$$
$$\kappa^2 = \eta^3(x - a) = +\eta^2 u \qquad\qquad u > 0 \tag{3.4.27}$$

Using $' = \frac{d}{dx}$, the WKB condition is $|k'| \ll |k^2|$ From ...

$$|2kk'| = \eta^3 \implies |k'| = \frac{\eta^3}{2|k|} = \frac{\eta^3}{2\eta|u|} = \frac{\eta^2}{2|u|} \tag{3.4.28}$$

$k^2 = \eta^2|u|$ thus

$$|k'| \ll k^2, \frac{\eta^2}{2|u|} \ll \eta^2|u| \implies |u|^{\frac{3}{2}} \gg \frac{1}{2} \implies |u| \gg 0.63 \tag{3.4.29}$$

Two integrals to estimate

$$x > a: \qquad \int_a^x \kappa(x')dx' = \int_a^x \sqrt{\eta^3(x' - a)}dx' = \frac{2}{3}\eta^{\frac{3}{2}}(x' - a)^{\frac{3}{2}}\Big|_a^x$$
$$= \frac{2}{3}\eta^{\frac{3}{2}}(x - a)^{\frac{3}{2}} = \frac{2}{3}u^{\frac{3}{2}} = \frac{2}{3}|u|^{\frac{3}{2}} = \xi \tag{3.4.30}$$

$$x < a: \qquad \int_x^a k(x')dx' = \int_x^a \sqrt{\eta^3(a - x')}dx' = \eta^{\frac{3}{2}}\left[-\frac{2}{3}(a - x')^{\frac{3}{2}}\right]_x^a$$
$$= \frac{2}{3}\eta^{\frac{3}{2}}(a - x)^{\frac{3}{2}} = \frac{2}{3}|u|^{\frac{3}{2}} = \xi \tag{3.4.31}$$

both integrals are equal to ξ.

$$\frac{1}{\sqrt{\kappa(x)}} = \frac{1}{\eta^{\frac{1}{2}}|u|^{\frac{1}{4}}}, \qquad \frac{1}{\sqrt{k(x)}} = \frac{1}{\eta^{\frac{1}{2}}|u|^{\frac{1}{4}}} \tag{3.4.32}$$

(3.4.11) and (3.4.12), let $\{A, B, C, D\} \to \eta^{\frac{1}{2}}\{A, B, C, D\}\frac{1}{\sqrt{\pi}}$ to cancel the extra factor and produce the ... constants

$$\psi(x) = A\frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{-\xi} + B\frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{\xi} \qquad\qquad u \gg 1$$
$$= 2AA_i(u) + BB_i(u) \tag{3.4.33}$$

$$\psi(x) = C\frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{i\xi} + D\frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{-i\xi} \qquad\qquad u \ll -1 \qquad (3.4.34)$$

Note that

$$A_i + iB_i = \frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{-i\left(\xi-\frac{\pi}{4}\right)} \tag{3.4.35}$$

$$A_i - iB_i = \frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{i\left(\xi-\frac{\pi}{4}\right)} \tag{3.4.36}$$

thus

$$e^{i\frac{\pi}{4}}\left(A_i - iB_i\right) = \frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{i\xi} \tag{3.4.37}$$

$$e^{-i\frac{\pi}{4}}\left(A_i + iB_i\right) = \frac{|u|^{-\frac{1}{4}}}{\sqrt{\pi}}e^{-i\xi} \tag{3.4.38}$$

Now back in (3.4.34):

$$\psi(x) = Ce^{i\frac{\pi}{4}}\left(A_i - iB_i\right) + De^{-i\frac{\pi}{4}}\left(A_i + iB_i\right)$$
$$= \left(Ce^{i\frac{\pi}{4}} + De^{-i\frac{\pi}{4}}\right)A_i + \left(iDe^{-i\frac{\pi}{4}} - iCe^{i\frac{\pi}{4}}\right)B_i \tag{3.4.39}$$

Finally equate (one solution):

$$2A = Ce^{i\frac{\pi}{4}} + De^{-i\frac{\pi}{4}} \tag{3.4.40}$$
$$iB = Ce^{i\frac{\pi}{4}} - De^{-i\frac{\pi}{4}} \implies \tag{3.4.41}$$

$$C = \frac{1}{2}e^{-i\frac{\pi}{4}}(2A + iB) \tag{3.4.42}$$

$$D = \frac{1}{2}e^{i\frac{\pi}{4}}(2A - iB) \tag{3.4.43}$$
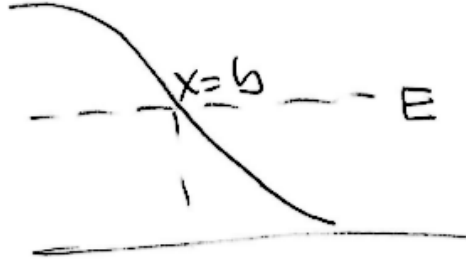
back in (3.4.12)

$$\psi(x) = \frac{1}{2}\frac{(2A + iB)}{\sqrt{k(x)}}\exp\left(i\int_x^a k(x')dx' - \frac{\pi}{4}\right) + \frac{1}{2}\frac{(2A - iB)}{\sqrt{k(x)}}\exp\left(-i\int_x^a k(x')dx' - \frac{\pi}{4}\right) \implies$$

$$\boxed{\psi(x) = \frac{2A}{\sqrt{k(x)}} \cos\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right) - \frac{B}{\sqrt{k(x)}} \sin\left(\int_x^a k(x')dx' - \frac{\pi}{4}\right)} \qquad (3.4.44)$$

Now discuss a subtlety. The formulas are in reality only usable in one direction with partial results. Some terminology helps. We always speak having in mind a fixed turning point. If we say we have a growing exponential at a turning point we mean we have a solution that grows as we move *away* from the turning point towards the classically forbidden region. Similarly, a decaying exponential means our solution decays as we move *away* from the turning point towards the classically forbidden region. In summary the connection arrow can go from a decaying exponential into an oscillatory solution and can go from an oscillatory solution into a growing exponential.

3.4.2   The other connection conditions

This time the turning point is at $x = b$, with the classically allowed region to the right of it and the classically forbidden region to the left of it.

$$\frac{1}{\sqrt{\kappa(x)}} \exp\left(-\int_x^b \kappa(x')dx'\right) \implies \frac{2}{\sqrt{k(x)}} \cos\left(\int_b^x k(x')dx' - \frac{\pi}{4}\right) \qquad (3.4.45)$$

$$-\frac{1}{\sqrt{\kappa(x)}} \exp\left(\int_x^b \kappa(x')dx'\right) \impliedby \frac{1}{\sqrt{k(x)}} \sin\left(\int_b^x k(x')dx' - \frac{\pi}{4}\right) \qquad (3.4.46)$$

For the first relation, if there is *only* a decaying exponential to the left, the wavefunction is definitely without the growing exponential, and the wavefunction to the right of $x = b$ is accurately determined. This does not work in the reverse direction because a small error in the oscillatory function would give a growing exponential to the left of for $x = b$ that would overtake the predicted decaying solution.

For the second relation, the stated direction (from right to left) is reliable: an small error on the right side of $x = b$ would produce a decaying exponential, thus a small error on the left-side of $x = b$. The reverse direction does not work: a small error to the left of $x = b$, a decaying exponential, would produce a large error in the right-hand side.

In summary, in *all cases* of the connection conditions, relative to a turning point,

> We can connect away from a decaying exponential and into a growing exponential.

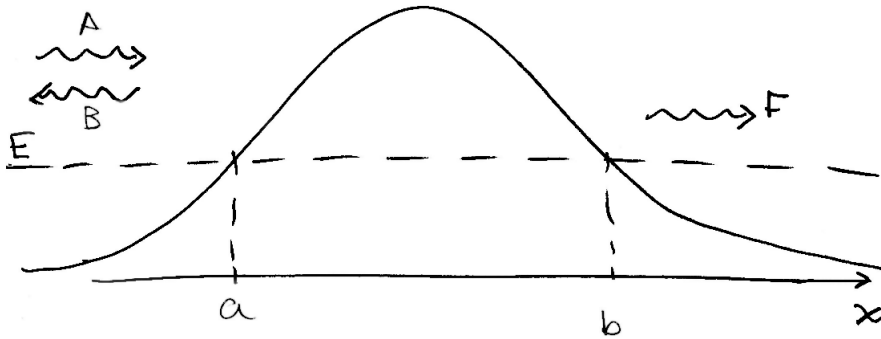$$(3.4.47)$$

3.5   Tunnelling through a barrier

Figure 3.4: Tunneling in the WKB approximation. The energy E must be smaller than the height of the potential, and the barrier must be wide and smooth.

We want to find the tunneling probability T for a wave of energy incident on a smoothly varying wide barrier. The energy E of the wave must be smaller than the height of the potential. In this problem there is an incident wave, a reflected wave and a transmitted wave, and the associated WKB expressions will have amplitudes controlled by constants A, B, and F, respectively. The situation is illustrated in Figure 3.4.
Remarks:

1) Expect T to be small. Little probability flux goes through and $|A| \approx |B|$.

2) For $x \gg b$ there is just an outgoing wave with amplitude controlled by F.

3) Within the barrier the component that decays as x grows is more relevant that the component that grows. It is the only component that can be estimated reliably.

Consider the transmitted right-moving wave valid for $x \gg b$

$$\psi_{tr}(x) \;=\; \frac{F}{\sqrt{k(x)}} \exp\left(i \int_b^x k(x')dx' - i\tfrac{\pi}{4} \right) \;, \quad x \gg b\,. \qquad (3.5.1)$$

This is a WKB solution with an extra phase of $\pi/4$ chosen to make the argument of the exponential have the familiar form appearing in the connection formulae. Expanding the

exponential

$$\psi_{tr}(x) = \frac{F}{\sqrt{k(x)}} \cos\left(\int_b^x k(x')dx' - \tfrac{\pi}{4}\right) + \frac{iF}{\sqrt{k(x)}} \sin\left(\int_b^x k(x')dx' - \tfrac{\pi}{4}\right) , \quad x \gg b . \quad (3.5.2)$$

This is in *standard form*. We can now match the second term to an exponential that grows as we move to the left of $x = b$, by using (3.4.46)

$$\psi(x)_{barr} = -\frac{iF}{\sqrt{\kappa(x)}} \exp\left(\int_x^b \kappa(x')dx'\right) , \quad a \ll x \ll b . \quad (3.5.3)$$

The subscript 'barr' indicates a solution in the barrier region. If we attempted to match the first term in (3.5.2) we would get an exponential that decays as we move to the left of $x = b$ and it is unreliable given the growing exponential. We can now refer this solution to the point $x = a$

$$\psi(x)_{barr} = -\frac{iF}{\sqrt{\kappa(x)}} \exp\left(\int_a^b \kappa(x')dx' - \int_a^x \kappa(x')dx'\right) \quad a \ll x \ll b . \quad (3.5.4)$$

Defining

$$\theta \equiv \int_a^b \kappa(x')dx' \quad (3.5.5)$$

we have

$$\psi(x)_{barr} = -\frac{iFe^\theta}{\sqrt{\kappa(x)}} \exp\left(-\int_a^x \kappa(x')dx'\right) \quad a \ll x \ll b . \quad (3.5.6)$$

Since this is a decaying exponential to the right of $x > a$ we can connect it to a solution to the left of $x < a$ using (3.3.1)

$$\psi(x) = -\frac{2iFe^\theta}{\sqrt{k(x)}} \cos\left(\int_x^a k(x')dx' - \tfrac{\pi}{4}\right) . \quad (3.5.7)$$

This is a superposition of two waves, a wave ψ_{inc} incident on the barrier and a wave ψ_{ref} reflected from the barrier. The incident part is

$$\psi_{inc}(x) = -\frac{iFe^\theta}{\sqrt{k(x)}} \exp\left(-i\int_x^a k(x')dx' + i\tfrac{\pi}{4}\right) . \quad (3.5.8)$$

The sign in front of the integral may seem unusual for a wave moving to the right, but it is correct because the argument x appears in the lower limit of the integration. The transmission coefficient T is the ratio of the transmitted probability current over the incident probability current. Given the result in (3.2.19) we have

$$T = \frac{\text{probability current for } \psi_{tr}}{\text{probability current for } \psi_{inc}} = \frac{|F|^2}{|-iFe^\theta|^2} = e^{-2\theta} . \quad (3.5.9)$$

This is the well-known exponential suppression of the transmission coefficient. Using the earlier definition of θ the result is

$$T_{\text{wkb}} \;=\; \exp\!\left(-2 \int_a^b \kappa(x')dx'\right). \tag{3.5.10}$$

We added the subscript 'wkb' to emphasize that this is the WKB approximation to the exact transmission coefficient. The integral extends in between the two turning points and captures information about the height and the width of the barrier. The integrand, as well as the turning points, depend on the energy as we can display by using the explicit value of $\kappa(x)$:

$$T_{\text{wkb}} \;=\; \exp\!\left(-2 \int_a^b \sqrt{\frac{2m}{\hbar^2}(V(x') - E)} \; dx'\right). \tag{3.5.11}$$

The WKB approximation only captures the exponentially decaying part of the transmission coefficient. There are corrections that are written as a prefactor to the exponential. These are not determined in this approximation.

Example. Use the WKB approximation to estimate the transmission probability T for the rectangular barrier

$$V(x) \;=\; \begin{cases} V_0 & \text{for} \;\; |x| < a\,, \\ 0\,, & \text{otherwise.} \end{cases} \tag{3.5.12}$$

Assume the barrier is large. In terms of the familiar unit-free constant z_0 used to characterize square wells, this means that

$$z_0^2 \;\equiv\; \frac{2mV_0 a^2}{\hbar^2} \;\gg\; 1\,. \tag{3.5.13}$$

Large barrier means large z_0 or large $V_0 a^2$. Moreover we assume E smaller than V_0; we cannot expect the approximation to work as the energy approaches the top of the barrier. Compare the WKB result for T with the exact result.
Solution. The WKB estimation, using (3.5.11) is immediate. Since the barrier extends from $x = -a$ to $x = a$ and the potential is constant we have

$$T_{\text{wkb}} \;=\; \exp\!\left(-2 \int_{-a}^a \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} \; dx'\right). \tag{3.5.14}$$

The integral can be done and we find

$$T_{\text{wkb}} \;=\; \exp\!\left(-\frac{4a}{\hbar} \sqrt{2m(V_0 - E)} \;\right). \tag{3.5.15}$$

This is the answer in the WKB approximation. In terms of z_0 this reads

$$T_{\text{wkb}} \;\simeq\; \exp\!\left(-4z_0 \sqrt{1 - \frac{E}{V_0}} \;\right). \tag{3.5.16}$$

The validity of the WKB approximation requires the argument in the exponent to be large. This is why we need $z_0 \gg 1$ and the energy not to approach V_0. When E is very small compared to V_0, we have

$$T \sim \exp(-4z_0). \tag{3.5.17}$$

Since $z_0 \sim a\sqrt{V_0}$, this result is the basis for the claim that the exponential suppression of the tunneling probability is proportional to the width of the well and the square root of its height.

The exact formula for the tunneling probability of a square barrier has been calculated before, and it is given by

$$\frac{1}{T} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2\left(\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\right). \tag{3.5.18}$$

This formula will allow us to confirm the WKB exponential suppression and to find the prefactor. Under the conditions $z_0 \gg 1$ and $V_0 - E$ finite, the argument of the sinh function is large so this function can be replaced by its growing exponential ($\sinh x \sim \frac{1}{2}e^x$):

$$\frac{1}{T} \simeq 1 + \frac{V_0}{16E(1 - \frac{E}{V_0})} \exp\left(\frac{4a}{\hbar}\sqrt{2m(V_0 - E)}\right), \tag{3.5.19}$$

where we also replaced $V_0 - E \to V_0$ in the prefactor. The additive unit on the right-hand side can be neglected and we have

$$T \simeq 16\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)\exp\left(-\frac{4a}{\hbar}\sqrt{2m(V_0 - E)}\right). \tag{3.5.20}$$

This result gives the same in exponential suppression as the WKB result (3.5.15). It also gives us a good approximation to the prefactor.

The WKB approximation is often used for the estimation of lifetimes. The physical situation is represented in Figure 3.5. We have a particle of mass m and energy E localized between the turning points $x = a$ and $x = b$ of the potential. The classical particle cannot escape because of the energy barrier stretching from $x = b$ to $x = c$. The quantum particle, however, can tunnel. The state of the quantum particle when localized between a and b is not strictly an energy eigenstate because the wavefunction for any energy eigenstate is nonzero for $x > c$. Our goal is to determine the lifetime τ of the particle. This is done by using some classical estimates as well as the quantum transmission probability.

We first show that the lifetime τ is the inverse of $\mathcal{B}$, the tunneling probability per unit time. To see this we examine the function $P(t)$ that represents the probability to have the particle localized within $[a, b]$ at time t, if it was there at $t = 0$. The lifetime is said to be τ if $P(t)$ has the time dependence $P(t) = e^{-t/\tau}$. To see that we have such a situation when the tunneling rate $\mathcal{B}$ is constant note that

$$P(t + dt) = P(t) \cdot \left(\text{probability that it does not tunnel in the next } dt\right). \tag{3.5.21}$$

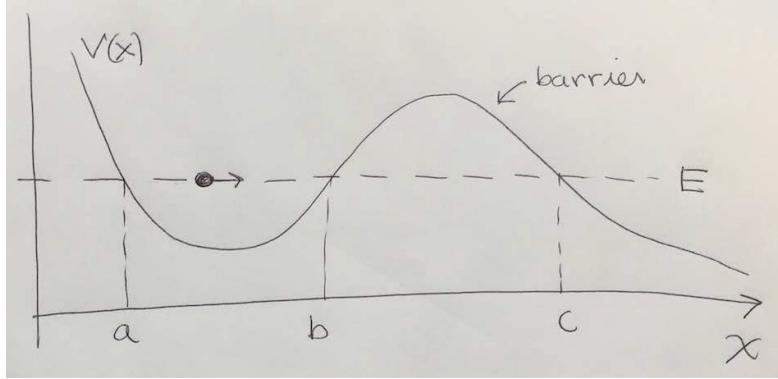Figure 3.5: Estimating the lifetime of a particle with energy E temporarily localized in $x \in [a, b]$.

Therefore

$$P(t + dt) = P(t) \cdot \left(1 - \mathcal{B}dt\right) \quad \rightarrow \quad P(t + dt) - P(t) = -\mathcal{B}P(t)\,dt\,. \tag{3.5.22}$$

We thus have the differential equation, and solution,

$$\frac{dP}{dt} = -\mathcal{B}\,P(t) \quad \rightarrow \quad P(t) = e^{-\mathcal{B}t}\,, \tag{3.5.23}$$

from which we identify, as claimed, that

$$\tau = \frac{1}{\mathcal{B}}\,. \tag{3.5.24}$$

The tunneling rate $\mathcal{B}$ or tunneling probability per unit time is estimated by counting the number of times n_{hit} the classical particle, bouncing between $x = a$ and $x = b$, hits the barrier at $x = b$ per unit time, and multiplying this number by the tunneling probability T:

$$\mathcal{B} = n_{\text{hit}}\, T = \frac{T}{\Delta t}\,, \tag{3.5.25}$$

where Δt is the time the classical particle takes to go from b to a and back to b:

$$\Delta t = 2 \int_a^b \frac{dx}{v(x)} = 2m \int_a^b \frac{dx}{p(x)}\,. \tag{3.5.26}$$

We now can put all the pieces together, using the WKB approximation for T. We find

$$\tau = \frac{\Delta t}{T} \simeq 2m \int_a^b \frac{dx}{p(x)} \cdot \exp\left(2 \int_b^c \kappa(x)dx\right)\,. \tag{3.5.27}$$

The smaller the tunneling probability, the larger the lifetime of the localized state. Note that the factor Δt carries the units of the result. The above result can easily fail to be accurate, as the WKB approximation for T does not give the prefactor multiplying the exponential suppression.

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