Chapter 10

WKB Approximation

We now come to a much different kind of approximation, the *semi-classical approximation* for stationary state wave functions. This is also known as the WKB approximation, in honour of physicists Wentzel, Kramers, and Brillouin who developed the method in the mid 1920's. Unlike the approximation methods of the previous chapters, which were formulated in the abstract language of Hilbert spaces and observables, the semi-classical approximation that we will consider here is very much tailored to the study of wave functions in particular. Indeed, there is an entire branch of the analysis of PDEs known as *semi-classical analysis* that is closely related to the methods presented here.

We begin by describing an informal "derivation" of what we will soon come to understand as the zeroth order WKB approximation. Recall that the momentum operator acts on wave functions according to

$$(P\psi)(x) = -i\hbar\psi'(x) \,. \tag{10.1}$$

Now for a given potential energy function $V(x)$ and a given energy E, the *classical* momentum of a particle with that energy at a given x (assuming $E > V(x)$) would be given by

$$p(x) = \sqrt{2m(E - V(x))} \,. \tag{10.2}$$

One might then imagine that a wave function for a state with energy E would obey something like an equation of the form

$$P\psi(x) \stackrel{?}{=} \pm p(x)\psi(x) \,, \tag{10.3}$$

which is just a first order ordinary differential equation. This can be solved directly as follows,

$$\psi(x) \stackrel{?}{=} \exp\left(\pm\frac{i}{\hbar}\int_{x_0}^{x} p(s)\,\mathrm{d}s\right) \,. \tag{10.4}$$

In general, this analysis is obviously flawed; in particular, when we evaluate the kinetic energy operator $P^2/2m$ on such a wave function, the second action of P will not only bring down another copy of $p(x)$ but by the product rule will also differentiate $p(x)$. Consequently, this analysis exactly valid only when $p(x)$ is a constant, in which case we just have a plane wave solution, *i.e.*, a generalised momentum/energy eigenstate.

Nevertheless, there is some appeal to the idea that the operator P should more or less look like the classical momentum as a function of x, at least in some kind of limit. Indeed, if there is a limiting situation in which quantum mechanics starts to systematically reduce to classical mechanics, one might very well expect such a relation to hold. It turns out there is often such a limit—it is known as the *semi-classical limit*—and the above *ad hoc* wave function is just the first approximation in a systematic expansion.

10.1 The semi-classical expansion and WKB approximation

The starting point for making the previous procedure more systematic is to rewrite a stationary state wave function in terms of (the exponential of) its logarithm,

$$\psi(x) = \exp\left(\frac{iS(x)}{\hbar}\right) \,. \tag{10.5}$$

In light of the heuristic discussion before, we anticipate that the phase S might be related to the integral of the classical momentum in some regime. The time-independent Schrödinger equation in terms of this polar expression takes the

form (after dividing through by $\psi(x)$ and rearranging some terms),[53]

$$S'(x)^2 - i\hbar S''(x) = 2m(E - V(x)) = p^2(x) \,. \tag{10.6}$$

The key assumption that we make at this point is that *as an expansion in* $\hbar$, we have

$$S(x) = S^{(0)}(x) + \hbar S^{(1)}(x) + \dots \,. \tag{10.7}$$

This is sometimes referred to as a *semi-classical expansion*, since the parameter $\hbar$ can be thought of as characterising a scale where quantum effects become important, so the $\hbar \to 0$ limit should in some sense be a classical limit.[54]

Solving order by order in $\hbar$, we find that the first two terms in the semi-classical expansion of (10.6) and are given by

$$S_0'(x)^2 = p(x)^2 \,, \tag{10.8}$$
$$2S_0'(x)S_1'(x) = iS_0''(x) \,. \tag{10.9}$$

The first equation (10.8) can be solved to give

$$S_0(x) = \pm \int_{x_0}^{x} p(s)\, \mathrm{d}s \,, \tag{10.10}$$

where, as before, p represents the classical momentum as a function of position (and, implicitly, energy). This reproduces our heuristic result (10.4), as promised. Continuing to the first correction (10.9), we compute

$$iS_1'(x) = -\frac{p'(x)}{2p(x)} \,, \tag{10.11}$$

which we can integrate to find

$$iS_1(x) = -\log\left(\sqrt{p(x)}\right) \,. \tag{10.12}$$

The WKB approximation refers to the situation where we truncate the series at this order, giving us the approximate *WKB wave functions*

$$\psi_\pm(x) = \frac{1}{\sqrt{p(x)}} \exp\left(\pm \frac{i}{\hbar} \int_{x_0}^{x} p(s)\, \mathrm{d}s\right) \,. \tag{10.13}$$

In general, this is a local approximation for the wave function and we need to be careful about what happens in the various regions of space, as we will see in a bit. However, there is a simple example where the analysis to this point is entirely sufficient to proceed.

Example 10.1.1 (WKB for particle in a box with a bumpy bottom). Consider the case of infinite potential barriers at, say, $x = a$ and $x = b$ with $a < b$, and assume $E > V(x)$ for $x \in (a, b)$, though $V(x)$ may be a nontrivial function. We then have WKB wave functions that, by our previous analysis, take the form

$$\psi_{\mathrm{WKB}}(x) = C_+\psi_+(x) + C_-\psi_-(x) \,, \qquad a \leqslant x \leqslant b \,, \tag{10.14}$$

and we need to impose the boundary conditions $\psi(a) = \psi(b) = 0$. Letting $x_0 = a$ in our expressions (10.13), the boundary condition at $x = a$ requires that we set $C_+ + C_- = 0$, so we have

$$\psi_{\mathrm{WKB}}(x) = \frac{C}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar} \int_{a}^{x} p(s)\, \mathrm{d}s\right) \,. \tag{10.15}$$

[53] This equation is an instance of the so-called *Riccati equation* for $S'(x)$.

[54] In a physical context, one must be wary about the notion of taking $\hbar \to 0$, since $\hbar$ is a dimensionful parameter with units of angular momentum; one should instead take an appropriate collection of other dimensionful parameters in the problem and form a dimensionless combination involving $\hbar$ that can then be taken to zero by scaling the other variables relative to $\hbar$. For our analysis here it won't be important to keep track of this issue and we will instead treat $\hbar$ as a small parameter; this is what is usuall done in the mathematical treatment of this subject.

Then the requirement $\psi(b) = 0$ gives the *quantisation condition*,

$$\frac{1}{\hbar}\int_a^b p(x)\,\mathrm{d}x = n\pi\,, \qquad n = 1, 2, 3, \ldots\,. \tag{10.16}$$

For the case of constant potential $V = V_0$, this is just the conventional particle in a box and the WKB wave functions are the true stationary states; (10.16) gives exactly the correct energy levels:

$$\sqrt{2m(E - V_0)}(b - a) = n\pi\hbar \quad\Longrightarrow\quad E = V_0 + \frac{n^2\pi^2\hbar^2}{2m(b-a)^2}\,. \tag{10.17}$$

In the case of a non-constant potential, (10.16) gives an approximation to the energy levels of the system.

Estimating the accuracy of the WKB approximation can require some subtle analysis, but to produce a rough proxy for the domain of the validity of the approximation we can inspect when the typical term in the leading equation (10.8) is much larger than the typical term in the subleading equation (10.9),

$$\left(S_0'(x)\right)^2 \gg \hbar\,|S_0''(x)|\,. \tag{10.18}$$

Putting in our solution for $S_0(x)$, we have

$$p(x)^2 \gg \hbar\,|p'(x)|\,, \tag{10.19}$$

which we rewrite presciently as

$$\frac{\hbar}{p(x)^2}\,|p'(x)| = \left|\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\hbar}{p(x)}\right)\right| \ll 1\,, \tag{10.20}$$

Now if we introduce the *local de Broglie wavelength* $\lambda(x) = h/p = 2\pi\hbar/p$, which represents the wavelength of the generalised momentum eigenstate of momentum $p(x)$, then we have for our condition (dropping a factor of 2π since we are dealing with an extreme inequality),

$$\left|\frac{\mathrm{d}}{\mathrm{d}x}\left(\lambda(x)\right)\right| \ll 1\,. \tag{10.21}$$

To reach an intuitive interpretation of our condition, we further multiply again by the de Broglie wavelength,

$$\lambda(x)\left|\frac{\mathrm{d}}{\mathrm{d}x}\left(\lambda(x)\right)\right| \ll \lambda(x)\,. \tag{10.22}$$

This says that the WKB approximation has a chance of being reliable when the *change of the local de Broglie wavelength over the course of one such wavelength is small compared to that wavelength*. So in terms of percentages, the local de Broglie wavelength should be slowly varying.

We can re-express this condition directly in terms of energies. Using the expression for the classical momentum, we have

$$p'(x) = \frac{mV'(x)}{p(x)} = \frac{m\lambda(x)V'(x)}{2\pi\hbar}\,, \tag{10.23}$$

which, when we plug it into (10.19), yields the consistency condition (this time dropping a factor of 4π),

$$|\lambda(x)V'(x)| \ll \frac{p(x)^2}{2m}\,. \tag{10.24}$$

This says that over the course of a de Broglie wavelength, the potential energy should be slowly varying relative to the kinetic energy. Thus we expect the WKB approximation to do well for high energies and slow-varying potentials.

10.2 WKB in forbidden regions

For more general potentials (see Figure 4, for example), for a fixed value of E, $E - V(x)$ will become negative for some values of x. These regions in space are referred to as the *classically forbidden regions*, and as $p^2/2m = E - V < 0$, for

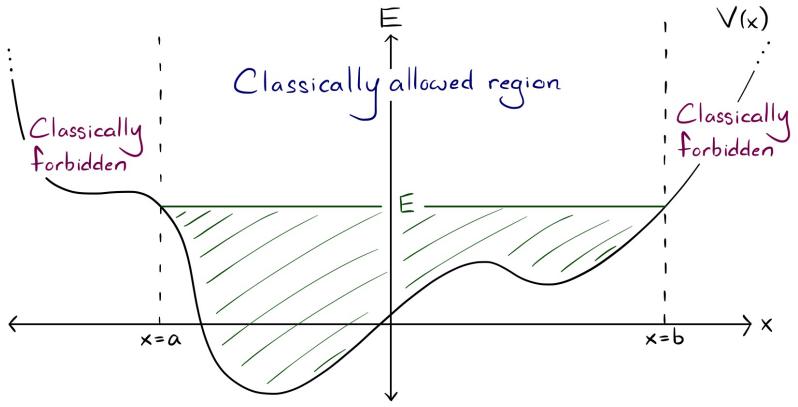

Figure 4. Example of a general potential with a single classically allowed region for the given value of energy (between $x = a$ and $x = b$). A WKB wave function for this type of potential and energy level will be defined in three separate regions and subjected to connection conditions at the classical turning points $x = a$ and $x = b$.

these regions the classical momentum defined by (10.2) becomes pure imaginary. Instead of the momentum we then introduce the real quantity

$$q(x) = \sqrt{2m(V(x) - E)}\,, \tag{10.25}$$

which is an analogue of the classical momentum in the forbidden region. We then solve (10.8) with an *imaginary* $S_0(x)$,

$$S_0(x) = \pm i \int_{x_0}^{x} q(s)\,\mathrm{d}s\,. \tag{10.26}$$

The $O(\hbar)$ term proceeds analogously, and we arrive at the WKB wave functions for classically forbidden regions,

$$\psi_{\pm}^{\text{forbidden}}(x) = \frac{1}{\sqrt{q(x)}} \exp\left(\pm \frac{1}{\hbar} \int_{x_0}^{x} q(s)\,\mathrm{d}s\right)\,. \tag{10.27}$$

Instead of being oscillatory, these are exponentially growing or decaying as a function of x. Though it is less intuitive, the analysis of validity performed above still applies in this case, with the de Broglie wavelength being replaced by the distance over which the exponentially growing/decaying solution increases/decreases by a factor of e.

10.3 WKB connection formulæ

We assume that, as in the figure, $E - V(x) \geqslant 0$ on the interval $[a, b]$ with $b > a$, and is negative outside and vanishes at a and b. These two points are referred to as the *classical turning points*, in reference to the classical trajectory at this energy. In order for our approximate solution to be normalisable, the solution in the left-most classically forbidden region must be exponentially growing with x (so decaying as $x \to -\infty$), and in the right-most forbidden region must be exponentially decaying with x. We therefore seek a solution of the form[55]

$$\psi(x) = \begin{cases} \frac{C_I}{\sqrt{q(x)}} \exp\left(-\frac{1}{\hbar}\int_x^a q(s)\,\mathrm{d}s\right)\,, & x < a\,, \\ \frac{C_+}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar}\int_a^x p(s)\,\mathrm{d}s\right) + \frac{C_-}{\sqrt{p(x)}} \exp\left(-\frac{i}{\hbar}\int_a^x p(s)\,\mathrm{d}s\right)\,, & a < x < b\,, \\ \frac{\tilde{C}_+}{\sqrt{p(x)}} \exp\left(\frac{i}{\hbar}\int_x^b p(s)\,\mathrm{d}s\right) + \frac{\tilde{C}_-}{\sqrt{p(x)}} \exp\left(-\frac{i}{\hbar}\int_x^b p(s)\,\mathrm{d}s\right)\,, & a < x < b\,, \\ \frac{C_{II}}{\sqrt{q(x)}} \exp\left(-\frac{1}{\hbar}\int_b^x q(s)\,\mathrm{d}s\right)\,, & x > b\,. \end{cases} \tag{10.28}$$

[55] Notice the strategic choice of limits of integration adopted here. We have given two versions of the wave function in the classically allowed region, one adapted for comparing to the left-most forbidden region and the other adapted for comparing to the right-most forbidden region.

There is a key subtlety having to do with deciding how to *connect* the exponentially increasing/decreasing solutions across the classical turning points at a and b to the oscillatory WKB wave functions in the classically allowed region. Indeed, all of our WKB wave functions actually diverge at a and b due to the denominator vanishing when $E = V(x)$. This represents is a *breakdown in the WKB approximation* in the vicinity of classical turning points.

To investigate the situation, we perform an additional approximate analysis in a *small neighbourhood of the classical turning point*. For $x \approx b$, say, we approximate the potential (assuming it is sufficiently smooth) as a linear function,

$$V(x) \approx V(b) + (x-b)V'(b)\,, \tag{10.29}$$

where in this case $V'(b)$ is positive. We then consider the Schrödinger equation for this approximation. Setting $y = x - b$ and $\tilde{\psi}(y) = \psi(x)$, we have

$$-\frac{\hbar^2}{2m}\tilde{\psi}''(y) = (E - V(b) - yV'(b))\,\tilde{\psi}(y) = -yV'(b)\tilde{\psi}(y)\,. \tag{10.30}$$

Introducing a further variable $z = \left(2mV'(b)/\hbar^2\right)^{1/3} y$ and defining $\varphi(z) = \tilde{\psi}(y)$, this becomes a famous ordinary differential equation, the *Airy equation*,

$$\varphi''(z) = z\varphi(z)\,. \tag{10.31}$$

We will take for granted the following integral expressions for a basis of solutions of the Airy equation (you can try to confirm for yourself that these solve the Airy equation by differentiating under the integral).

$$\begin{aligned} \mathrm{Ai}(z) &= \frac{1}{\pi}\int_0^\infty \cos\left(\frac{t^3}{3} + zt\right)\,\mathrm{d}t\,, \\ \mathrm{Bi}(z) &= \frac{1}{\pi}\int_0^\infty \left(\sin\left(\tfrac{t^3}{3} + zt\right) + \exp\left(-\tfrac{t^3}{3} + zt\right)\right)\,\mathrm{d}t\,. \end{aligned} \tag{10.32}$$

What will be important for our purposes here is the large $|z|$ asymptotics of these functions, which take the form (again, feel free to take this for granted),

$$\mathrm{Ai}(z) \sim \frac{\exp\left(-\frac{2}{3}z^{\frac{3}{2}}\right)}{2\sqrt{\pi}z^{\frac{1}{4}}}\,, \qquad \mathrm{Bi}(z) \sim \frac{\exp\left(\frac{2}{3}z^{\frac{3}{2}}\right)}{\sqrt{\pi}z^{\frac{1}{4}}}\,, \qquad z \gg 1\,, \tag{10.33}$$

$$\mathrm{Ai}(z) \sim \frac{\cos\left(\frac{2}{3}(-z)^{\frac{3}{2}} - \frac{\pi}{4}\right)}{\sqrt{\pi}(-z)^{\frac{1}{4}}}\,, \quad \mathrm{Bi}(z) \sim \frac{\cos\left(\frac{2}{3}(-z)^{\frac{3}{2}} + \frac{\pi}{4}\right)}{\sqrt{\pi}(-z)^{\frac{1}{4}}}\,, \quad z \ll -1\,, \tag{10.34}$$

We see that it is $\mathrm{Ai}(z)$ that behaves like a decaying exponential for large positive z, while $\mathrm{Bi}(z)$ instead behaves like a growing exponential. This suggests that we should want to use the $\mathrm{Ai}(z)$ solution to interpolate between the forbidden and allowed regions.[56]

Indeed, if we consider the forbidden-region decaying exponential WKB wave function in the right region and use the same approximation (10.29) for the potential near $x = b$, then we find

$$\begin{aligned} \frac{C_{II}}{\sqrt{q(x)}}\exp\left(-\frac{1}{\hbar}\int_b^x q(s)\,\mathrm{d}s\right) &\approx \frac{C_{II}}{(2mV'(b)y)^{\frac{1}{4}}}\exp\left(-\left(\frac{2mV'(b)}{\hbar^2}\right)^{\frac{1}{2}}\int_0^x s^{\frac{1}{2}}\,\mathrm{d}s\right)\,, \\ &= \frac{C_{II}\exp\left(-\frac{2}{3}z^{\frac{3}{2}}\right)}{(2mV'(b)\hbar)^{\frac{1}{6}}z^{\frac{1}{4}}}\,, \\ &\approx C_{II}\,\kappa\,\mathrm{Ai}(z)\,. \end{aligned} \tag{10.35}$$

[56] In a careful treatment, we should further subdivide our space to include turning point regions where we use this Airy approximation, and these should overlap with the regions where the WKB wave functions are valid. This level of detail is important for an estimation of the size of errors in the WKB approximation, but will not be necessary for us.

where $\kappa = 2\sqrt{\pi}/(2mV'(b)\hbar)^{\frac{1}{6}}$ is a numerical constant that we could also have absorbed into our overall constant. This matches precisely with the asymptotics of the $\mathrm{Ai}(z)$ function up to an overall numerical factor, so we will use $\mathrm{Ai}(z)$ to interpolate from the forbidden to the allowed region.

In the allowed region, then, we have to match to an appropriate combination of oscillatory WKB wave functions. To this end, we observe that in the allowed region we have, under the approximation (10.29) for $x \approx b$,

$$\begin{aligned}\frac{2C_{II}}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_x^b p(s)\,\mathrm{d}s - \frac{\pi}{4}\right) &\approx \frac{2C_{II}}{(-2mV'(b)y)^{\frac{1}{4}}}\cos\left(\left(\frac{2mV'(b)}{\hbar^2}\right)^{\frac{1}{2}}\int_y^0 (-s)^{\frac{1}{2}}\,\mathrm{d}s - \frac{\pi}{4}\right)\\ &= \frac{2C_{II}\cos\left(\frac{2}{3}(-z)^{\frac{3}{2}} - \frac{\pi}{4}\right)}{(2mV'(b)\hbar)^{\frac{1}{6}}(-z)^{\frac{1}{4}}}\,,\\ &\approx \kappa\, C_{II}\mathrm{Ai}(z)\,.\end{aligned} \tag{10.36}$$

We conclude that to interpolate with the $\mathrm{Ai}(z)$ Airy function, we should choose $\tilde{C}_\pm$ in the allowed region so that they combine to give the first expression in (10.36). An analogous treatment at the turning point $x = a$ implies that the allowed-region WKB wave function on the right hand side of that turning point should be given by

$$\psi(x) = \frac{2C_I}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_a^x p(s)\,\mathrm{d}s - \frac{\pi}{4}\right)\,. \tag{10.37}$$

The resulting connection formulæ are summed up in the following.

Proposition 10.3.1. For continuation to the exponentially decreasing solution past the turning point at b we must have

$$\tilde{C}_+ = C_{II}\,\mathrm{e}^{-\frac{\pi i}{4}}\,,\quad \tilde{C}_- = C_{II}\,\mathrm{e}^{\frac{\pi i}{4}} \quad\Longrightarrow\quad \psi(x) = \frac{2C_{II}}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_x^b p(s)\,\mathrm{d}s - \frac{\pi}{4}\right)\,, \tag{10.38}$$

Similarly, for continuation to the solution that exponentially decays as $x \to -\infty$ past the turning point at a we must have

$$C_+ = C_I\,\mathrm{e}^{-\frac{\pi i}{4}}\,,\quad C_- = C_I\,\mathrm{e}^{\frac{\pi i}{4}} \quad\Longrightarrow\quad \psi(x) = \frac{2C_I}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_a^x p(x)\,\mathrm{d}s - \frac{\pi}{4}\right)\,, \tag{10.39}$$

Remark 10.3.2. Though not important in this particular analysis, one does run into situations where one wants to match onto the exponentially *growing* solution on the other side of the classical turning point. In this case we have, by an analogous analysis, that if the wave functions in the forbidden regions are of the form

$$\psi_I(x) = \frac{D_I\exp\left(\frac{1}{\hbar}\int_x^a q(s)\,\mathrm{d}s\right)}{\sqrt{q(x)}}\,,\qquad \psi_{II}(x) = \frac{D_{II}\exp\left(\frac{1}{\hbar}\int_b^x q(s)\,\mathrm{d}s\right)}{\sqrt{q(x)}}\,, \tag{10.40}$$

then the matching must be done with the $\mathrm{Bi}(z)$ Airy function and one has in the classically allowed region

$$\tilde{C}_+ = \frac{D_{II}}{2}\,\mathrm{e}^{\frac{\pi i}{4}}\,,\quad \tilde{C}_- = \frac{D_{II}}{2}\,\mathrm{e}^{-\frac{\pi i}{4}} \quad\Longrightarrow\quad \psi(x) = \frac{D_{II}}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_x^b p(s)\,\mathrm{d}s + \frac{\pi}{4}\right)\,, \tag{10.41}$$

for matching to the right and

$$C_+ = \frac{D_I}{2}\,\mathrm{e}^{\frac{\pi i}{4}}\,,\quad C_- = \frac{D_I}{2}\,\mathrm{e}^{-\frac{\pi i}{4}} \quad\Longrightarrow\quad \psi(x) = \frac{D_I}{\sqrt{p(x)}}\cos\left(\frac{1}{\hbar}\int_a^x p(x)\,\mathrm{d}s + \frac{\pi}{4}\right)\,, \tag{10.42}$$

for matching to the left. Taken together, this full set of connection formulæ allow us to match an arbitrary solution across turning points.

Remark 10.3.3. An important feature of this result is that, when all is said and done, we can forget about the Airy

functions and the interpolation region; the relation between the coefficients in the allowed and forbidden regions is fixed *universally* subject to only the assumption that the potential is smooth at the turning points.

Remark 10.3.4. There is another way of deducing these connection formulæ that is quite elegant, though the justification is not entirely transparent. The idea is to *analytically continue* the WKB wave functions around the classical turning point, avoiding the singularity, and matching on either side. In other words, for (say) the turning point at $x = a$, set $x - a = \rho e^{i\varphi}$, with ρ sufficiently large that the WKB approximation can plausibly stays reliable. Starting with the exponential solution in the forbidden region, we continue along the path in the upper half plane ($\varphi \in (0, \pi)$) and this produces the coefficient C_- near a; the C_+ term is instead obtained by analytic continuation in the lower half plane ($\varphi \in (\pi, 2\pi)$). In this treatment, the important phase shift by $\pi/4$ arises from the analytic continuation of the $1/\sqrt{p} \simeq (x-a)^{-\frac{1}{4}}$ factor. A similar analysis follows at $x = b$.

10.4 Bohr–Sommerfeld quantisation

We produced two expressions for the WKB wave function in the classically allowed region by matching to the appropriate exponential wave functions in both forbidden regions. The requirement that these two expressions agree gives the *Bohr–Sommerfeld quantisation rule*, which generalises the quantisation condition from our example to the case with finite potential in the classically forbidden regions.

Corollary 10.4.1 (Bohr–Sommerfeld quantisation rule)**.** Normalisable semiclassical solutions satisfying the connection formulæ at classical turning points exist if and only if

$$\int_a^b p(x)\,\mathrm{d}x = \left(n + \frac{1}{2}\right)\pi\hbar\,. \tag{10.43}$$

Proof. Equating the two expressions for the allowed-region WKB wave function we have

$$\frac{C_I}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_a^x p(s)\,\mathrm{d}s - \frac{\pi}{4}\right) = \frac{C_{II}}{\sqrt{p}}\cos\left(\frac{1}{\hbar}\int_x^b p\,\mathrm{d}s - \frac{\pi}{4}\right)\,. \tag{10.44}$$

Rewriting

$$\frac{1}{\hbar}\int_x^b p(s)\,\mathrm{d}s - \frac{\pi}{4} = \frac{1}{\hbar}\int_a^b p(s)\,\mathrm{d}s - \frac{1}{\hbar}\int_a^x p(s)\,\mathrm{d}s - \frac{\pi}{4}\,, \tag{10.45}$$

and using evenness of cos, we have that one of the following must hold

$$\begin{aligned} &C_I = +C_{II}\,, \qquad \frac{1}{\hbar}\int_a^b p(x)\,\mathrm{d}x = \frac{\pi}{2} + 2\pi n\,, \qquad n = 0,1,2,\ldots \\ &C_I = -C_{II}\,, \qquad \frac{1}{\hbar}\int_a^b p(x)\,\mathrm{d}x = \frac{3\pi}{2} + 2\pi n\,, \qquad n = 0,1,2,\ldots \end{aligned} \tag{10.46}$$

which, allowing for either sign, gives the expected condition

$$\int_a^b p(x)\,\mathrm{d}x = \left(n + \frac{1}{2}\right)\pi\hbar\,, \qquad n = 0,1,2,\ldots\,. \tag{10.47}$$

The correction factor of $1/2$ coming from the connection conditions is known as the *Maslov correction*. ■

This condition is capable of giving surprisingly good answers. For example, it is *exact* for the simple harmonic oscillator.

A frequent interpretation/application of (10.43) arises from expressing the same quantity as an area integral. Indeed, if we identify the region $A(E) \subset \mathbb{R}^2_{x,p}$ where $p^2 \leqslant 2m(E - V(x))$, then we estimate the *number of quantum states*

corresponding to the classical states whose trajectories are confined to this region in phase space by

$$\#\text{ states}(E) \approx n(E) = \frac{1}{\pi\hbar}\int_{a(E)}^{b(E)} p\,\mathrm{d}x = \frac{1}{2\pi\hbar}\iint_{A(E)} \mathrm{d}p\,\mathrm{d}x\,, \tag{10.48}$$

where the final equality involves a factor of two because the area of the region includes both the area above the x-axis and the area below it. Since wave functions decay exponentially fast outside the region, this number can also be thought of as an estimate of the number of states whose wave functions are supported in $A(E)$.

This formula is often summarised by saying that there is, roughly, a quantum state for each $2\pi\hbar$ unit of area in phase space; this can be generalised to systems in higher dimensions, in which case there is roughly one quantum state for each $(2\pi\hbar)^d$ unit of volume in phase space.

10.5 The radial WKB approximation

The WKB method we've been studying is particularly suited to the case of one-dimensional systems. We can easily extend this to three dimensional problems in the case where spherically symmetry allows us to restrict to definite angular momentum eigenstates and then solve a one-dimensional radial problem. Indeed, with central potential $V(\mathbf{x}) = V(r)$, we have for $\psi(\mathbf{x}) = R(r)Y_\ell^m(\theta,\varphi)$ the radial (time-independent) Schrödinger equation,

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial^2}{\partial r^2}(rR)\right] + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}R(r) = (E - V(r))\,R(r)\,, \tag{10.49}$$

which can be rewritten as a one-dimensional Schrödinger equation for $rR(r)$ (with a modified potential for nonzero angular momentum),

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}(rR) = \left(E - V(r) - \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right)(rR)\,. \tag{10.50}$$

Consequently we have radial WKB wave functions given by

$$R_\pm(r) = \frac{1}{rp(r)^{\frac{1}{2}}}\exp\left(\pm\frac{i}{\hbar}\int^r p(r)\right)\,, \tag{10.51}$$

where

$$p(r)^2 = 2m\left(E - V(r) - \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\right)\,. \tag{10.52}$$

In the case where $V(r)$ is a strictly increasing function of r (such as the harmonic oscillator or the Hydrogen atom), there is an important distinction between the case where $\ell = 0$ (spherically symmetric states), for which there is no inner turning point, and the case where $\ell \neq 0$, for which for any energy there will be an inner turning point as long as the potential diverges less than quadratically with radius at the origin. (See Figure 5.)

The semiclassical wave function must still satisfy the connection conditions of 10.3.1 at $r = r_{\text{outer}}$. However, there is a new ingredient in the case when $\ell = 0$, which is that for $R(r)$ to be bounded, $rR(r)$ should vanish at the origin. As a result, we must have the sin combination of $R_\pm$ wave functions,

$$R(r) = \frac{C}{rp(r)^{\frac{1}{2}}}\sin\left(\frac{1}{\hbar}\int_0^r p(s)\,\mathrm{d}s\right) = \frac{\tilde{C}}{rp(r)^{\frac{1}{2}}}\cos\left(\frac{1}{\hbar}\int_r^{r_{\text{outer}}} p(s)\,\mathrm{d}s - \frac{\pi}{4}\right)\,, \tag{10.53}$$

and to match both expressions we need

$$\frac{1}{\hbar}\int_0^{r_{\text{outer}}} p(s)\,\mathrm{d}s = \left(n + \frac{3}{4}\right)\pi\,, \qquad n = 0, 1, 2, \ldots\,. \tag{10.54}$$

For the Hydrogen atom, this yields good estimates for the energies of s-orbitals, as you will see on Problem Sheet 4.

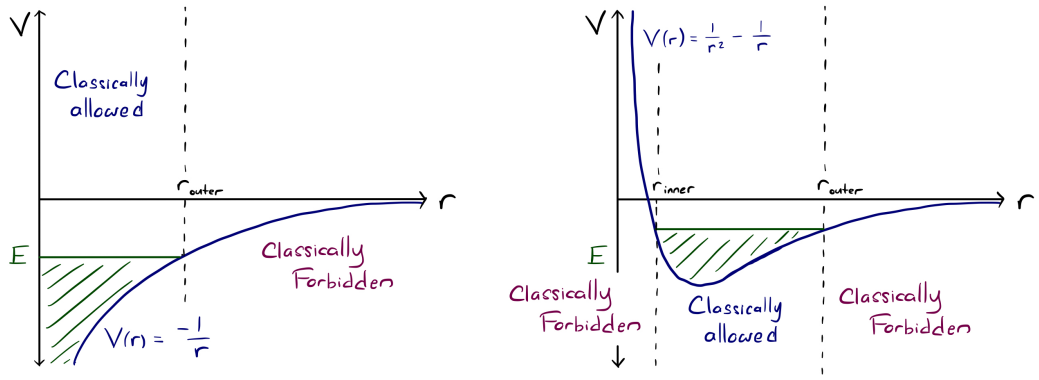

Figure 5. Radial potentials (in this case similar to the Coulomb potential) with and without "centrifugal" term from angular momentum. In the case without, there is a single classical turning point at r_{outer}, while for the case with angular momentum there is also an inner turning point at r_{inner}.

Remark 10.5.1. For states with nonzero angular momentum, one has an inner turning point so there is a naive quantisation condition of the usual form,

$$\frac{1}{\hbar}\int_{r_{\text{inner}}}^{r_{\text{outer}}} p(s)\,\mathrm{d}s = \left(n+\frac{1}{2}\right)\pi\,, \qquad n=0,1,2,\ldots\,. \tag{10.55}$$

There is a subtlety here, because the resulting exponentially decaying WKB wave function in the interior forbidden region won't actually be bounded at $r=0$ due to the enhanced singularity in the effective potential. There is a curious correction known as the *Langer correction* that can be implemented to improve errors arising from this problem at the origin, and you will encounter this as well on Problem Sheet 4.

10.6 Time-dependent WKB*

The relationship between the WKB approximation and classical physics can be drawn out further by considering the analogous approximation to solutions of the time-*dependent* Schrödinger equation. Below we will freely cite concepts from **B7.1 Classical Mechanics**.

Lemma 10.6.1. Parameterising a quantum-mechanical wave function according to

$$\Psi(\mathbf{x},t) = A(\mathbf{x},t)\exp\left(\frac{i}{\hbar}S(\mathbf{x},t)\right)\,, \tag{10.56}$$

where A and S are both real, the Schrödinger equation with Hamiltonian $H = P^2/2m + V(X)$ is equivalent to the following pair of equations,

$$\frac{\partial S}{\partial t} + \frac{|\nabla S|^2}{2m} + V = \frac{\hbar^2}{2m}\frac{\nabla^2 A}{A}\,, \tag{10.57}$$

$$\frac{\partial A^2}{\partial t} + \nabla\cdot\left(\frac{A^2}{m}\nabla S\right) = 0\,. \tag{10.58}$$

Proof. Direct calculation yields

$$\nabla\Psi = \left(\frac{\nabla A}{A} + \frac{i}{\hbar}\nabla S\right)\Psi\,, \qquad \frac{\partial\Psi}{\partial t} = \left(\frac{1}{A}\frac{\partial A}{\partial t} + \frac{i}{\hbar}\frac{\partial S}{\partial t}\right)\Psi\,, \tag{10.59}$$

and continuing,

$$\nabla^2\Psi = \left(\frac{\nabla^2 A}{A} + \frac{i}{\hbar}\nabla^2 S + 2\frac{i}{\hbar}\frac{\nabla A}{A}\cdot\nabla S - \frac{1}{\hbar^2}|\nabla S|^2\right)\Psi\,. \tag{10.60}$$

Substituting these into Schrödinger's equation and dividing by Ψ yields a complex equation whose real and imaginary parts are, after a little manipulation, the desired pair of equations. ■

The probability density is $|\Psi|^2 = A^2$ and the probability current is

$$\mathbf{j} := i\frac{\hbar}{2m}\left(\Psi\nabla\overline{\Psi} - \overline{\Psi}\nabla\Psi\right) = \frac{A^2}{m}\nabla S\,, \tag{10.61}$$

so we can interpret (10.58) as exactly the conservation of probability. The first equation is more subtle to interpret, and is the site of the WKB assumption. Indeed, the $\hbar \to 0$ limit is implemented by ignoring the right hand side of (10.57). This yields:

Definition 10.6.2 (The semi-classical approximation of the time-dependent Schrödinger equation)**.** This determines the wave function $\Psi = Ae^{iS/\hbar}$ satisfying

$$\frac{\partial S}{\partial t} + \frac{|\nabla S|^2}{2m} + V = 0\,, \tag{10.62}$$

known as the *Hamilton–Jacobi* equation, and

$$\frac{\partial A^2}{\partial t} + \nabla\cdot\left(\frac{A^2}{m}\nabla S\right) = 0\,, \tag{10.63}$$

the continuity equation.

Remark 10.6.3. This approximation has the best chance to be valid when the right hand side $\hbar^2\nabla^2 A/A$ of (10.57) is small, so in particular, $A \neq 0$.

We recall that the Hamilton–Jacobi equation arises in *classical mechanics* as the equation satisfied by the *action* of the classical trajectory ending at the point $\mathbf{x}$ at time t. For our Hamiltonian, the classical equations of motion are

$$m\ddot{\mathbf{X}} = -\nabla V\,, \tag{10.64}$$

which arise as the Euler–Lagrange equations that follow from extremising the action functional,

$$S[\mathbf{X}(t)] = \int_{t_0}^{t} \mathcal{L}\left(\mathbf{X}(s), \dot{\mathbf{X}}(s)\right)\,\mathrm{d}s\,, \quad \text{where} \quad \mathcal{L}(\mathbf{X}, \dot{\mathbf{X}}) = \frac{m}{2}|\dot{\mathbf{X}}|^2 - V(\mathbf{X})\,. \tag{10.65}$$

The solution to the Hamilton–Jacobi equation $S(t, \mathbf{x})$ arises as the value of $S[\mathbf{X}_{\mathbf{x}}(t)]$ when $\mathbf{X}_{\mathbf{x}}(s)$ are a family of solutions to the classical equations of motion (10.64) chosen so that $\mathbf{X}_{\mathbf{x}}(t) = \mathbf{x}$. One might, for example, consider the family of trajectories for which $\mathbf{x}(0) = \mathbf{y}$ for a fixed $\mathbf{y}$.

With the suggested boundary condition, evaluating $S(\mathbf{x}, t)$ requires us to integrate along the classical trajectory that joins $\mathbf{y}$ to $\mathbf{x}$. Thus the initial velocity is chosen so that the classical trajectory arrives at $\mathbf{x}$ at time t. The momentum of the trajectory when it passes through $\mathbf{x}$ at time t is then determined by

$$\mathbf{p} = \nabla S\,. \tag{10.66}$$

For a free classical particle (*i.e.*, $V = 0$) our prescription leads to

$$S = \int_0^t \frac{m}{2}\dot{\mathbf{x}}^2\,\mathrm{d}t = \frac{m|\mathbf{x}-\mathbf{y}|^2}{2t}\,, \qquad \text{where} \qquad \dot{\mathbf{x}} = (\mathbf{x}-\mathbf{y})/t\,. \tag{10.67}$$

It can be easily verified that this satisfies (10.62) with $V = 0$.

Theorem 10.6.4. Given a solution $S(\mathbf{x}, \mathbf{y})$ to the Hamilton–Jacobi equation with the aforementioned boundary conditions, a solution to the continuity equation is given by

$$A^2 = \det\left(\frac{\partial^2 S}{\partial x_j \partial y_k}\right)\,. \tag{10.68}$$

Proof. For simplicity we only prove the one-dimensional case, which follows from direct calculation. The calculation in higher dimensions is more involved but not in a deep way.

$$\begin{aligned}\frac{\partial A^2}{\partial t} &= \frac{\partial^3 S}{\partial x \partial y \partial t}\,, \\ &= -\frac{\partial^2}{\partial x \partial y}\left[\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V\right]\,, \\ &= -\frac{\partial}{\partial x}\left(\frac{1}{m}\frac{\partial S}{\partial x}\frac{\partial^2 S}{\partial x \partial y}\right)\,, \\ &= -\frac{1}{m}\frac{\partial}{\partial x}\left(\frac{\partial S}{\partial x}A^2\right)\,.\end{aligned}$$

which gives the continuity condition. ∎

Thus for the free particle, we obtain

$$A^2 = \det\left(-\frac{m}{t}1_{3\times 3}\right) = -\left(\frac{m}{t}\right)^3\,, \tag{10.69}$$

so that the WKB wave function at a future time t is given by

$$\Psi(\mathbf{x},t) = \left(\frac{m}{t}\right)^{3/2}\exp\left(\frac{im|\mathbf{x}-\mathbf{y}|^2}{2\hbar t}\right)\,. \tag{10.70}$$

Comparing to our result for the propagator (2.53), we see that up to overall normalisation this is exactly the evolution to time t of the generalised position eigenstate for position $\mathbf{y}$ at time zero. That we get the exact answer is actually no surprise, because we can check that in this case $\nabla^2 A = 0$, so the WKB equations reproduce the full time-dependent Schrödinger equation.

For time-independent systems and states of definite energy, one can separate out the time dependence and, in the one-dimensional case, recover our previous time-independent analysis.

Proposition 10.6.5. For a time-independent potential $V(\mathbf{x},t) = V(\mathbf{x})$, the Hamilton–Jacobi equation has solutions of the form

$$S(\mathbf{x},t) = W(\mathbf{x}) - Et\,, \tag{10.71}$$

provided that

$$\frac{|\nabla W|^2}{2m} + V = E\,. \tag{10.72}$$

The corresponding wave functions,

$$\Psi(\mathbf{x},t) = A(\mathbf{x},t)\exp\left(\frac{i(W(\mathbf{x})-Et)}{\hbar}\right)\,, \tag{10.73}$$

give the approximate eigenstates of energy with eigenvalue E.

Proof. This follows by direct substitution. ∎